

Reconstruction of the muon content of extensive air showers at the IceCube Neutrino Observatory

Rekonstruktion des Myonenanteils von ausgedehnten
Luftschauern mit dem IceCube Neutrino Observatorium

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I declare that I have developed and written the enclosed thesis completely by myself, and have not used sources or means without declaration in the text.

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Abstract

Reconstruction of the muon content of extensive air showers at the IceCube Neutrino Observatory

Due to their low flux, high-energy cosmic rays entering the Earth's atmosphere are measured indirectly by means of the particle cascades (extensive air showers) that are initiated upon interaction with the atmosphere. The footprint of the cascades can be observed with ground-based detector arrays, where information about the nature of the cosmic rays is convoluted in the characteristics of the measured particle distributions. Because of its direct connection to the hadronic part of the cascade and, therefore, to the cosmic-ray mass, the muon content in air showers is one key observable.

The IceCube Neutrino Observatory allows, in particular, measurements of air-shower muons in two different energy regimes. While its surface instrumentation, IceTop, is sensitive to the electromagnetic and low-energy ($\sim \text{GeV}$) muon component of air showers, high-energy ($\gtrsim 400 \text{ GeV}$) muons can be observed with its deep in-ice detector.

In this work, the muon content in air showers measured with IceTop is analyzed using a novel likelihood-based reconstruction algorithm. Dedicated detector response simulations to muons are performed and build the basis of the *two-component* reconstruction, which aims to disentangle the electromagnetic and muon contribution to the measured signal distributions. The two-component reconstruction provides a simultaneous reconstruction of the primary energy and muon number with a resolution of $< 10\%$ and $\lesssim 20\%$, respectively, around 100 PeV primary cosmic-ray energy for near-vertical showers with a minimal dependence on the cosmic-ray mass, and is therefore of general interest for cosmic-ray composition analyses. In this work, using the primary energy estimation, different cosmic-ray mass-dependent parameters as well as the muon number in near-vertical air showers are studied as a function of energy between a few PeV to 100 PeV and interpreted using different models for the description of the high-energy hadronic interactions in the air-shower development. This includes state-of-the-art hadronic interaction models that are tuned to data from the Large Hadron Collider (LHC), named *post-LHC* models like EPOS-LHC and QGSJet-II-04, and the *pre-LHC* model Sibyll 2.1.

It is shown that the average cosmic-ray composition obtained on the basis of the muon content measured with IceTop is in tension with modern cosmic-ray composition models when interpreted with post-LHC models, suggesting a predicted muon content that is too large compared to measured data in the considered primary energy and zenith range. At the same time, for some mass-sensitive parameters, the pre-LHC model leads to a predicted average composition that is outside the expected range for primary energies around 100 PeV . Therefore, none of the considered hadronic interaction models leads to a self-consistent description of the entirety of the air-shower development.

Zusammenfassung

Rekonstruktion des Myonenanteils von ausgedehnten Luftschauern mit dem IceCube Neutrino Observatorium

Aufgrund ihrer geringen Flussrate werden hochenergetische kosmische Strahlen, die in die Erdatmosphäre eindringen, indirekt durch die Teilchenkaskaden (Luftschauer) gemessen, die bei der Wechselwirkung mit der Atmosphäre entstehen. Die Signaturen der Schauer können mit bodengebundenen Detektor-Arrays beobachtet werden, wobei Informationen über die Eigenschaften der kosmischen Strahlen in den Merkmalen der gemessenen Teilchenverteilungen enthalten sind. Der Myonengehalt im Luftschauer ist eine der wichtigsten Messgrößen, da er eine direkte Verbindung zum hadronischen Teil des Luftschauers und damit zur Masse der kosmischen Strahlung aufweist.

Mit dem IceCube-Neutrino-Observatorium sind Messungen von Myonen in zwei verschiedenen Energiebereichen möglich. Während dessen Oberflächenkomponente, IceTop, sensitiv gegenüber dem elektromagnetischen- und niederenergetischen ($\sim \text{GeV}$) Myonenbeitrags des Schauers ist, können hochenergetische ($\gtrsim 400 \text{ GeV}$) Myonen mit seinem tiefen In-Eis-Detektor beobachtet werden.

In dieser Arbeit wird der Myonengehalt in Luftschauern gemessen mit IceTop, unter Verwendung eines neu entwickelten wahrscheinlichkeitbasierten Rekonstruktionsalgorithmus analysiert. Spezielle Simulationen der Detektorantwort zu Myonen werden durchgeführt und bilden die Grundlage der sogenannten *Zwei-Komponenten*-Rekonstruktion, die darauf abzielt, den elektromagnetischen- und Myonenanteil der gemessenen Signalverteilungen zu separieren. Die Zwei-Komponenten-Rekonstruktion ermöglicht eine simultane Rekonstruktion der Primärenergie und der Myonenanzahl mit einer Auflösung von $< 10\%$ bzw. $\lesssim 20\%$ bei etwa 100 PeV für nahezu vertikale Schauer und einer minimalen Abhängigkeit von der Masse der kosmischen Strahlung und ist daher von großem Interesse für Analysen der Massenzusammensetzung der kosmischen Strahlung. In dieser Arbeit wird unter Verwendung der entwickelten Primärenergieabschätzung der GeV -Myonenanteil sowie weitere Parameter, die von der Masse der kosmischen Strahlung abhängen, in nahezu vertikalen Luftschauern im Primärenergiebereich von einigen PeV bis 100 PeV untersucht und mittels verschiedener hadronischer Wechselwirkungsmodelle zur Beschreibung der hochenergetischen hadronischen Wechselwirkungen in der Schauerentwicklung interpretiert. Dies umfasst sowohl moderne (*post-LHC*) hadronische Wechselwirkungsmodelle wie EPOS-LHC und QGSJet-II-04, die mit Daten des Large Hadron Collider (LHC) kalibriert sind, als auch das *pre-LHC*-Modell Sibyll 2.1.

Es wird gezeigt, dass die mittlere Massenzusammensetzung der kosmischen Strahlung, die auf Basis des mit IceTop gemessenen Myonengehalt rekonstruiert wurde, bei der Interpretation mit *post-LHC*-Modellen im Widerspruch zu aktuellen Modellen der Massenzusam-

mensetzung und des astrophysikalischen Flusses steht, was, im betrachteten Primärenergie- und Zenitbereich, verglichen mit den Messdaten einen zu hohen vorhergesagten Myonengehalt suggeriert. Gleichzeitig führt das pre-LHC-Modell für einige massenabhängige Parameter zu einer vorhergesagten mittleren Zusammensetzung, die, für Primärenergien von etwa 100 PeV, außerhalb des physikalisch erwarteten Bereichs liegt. Daher führt keines der betrachteten hadronischen Wechselwirkungsmodelle zu einer in sich widerspruchsfreien Beschreibung der Gesamtheit der Schauarentwicklung.

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1

Introduction

More than 110 years ago, charged particles were discovered to arrive at Earth in addition to photons in the visible range. One widely known phenomenon created by charged particles traversing the Earth's atmosphere are the polar lights. These photons are created by the excitation of gas molecules by mainly electrons and protons at low energies produced in the solar winds. Outside of our Solar System, the most energetic processes in the universe can generate charged particles with orders of magnitude larger energy that are observed at Earth with a much lower abundance. Such highly energetic charged particles are called *cosmic rays*.

Cosmic rays are therefore messenger particles for high-energetic phenomena in our Universe. However, because of their nature as fully ionized nuclei, they are deflected along their path by Galactic and extragalactic magnetic fields. Neutral messenger particles are high-energy gamma rays and neutrinos, both secondary particles from the accelerated cosmic rays. While gamma rays can be absorbed by dust clouds in the interstellar medium, neutrinos, as weakly interacting particles, are not influenced by dust or magnetic fields. In addition, gravitational waves produced in violent astrophysical processes contain valuable information about the sources of such high-energetic phenomena. The combination of different messenger channels is the state-of-the-art strategy for the observation of respective source candidates and is known as *multi-messenger astrophysics*.

The focus of the work presented in this thesis is the measurement and understanding of high-energy cosmic rays. One of the first indications of the existence of cosmic rays was found from ionization measurements during balloon flights conducted in the early 20th century by Victor Hess [1]. From these measurements, it was found that the amount of charged radiation increases with increasing altitude and was therefore concluded to be of extraterrestrial origin. Additionally, since the intensity did not show significant differences for measurements during the day and at night, the Sun was excluded as a possible source. Today we know that the measured charged particles (mainly muons) are secondaries of primary cosmic rays interacting in the Earth's atmosphere. Although, since their initial discovery, cosmic rays have been observed over 11 orders of magnitude in energy, until today their composition remains one of the central questions to be answered

to gain insights about their sources, acceleration, and propagation mechanisms.

While at energies below a few 100 TeV their flux is sufficient for balloon- or satellite-based direct detection, at higher energies the cosmic-ray flux is so low that detectors with significantly larger exposure are required. For this purpose, ground-based detector arrays on the surface of Earth are employed, which measure the particle cascades produced by cosmic rays interacting with atoms of the Earth's atmosphere. Detector arrays for these extensive air-showers (EASs) can comprise thousands of square kilometers and can therefore measure the high-energy region of the cosmic-ray spectrum with sufficient statistics. Because cosmic rays can exhibit energies that exceed the scales reachable with human-made accelerators, the measurement of cosmic rays as probes of a phase space beyond accelerator scales is also of high interest for high-energy physics. Though, the reconstruction of the cosmic-ray characteristics in indirect measurements is connected to large uncertainties. This is because the interpretation of the measured data depends on the description of the EAS development in simulations. However, the description of high-energy hadronic interactions within EASs through *hadronic interaction models* is associated with large uncertainties, since corresponding models need to extrapolate from accelerator data to the phase space relevant for air showers. These model uncertainties are the main contribution to the systematic uncertainty in the interpretation of cosmic-ray data at the highest energies and therefore to the implications of astrophysics and particle physics. The reconstruction of EASs and validation of hadronic interaction models is the target of the work. For this, air-shower measurements at the IceCube Neutrino Observatory are used.

The IceCube Neutrino Observatory, situated at the geographic South Pole, constitutes an ideal facility to test the validity of hadronic interaction models. Its combination of a surface array, IceTop, for the detection of EASs with primary energies of a few hundred TeV to EeV and a deep optical in-ice array allows for the measurement of electromagnetic particles and low-energy ($\sim$ GeV) muons as well as accompanying high-energy ($\gtrsim$ 400 GeV) muons produced in EASs. This coincident measurement allows for the test of the description of different shower components inferred from hadronic interaction models. In particular, the low- and high-energy muon content of EASs is a probe of hadronic interactions at different energy regimes and is a valuable input for the reconstruction of the cosmic-ray composition.

The focus of this work is the derivation of the low-energy muon content with IceTop. For this purpose, a novel approach for the single-event based reconstruction of the primary energy and the muon number in EASs is developed and used to analyze measured data.

In this thesis, first, the necessary background information and motivation are provided before the methodical details and the analysis results are discussed.

In chapter 2, an introduction to cosmic rays and the connected open questions is given. Additionally, the relevant experimental results and their implications are discussed. Moreover, in chapter 3, the principle of indirect cosmic-ray detection through air-shower observatories is detailed. This includes a description of the development of the particle cascade through the Earth’s atmosphere and the important air-shower observables. In addition, different detection channels for EASs are introduced. Since the interpretation of EAS data relies on simulations, the simulation code and hadronic interaction models relevant for this thesis are discussed. For the latter, various discrepancies in the description of the muon component in EASs between measured data and simulations are described within the context of the *Muon Puzzle* in air showers [2]. The Muon Puzzle constitutes one main motivation for the work presented in this thesis.

An overview of the detector components of the IceCube Neutrino Observatory is given in chapter 4. Here, the measurement principle with a focus on EAS detection and the data acquisition and reconstruction chains are discussed. Furthermore, relevant analysis results related to muon measurements and the simulation set used for this work are introduced. Lastly, the ongoing and planned future advances of IceCube are briefly outlined.

In chapter 5, the response of the detectors employed in IceTop to muons is investigated. By means of a full detector response simulation, muon response distributions are derived that build the foundation for the novel likelihood-based method used in this work.

A novel methodical approach is developed and introduced in chapter 6, where, first, the basic principle of the air-shower reconstruction via the application of lateral distribution functions (LDFs) is explained. After the introduction and optimization of the LDFs used for this work, the technical details of the construction of a combined likelihood within a two-component model for the description of the electromagnetic and muon component of EASs measured with IceTop are discussed.

The specifics of the reconstruction of the primary energy and muon number in EASs based on the two-component model are discussed in chapter 7. In addition, the validity of the underlying assumptions of the model is tested. Finally, the reconstruction performance of the primary energy, muon number, and air-shower geometry is quantified and compared to the standard reconstruction of IceTop.

In chapter 8, the internal consistency of different hadronic interaction models in the prediction of the average cosmic-ray composition is tested based on different composition-sensitive reconstruction parameters of the two-component model. The results are compared to a previous analysis that includes other composition-sensitive parameters obtained at IceCube.

Moreover, a first study of the average number of muons in EASs as a function of primary energy is performed in chapter 9 using the new reconstruction method. The average muon number is derived on the basis of model-dependent correction factors that account for reconstruction biases and is interpreted in the context of different hadronic interaction

models. The results are compared to previous measurements of the low-energy (GeV) muon density and high-energy (> 500 GeV) muon multiplicity with IceCube. Lastly, further applications of the two-component model already in work at IceCube are discussed in a more broad context.

Finally, in chapter [10](#), a summary and discussion of the results as well as an outlook for future studies are given.

Cosmic rays

Primary cosmic rays arriving at Earth consist mainly of nuclei ($\sim 98\%$) with only a small fraction of primary electrons ($\sim 2\%$) [3]. However, for this work, the term cosmic rays will be used only in reference to nuclei. Despite significant progress in the measurement of high-energy cosmic rays over the past several decades, their exact composition remains one of the central questions.

Cosmic rays can exhibit energies that far exceed the scales achievable with human-made accelerators such as the *Large Hadron Collider* (LHC) [4]. Aside from the astrophysical implications, the measurement of high-energy cosmic rays is therefore also of general interest for high-energy physics. For instance, measurements of high-energy cosmic rays can be used to probe phase spaces of particle interactions beyond accelerator scales, including the production of new physics.

Depending on the energy range of the cosmic rays, different methods are employed for their measurement. This is because of the steeply falling cosmic-ray energy spectrum that leads to extremely low fluxes at high energies (see section 2.3). For energies below ~ 100 TeV, the flux is large enough to measure cosmic rays directly via balloon or satellite experiments. Using magnetic spectrometers, these experiments can directly measure the nuclear and isotopic cosmic-ray composition. In combination with calorimeters and tracking detectors, the charge and momentum, as well as the energy of cosmic rays, can be determined. Examples are the CREAM [5], AMS-02 [6], and PAMELA [7] detector. For this work, only the characteristics of ultra-high-energy cosmic rays are of relevance. Low-energy ($\lesssim$ GeV) cosmic rays mainly stem from the Sun and are not included in the discussions presented in this chapter. Above these energies, the majority of cosmic rays are believed to be produced outside the solar system [8].

In this chapter, a general introduction to the characteristics of cosmic rays and their observation is given. For this purpose, first, source candidates and the propagation of high-energy cosmic rays are discussed in section 2.1. The energy spectrum and composition of cosmic rays arriving at Earth are discussed in section 2.3 and section 2.2. Finally, models for the description of the cosmic-ray spectrum relevant for this work, including different source and composition assumptions, are introduced in section 2.4. For a comprehensive overview of all topics discussed in this chapter, see [8].

2.1. Sources and propagation

Generally, two source contributions to the observed flux of cosmic rays are distinguished: Galactic sources and extragalactic sources. Candidates for both source classes are introduced in section 2.1 and section 2.1. A possible mechanism for the acceleration of charged particles in the cosmic ray sources was suggested by Fermi in 1949 [9]. In this mechanism, the elastic deflection caused by moving magnetic field structures in the interstellar medium transfers kinetic energy to a charged particle. However, this process is found to be only a second-order effect, since the average energy gain of the charged particles is proportional to $(v/c)^2$, where v is the velocity of the magnetized cloud and c is the speed of light [10]. The magnetic deflection off moving magnetized structures in the interstellar medium is therefore referred to as second-order Fermi acceleration. A more efficient acceleration mechanism is given by the first-order Fermi acceleration, referring to the Fermi acceleration in moving shock fronts. In this scenario, a back-over-the-envelope calculation can be performed assuming a net energy gain of $\Delta E = \zeta E$ for each deflection determined by a proportionality constant ζ , with the initial particle energy E . Note that this method relies on the presence of an inhomogeneous magnetic field in the vicinity of the shock front, as particles can escape more easily along homogeneous field lines [10]. For each deflection process, the particle has a probability p_{esc} to escape from the acceleration region. After n encounters, the energy is then given by

$$E_n = E_0(1 + \zeta)^n, \quad (2.1)$$

with the injection energy of the accelerator E_0 [8]. Consequently, the number of encounters needed to reach a given energy E becomes

$$n = \frac{\ln(E/E_0)}{\ln(1 + \zeta)}, \quad (2.2)$$

and the number of charged particles exceeding E is given by

$$N(> E) \propto \frac{1}{p_{\text{esc}}} \left(\frac{E}{E_0} \right)^{-\gamma}. \quad (2.3)$$

Here, $\gamma \approx p_{\text{esc}}/\zeta = \frac{T_{\text{cycle}}}{\zeta T_{\text{esc}}}$, with the characteristic time of the acceleration cycle and escape from the acceleration region T_{cycle} and T_{esc} , respectively. Note that with Eq. (2.3), the shock acceleration naturally leads to a power-law spectrum of cosmic-ray energies with $\gamma \approx 2$ at the source (see section 2.3).

Due to the probability of escape, the maximum energy of the particles depends on their confinement within the acceleration region and therefore on their gyroradius

$$r_L = \frac{R_m}{B}, R_m = \frac{pc}{Ze} \approx \frac{E}{Ze}, \quad (2.4)$$

Here, B is the magnetic field strength perpendicular to the direction of motion of the particle, and R_m is the magnetic rigidity, where its relativistic approximation is shown with the charge Ze of the nucleus, the momentum p , and the energy E . Based on this consideration, the *Hillas criterion* can be written as

$$E < \beta ZeBR, \quad (2.5)$$

describing the maximum particle energy to be magnetically confined within the accelerator region with radius R [11]. Here, β represents the velocity of the shock front. The practical implications of Eq. (2.5) are visualized in Fig. 2.1 in a *Hillas plot*, where the magnetic field strengths of different cosmic-ray source candidates are drawn against the respective spatial dimensions of the acceleration region. In this representation, the downward diagonal lines indicate the upper limits for the acceleration of cosmic rays to a given energy. Therefore, source candidates to the left of the lines are not able to accelerate protons to the given energy because of limited confinement. For instance, supernova remnants (SNRs) are source candidates for the acceleration of cosmic rays up to energies of the knee¹ of the cosmic-ray spectrum (see section 2.3). At the same time, sources like Active Galactic Nuclei (AGNs) are more likely to produce higher energy particles.

Due to the dependence of the gyroradius on R_m , magnetic confinement is more effective for high charge nuclei. Consequently, heavier nuclei can be accelerated to higher energies. This has an important implication for the observation of cosmic rays, namely that a transition toward a heavier composition is expected once the dominant sources reach their energy limit in the acceleration of protons. Therefore, a rigidity-dependent cutoff is expected in the measured cosmic-ray spectrum. This effect is typically referred to as *Peters cycle* [12]. However, a certain ambiguity is introduced by the fact that propagation effects can cause a similar behavior [13].

Galactic cosmic rays

For the observation of sources in our own Galaxy, the cosmic rays diffusing through it have to be confined. Based on the gyroradius (Eq. (2.4)), the requirement of magnetic confinement of cosmic rays in our Galaxy can be estimated using the Galactic magnetic field strength ($\sim 3\mu\text{G}$) and radius ($\sim 15\text{kpc}$). It can be deduced that cosmic rays of heavy mass are retained up to EeV energies.

During the diffusion of cosmic rays through the Galaxy, they can interact with the interstellar medium. Due to the energy dependence of the diffusion, cosmic rays traverse different effective amounts of matter, or *grammage*. In the GeV region, on average, cosmic

¹For a detailed discussion of the features of the cosmic-ray energy spectrum like the *knee* and the *ankle* see section 2.3.

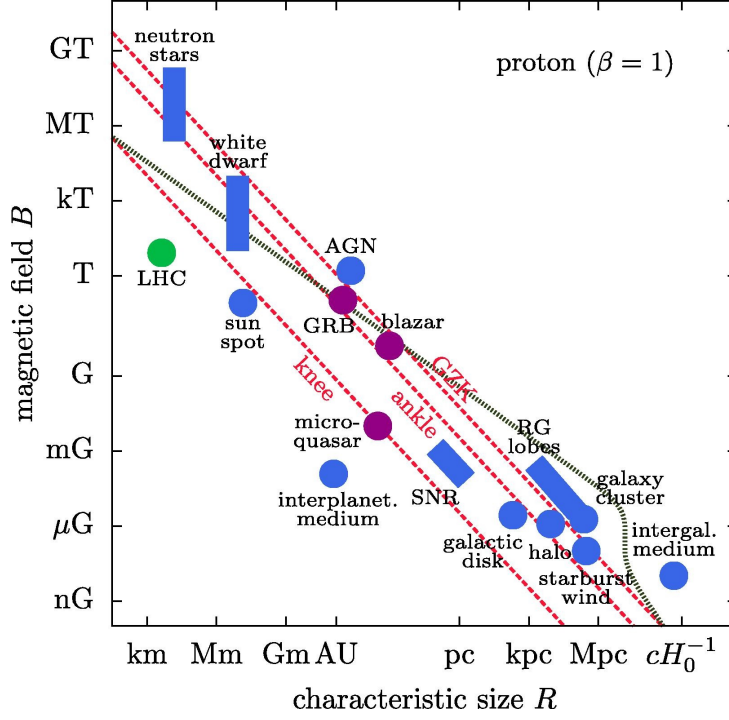


Figure 2.1.: Example of a Hillas plot for the consideration of different candidates for cosmic-ray (specifically proton) acceleration in dependence on the magnetic field strength of a given source as well as its spatial dimension. For reference, red dashed lines indicate the minimum requirements for possible source candidates to produce energies around the *knee*, the *ankle*, and the *GZK-cutoff* [14] of the cosmic-ray spectrum (see section 2.3 for details). Sources above the lines are able to accelerate protons to the respective energies. The gray dashed line shows a more realistic source requirement that includes synchrotron losses within the source and interactions with the cosmic microwave background. Figure taken from [15].

rays traverse a grammage of $\sim 5 - 10 \text{ g/cm}^2$ between acceleration and observation², while the effective grammage decreases with increasing cosmic ray energy [8]. With the thickness of the Milky Way disc ($\sim 10^{-3} \text{ g/cm}^2$, corresponding to a density of ~ 1 hydrogen atom per cubic centimeter), this implies an average path length of Galactic cosmic rays from their sources to Earth of thousands of times the thickness of the disc in the GeV region, suggesting diffusion in a volume containing the Galactic disc. It also implies that higher-energy cosmic rays spend comparably less time in the Galaxy.

The magnetic field of our Galaxy is roughly oriented parallel to the local spiral arm, where the ionized gas and the magnetic field can be described by a magneto-hydrodynamic fluid,

²Note, that this can be deduced from the ratio of primary to secondary nuclei, which will be discussed in section 2.2.

through which waves can travel with a characteristic *Alfvén velocity* v_A , with

$$0.5\rho v_A = \frac{B^2}{8\pi}, \quad (2.6)$$

where $B^2/8\pi \sim 0.4 \cdot 10^{-12} \text{ erg/cm}^3$ is the energy density of the magnetic field³ [8].

A simplified model for the diffusion of cosmic rays through the Galaxy is the *leaky box* model, in which cosmic rays propagate freely within a volume of containment but have a constant escape probability $\tau_{\text{esc}}^{-1} \ll c/h$ upon reaching the boundary, where h defines half of the thickness of the disc. The latter is modeled by a characteristic escape time τ_{esc} , which includes the diffusion and convection of cosmic rays. After a time t , the probability of remaining in the box is given as $\exp(-t/\tau_{\text{esc}})$. Consequently, the mean containment time of a cosmic ray is determined by τ_{esc} and the distribution of the path lengths of the cosmic rays is exponential. Assuming that the cosmic-ray spectrum measured at Earth is representative of the entire Milky Way, the power required to maintain an equilibrium of cosmic rays within the Galaxy can be estimated to be of the order of $7 \cdot 10^{40} \text{ erg/s}$ [8]. Furthermore, considering shock acceleration from Type II Supernovae occurring every 30 years with an ejected mass of $10 M_\odot$ expanding at a velocity of $5 \cdot 10^8 \text{ cm/s}$ into a medium with a density similar to the interstellar medium, a power of $3 \cdot 10^{42} \text{ erg/s}$ is produced. This makes it plausible that SNRs are indeed the powerhouse of Galactic cosmic rays, even if the efficiency of the acceleration is on the few percent level.

A more direct way of probing SNRs as sources of cosmic rays is by observing gamma rays. This is because accelerated cosmic rays, such as protons, can interact with the gas surrounding the source environment and produce, among others, neutral pions (π^0) that decay into two photons. Since gamma rays are not deflected by magnetic fields, they point back to their source. In the π^0 rest frame, the decay happens back-to-back and both photons receive an energy of $m_\pi/2 \approx 67.5 \text{ MeV}$. Therefore, a characteristic peak is produced in the spectrum of gamma rays. In fact, Fermi-LAT [16] reported evidence of the expected feature in the gamma-ray spectrum that cannot be explained by leptonic processes [17].

However, SNRs are likely not the sources of the highest-energy Galactic cosmic rays (see section 2.3). Observations from H.E.S.S [18] in 2016 suggest the Galactic center as region in which cosmic rays are accelerated to PeV energies [19]. Other *PeVatrons* were discovered by LHAASO [20, 21].

³Note, that the energy density of cosmic rays is of the same order with $\sim 0.8 \cdot 10^{-12} \text{ erg/cm}^3$. This is caused by the coupling of both, in which the propagation of cosmic rays can produce Alfvén waves, that can in turn lead to cosmic ray scattering [8].

Extragalactic cosmic rays

Following the discussion in the context of magnetic confinement, the highest-energy cosmic rays observed at Earth are likely not created in our own Galaxy. This is also motivated by the fact that such ultra-high energy cosmic rays (UHECRs) do not exhibit a significant anisotropy with respect to the Galactic disc [22, 23].

From Fig. 2.1, examples for potential sources for UHECRs are AGNs, gamma-ray bursts (GRBs) and neutron stars with a comparably strong magnetic field but limited size, or large structures with a small magnetic field, such as galaxy clusters. If the magnetic field is too large, protons lose a significant part of their energy through synchrotron radiation, and since they need to escape from the source region, the size of the object should not be too large in this case.

Since cosmic ray interactions can also produce neutrinos by means of charged pion decay, coincident observations of gamma rays and neutrinos can be used for the discovery of extragalactic sources. Evidence for such a scenario was found in 2017 via a multi-messenger observation of a candidate for an astrophysical neutrino with the IceCube Neutrino Observatory that points in the direction of a flaring blazar from which gamma-ray emission was detected [24].

UHECRs from extragalactic sources are influenced not only by our own Galaxy but also by extragalactic magnetic fields along their path to Earth. In addition, the interaction with the *cosmic microwave background* (CMB)⁴ becomes important, where highly energetic protons undergo photo-pion production with a CMB photon, $\gamma p \rightarrow \pi^0 p$ ⁵. The energy threshold for this process can be estimated from the π^0 rest mass and is of the order of $\sim 7 \cdot 10^{19}$ eV in the lab system for a head-on collision and for an energy of $\sim 10^{-3}$ eV of a CMB photon [8]. Greisen, Zatsepin, and Kuzmin concluded that this effect leads to an opaque Universe for UHECRs, which results in a cutoff at the high-energy end of the cosmic-ray spectrum, the *GZK cut-off* [14, 26]. In addition to the photo-pion production with CMB photons, interactions with photons can also lead to energy losses through electromagnetic production of electron-positron (e^+e^-) pairs. The energy threshold for this process is $\sim 6 \cdot 10^{17}$ eV. However, the effective energy loss per interaction is significantly smaller compared to the GZK effect. It should also be mentioned that the heavier nuclei of the UHECRs are affected by photodisintegration through background photons along their path.

⁴The energy spectrum of CMB photons is similar to that of black body radiation with a temperature of ~ 2.7 K and a photon density of $\sim 410 \text{ cm}^{-3}$ [25].

⁵Note, that in addition to the CMB also the infrared background and radio background constitute important target photons [8].

2.2. Composition

The relative abundance of different species of cosmic rays measured at Earth contains valuable information about the source properties and propagation effects. This is especially true when compared to the composition observed from the solar system. The difference in the relative abundances in low-energy cosmic rays and in the solar system is shown in Fig. 2.2. While some similarities like the *odd-even* effect⁶ and peaks in the products of stellar nucleosynthesis such as carbon, oxygen, and iron, are observed, important differences in the relative abundance of two elemental groups are visible. In particular, a higher abundance of elemental groups Li-B and Sc-Mn is observed in cosmic rays. Note that these are elements with mass right below the abundant elements carbon/oxygen and iron for the first and second group, respectively. This suggests that the higher abundance is the result of spallation processes of, e.g., primary carbon, oxygen, or iron, along their path to Earth. It also implies that the relative abundance of the spallation products contains information about the average time cosmic rays spend in the Galaxy, supporting the assumption of cosmic-ray confinement by the Galactic magnetic field. It should also be noted that the abundance of elements heavier than iron is suppressed by several orders of magnitude because they are not produced in stellar thermonuclear processes. For the lightest-mass nuclei, hydrogen and helium, a lower abundance is observed in cosmic rays compared to the solar system. However, the reason for this is still under discussion. For instance, the difference could be caused by a composition variation of the injection spectrum or by the acceleration characteristics for low charge nuclei.

As will be discussed in section 2.3, the cosmic-ray spectrum is steep and falls off over many orders of magnitude as a function of energy. Since the composition is also energy dependent, the relative elemental abundances depend on the cosmic ray energy and are dominated by cosmic rays of lower energies. The measurement of the composition of high-energy cosmic rays is much more complicated, as it is based on indirect detection (see chapter 3).

Note that in addition to the cosmic-ray composition, the anisotropy in their arrival direction also contains valuable insights into the sources, acceleration, and propagation of cosmic rays. For instance, the observation of the anisotropies of UHECRs can be used to pinpoint their source locations [8]. However, a discussion of the characteristics of cosmic-ray anisotropy is beyond the scope of this thesis.

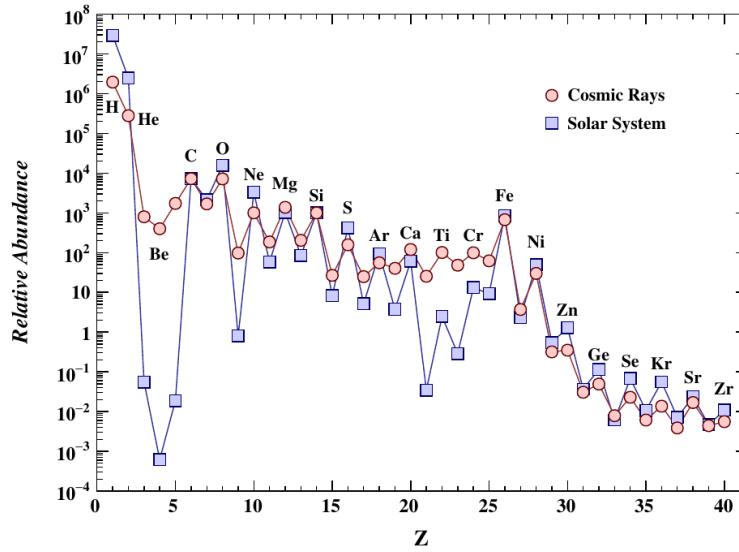


Figure 2.2.: Elemental composition of cosmic rays compared to the abundance in the solar system (relative to Silicon). Figure taken from [27].

2.3. Energy spectrum

The measurement of the cosmic-ray energy spectrum has been conducted over several decades by various experiments. As a result, the spectrum is measured over many orders of magnitude in energy from $\sim 10^{10}$ eV to $\sim 10^{20}$ eV. The cosmic-ray spectrum is shown in Fig. 2.3. The flux in the differential cosmic-ray spectrum is normalized per bin in energy, area, solid angle, and time:

$$J(E) \equiv \frac{dN}{dE dA d\Omega dt} (\text{GeV}^{-1} \text{m}^{-2} \text{sr}^{-1} \text{s}^{-1}). \quad (2.7)$$

Due to the steeply falling behavior of the cosmic-ray spectrum, the flux shown in Fig. 2.3 is multiplied by an additional factor of E^2 to better visualize its features. Up to ~ 200 TeV, the flux can be measured directly, with direct particle identification. However, at higher energies, only the all-particle spectrum is shown. Generally, the spectrum can be described by power laws of the form

$$J(E) \propto E^{-\alpha}, \quad (2.8)$$

where the power law index α changes depending on the energy range. Note that the shock front (first-order Fermi) acceleration naturally leads to a power law with a spectral index of 2 [8]. However, propagation effects on the way from the source to Earth additionally steepen the spectrum. At energies around $3 - 4 \cdot 10^6$ GeV, a steepening (softening) of the spectrum is visible, where a change of α from ~ 2.7 to ~ 3.1 occurs. This feature is well

⁶This effect describes the higher abundance of nuclei with an even proton and neutron number due to their larger binding energy and therefore increased stability.

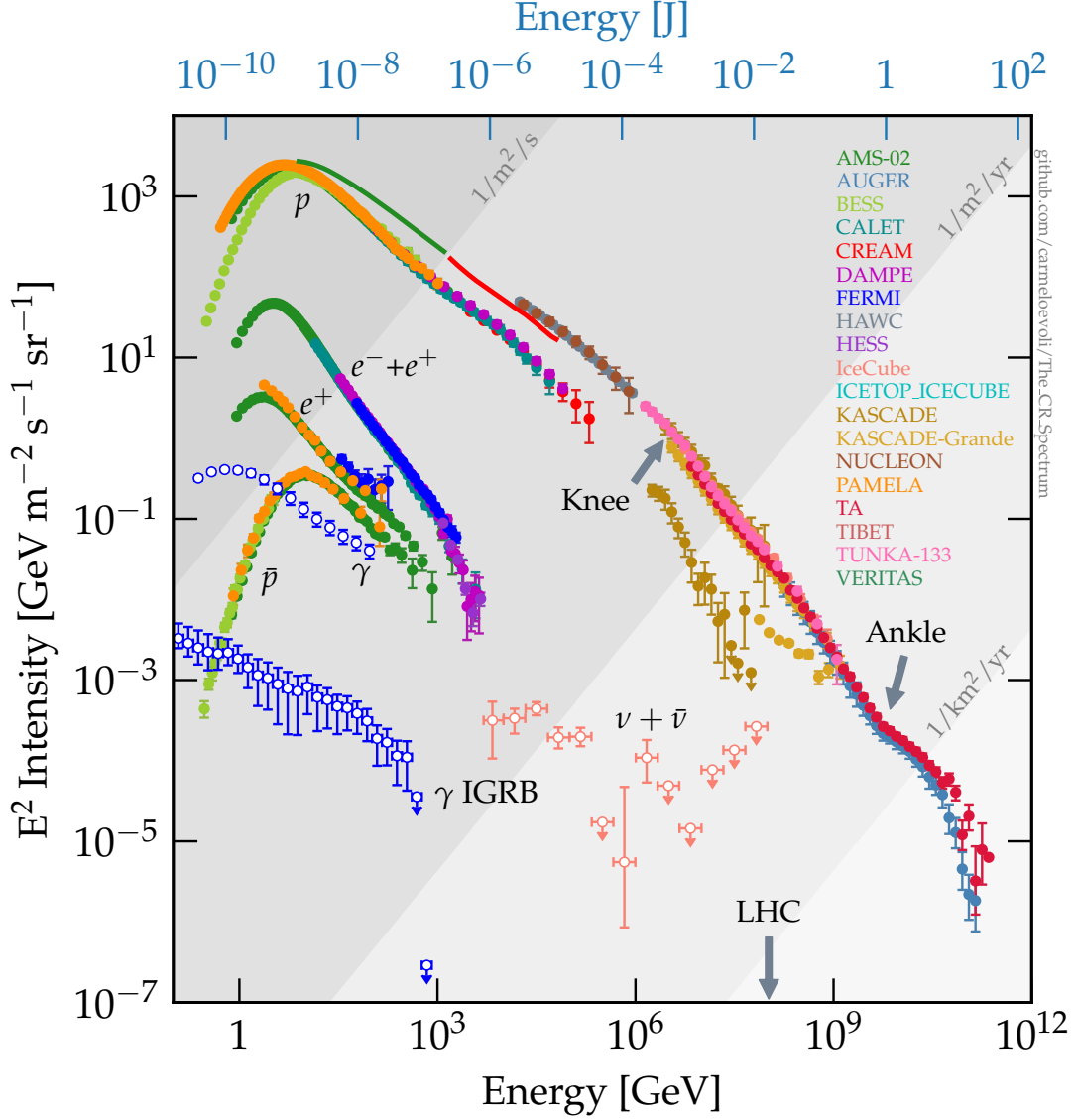


Figure 2.3.: Cosmic-ray energy spectrum measured over several orders of magnitude by different direct and indirect cosmic ray detectors. In direct detection of cosmic rays at low energies, the elemental composition can be deduced by experiments like AMS-02 [28] or CREAM [5]. At high energies, where cosmic rays can only be observed indirectly, the all-particle flux is shown as measured by different observatories. In addition, diffuse tracks and cascade measurements and upper limits of high-energy neutrinos from the IceCube Neutrino Observatories, as well as the isotropic gamma-ray background (IGRB) measured by Fermi-LAT [16] are shown. Figure taken from [29].

known as the *knee* of the cosmic-ray spectrum. After the knee, the spectrum becomes slightly flatter (harder), followed by another steepening around $\sim 10^{17}$ eV [30], the *second knee*. At higher energies $\sim 4 \cdot 10^{18}$ eV [31], the spectrum flattens (hardens) again, where the spectral index transitions to ~ 2.6 . This flattening is known as the *ankle*. Lastly, at

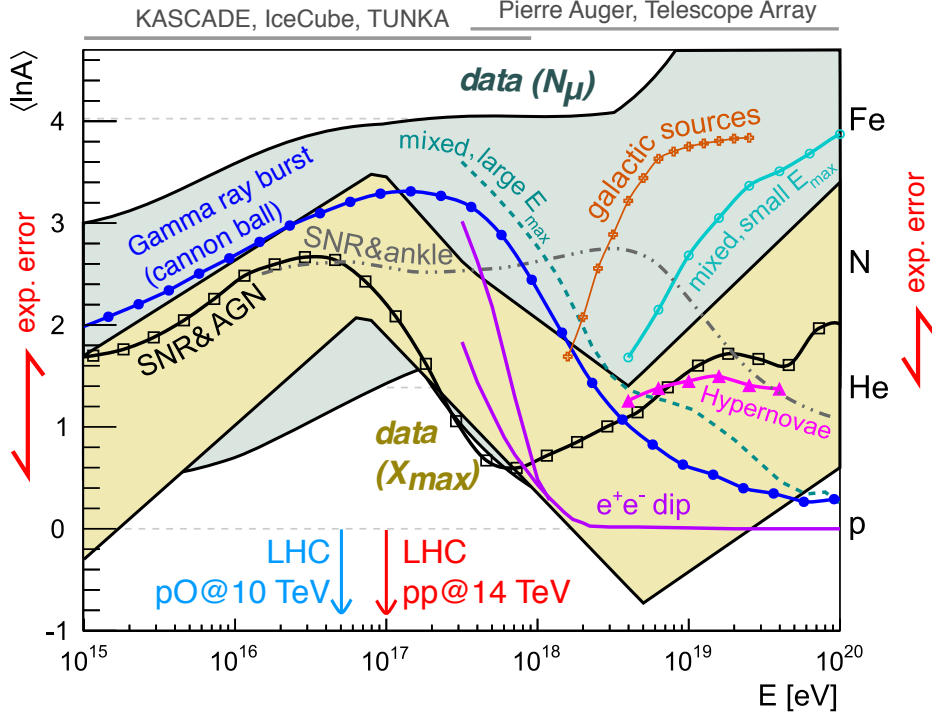


Figure 2.4.: Mean logarithmic mass $\langle \ln A \rangle$ as a function of cosmic ray energy. Data used in the figure taken from [36]. Figure taken from [37].

the highest energies ($\gtrsim 5 \cdot 10^{19}$ eV), a suppression is observed, the *GZK cut-off*.

KASCADE [32] and KASCADE-Grande [33] measurements indicated that the knee and the second knee are caused by subsequent dropout of light and heavy components [34, 35], which is supported by measurements from several observatories [36]. This suggests that at the position of the knee, a population of sources (e.g. SNRs) reaches its acceleration limit for protons, leading to a rigidity-dependent drop-off up to the second knee, as expected from the Peters cycle.

The ankle is often associated with the emergence of extragalactic cosmic rays. In this scenario, a second population of Galactic cosmic rays is required that accelerates protons to energies of $\sim 10^{17}$ PeV to explain the presence of Galactic protons until the transition is complete [8]. This is often referred to as *Population B*. However, alternative explanations for the ankle exist [4].

At the highest energies around $\sim 6 \cdot 10^{19}$ eV, a clear suppression is observed in the cosmic-ray flux. This could be produced by the GZK effect. However, as indicated by recent measurements from the Pierre Auger Observatory, the composition becomes increasingly heavy toward the highest energies [38]. This could suggest that the extragalactic sources reach their acceleration limit.

Due to the indirect nature of cosmic-ray measurements at high energies, their species can typically not be reconstructed on a single-event basis. Instead, data of high-energy

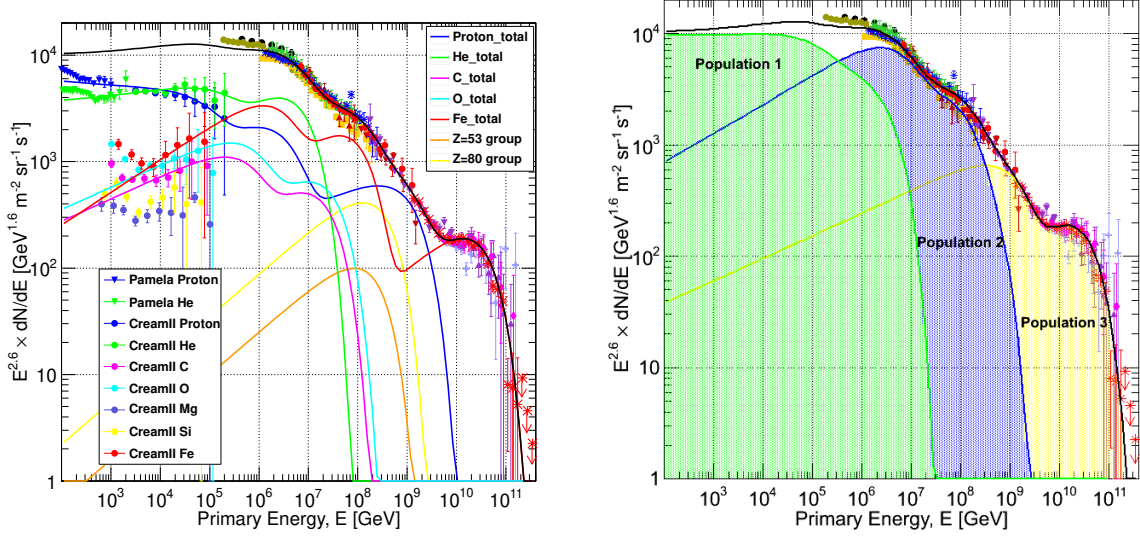


Figure 2.5.: Overview of the GST flux model. The energy spectra of individual elements from direct measurements are fitted and extrapolated toward higher energies to fit data from indirect measurements. The resulting contributions from individual mass groups and from the different populations are shown on the left and right, respectively. Figure taken from [4].

cosmic rays is interpreted by means of the mean logarithmic mass $\langle \ln A \rangle$. The two main observables for the reconstruction of the mean mass are the depth of the maximum of the air shower X_{max} produced by highly energetic cosmic rays interacting in the Earth's atmosphere, as well as its muon content N_{μ} (see chapter 3 for a detailed discussion). Both are visualized in Fig. 2.4 as yellow and green bands, respectively, where the width indicates connected experimental and hadronic model uncertainties (see section 3.6.2). Although the accuracies of $\sim 10\%$ of the difference between proton and iron are achieved through measurements of the observables, hadronic interaction models involved in their conversion to $\langle \ln A \rangle$ introduce large uncertainties (see sections 3.6.2 and 3.6.3 for a detailed discussion). This is unsatisfactory, as $\langle \ln A \rangle$ can strongly constrain different source scenarios, indicated as lines in Fig. 2.4.

2.4. Spectrum and composition models

Several astrophysical models describing the shape and composition of the cosmic-ray spectrum exist, attempting to better understand the spectral features and, by that, the sources, acceleration, and propagation mechanisms. In [39], Hillas proposed a model that assumes three source populations to describe the cosmic-ray spectrum. In this way, the

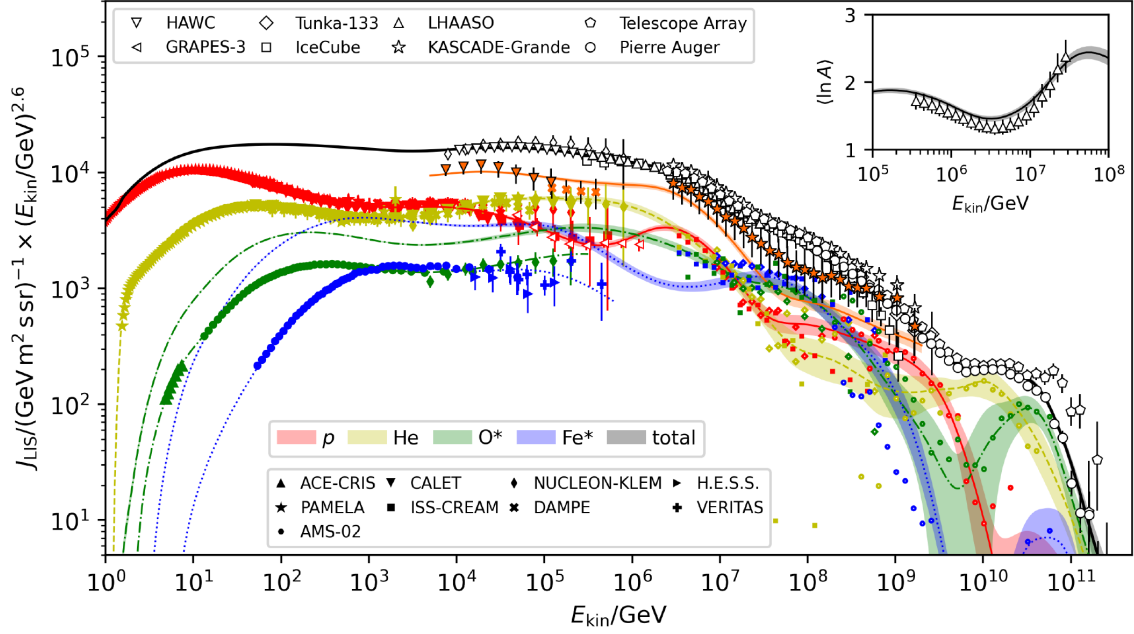


Figure 2.6.: Updated version of the GSF model compared to measured indirect data after correction for the energy scale through the fit. Colored (red, yellow, green, and blue, for proton, helium, oxygen, and iron, respectively) points and lines show the measurements and fit of different mass groups, where the bands indicate the resulting 1σ uncertainty. Figure taken from [40].

first population corresponds to the contribution of SNRs to the cosmic-ray flux, where the knee marks its limit for the acceleration of protons. As mentioned in section 2.3, the interpretation of the ankle as the transition from Galactic to extragalactic cosmic rays requires the contribution of a second, higher-energy Galactic source population. In this model, the second population leads to the observed shape of the spectrum between the knee and the second knee (see section 2.3 for a detailed discussion). Finally, the third population describes extragalactic sources. Note that in reality, significantly more source populations could be contributing.

Assuming a rigidity-dependent cutoff as motivated by the Peters cycle, the contributions of different mass groups to the all-particle spectrum can be described as

$$\phi_i(E) = \frac{dN_i}{d \ln E} = \sum_{j=1}^3 a_{i,j} E^{-\gamma_{i,j}} e^{-\frac{E}{Z_i R_{c,j}}}, \quad (2.9)$$

where R_c marks the characteristic rigidity of the cutoff and a and γ are the normalization constant and the integral spectral index of the three populations, respectively. Depending on the model, different numbers of mass groups are included. One example is the $H3a$ or $H4a$ models, which assume five mass groups, where $H4a$ uses a proton-only flux to

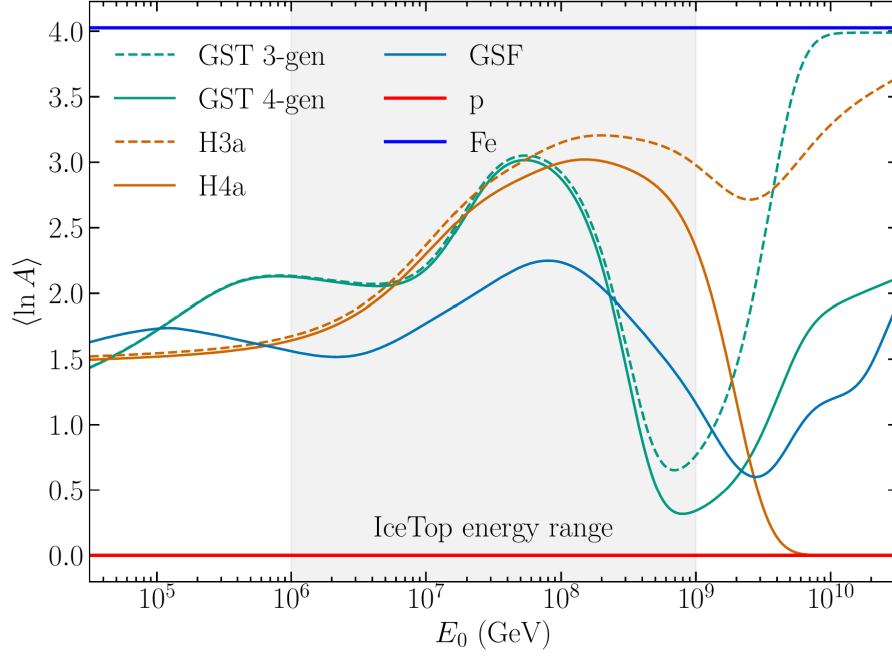


Figure 2.7.: $\langle \ln A \rangle$ predicted by different cosmic-ray flux models and compared to the respective pure proton and iron flux assumptions as a function of primary energy. The shaded area indicates the energy range relevant for the IceCube Neutrino Observatory (see chapter 4). Figure taken from [41].

model the extragalactic population⁷ Due to reliance on simulations for the interpretation of indirect cosmic-ray measurements, significant differences are observed in the cosmic-ray spectra reported by different experiments. This typically manifests itself in offsets in the spectrum due to differences in the absolute energy scale between different experiments. However, under the assumption that the features of the cosmic-ray spectrum are universal, the spectra of different experiments can be rescaled ($\mathcal{O}(10\%)$) to match each other. An example of a cosmic-ray flux model using a global fit to the rescaled spectrum of different experiments is the *Gaissner-Stanev-Tilav* (GST) model [4]. Individual mass group contributions and contributions from different source populations within the GST model are shown in Fig. 2.5. Another example is the *Global Spline Fit* (GSF) model [40], which is not based on theoretical assumptions, but fits the average of measurements from various experiments, taking into account the statistical and systematic uncertainties. The GSF model uses the four mass groups (H, He, O, Fe), which are often measured by different experiments and are roughly equidistant in $\langle \ln A \rangle$. Since uncertainties in the energy estimation in indirect cosmic ray measurements are large, the energy scale for the global spline fit is determined by direct observations, whereas offsets between different indirect

⁷As mentioned, more recent data indicate an increasingly heavy composition at the highest energies, which is in tension with a pure-proton assumption. However, in the energy range relevant for this work, the assumption does not have a significant impact (see Fig. 2.7).

experiments are taken into account by the fit. The GSF model is shown in Fig. 2.6. A unique feature of the GSF fit is the availability of a covariance matrix for the fit, which can be utilized to propagate uncertainties to observables.

A comparison of the prediction of $\langle \ln A \rangle$ of the cosmic-ray flux models H3a, H4a, GST, and GSF is shown in Fig. 2.7. The energy range considered in this work is $\sim 10^{15} - 10^{17}$ eV, which roughly corresponds to the region between the knee and the second knee. In this energy range, only small differences are visible between the different versions of the same model, such as H3a & H4a, and GST 3-gen & GST 4-gen. However, in the case of the GSF model, a significantly lighter average composition is predicted compared to the other models.

In the context of this work, these models are used for weighting purposes as well as to derive expectations from simulations for the interpretation of measured data.

Extensive air showers

After entering the Earth’s atmosphere, a cosmic ray interacts with an air nucleus. Since the interaction length of cosmic rays at around PeV energies is less than 100 g/cm^2 , while a full penetration of the atmosphere down to sea level amounts to $\sim 1000 \text{ g/cm}^2$ [42], practically all cosmic rays above this energy range interact and produce a cascade of secondary particles¹. Thus, the Earth’s atmosphere can be understood as a calorimeter, in which the primary energy is fragmented, resulting in the production of secondary particles [43]. The amount of secondary particles therefore is a measure of the primary energy. The secondary particles can undergo subsequent interactions and decays, which further evolves the particle cascade. At sufficient energy, the particle cascade reaches the Earth’s surface and can be measured via large ground-based detector arrays. The first measurement of such an extensive air shower (EAS) using spatially separated particle detectors was performed by Pierre Auger and collaborators in the 1930’s [44, 45, 46].

Based on such measurements, air-shower observatories try to infer the properties of the corresponding primary cosmic-rays. However, because of this indirect nature of cosmic-ray observations via air-shower measurements, the reconstruction of cosmic-ray properties is subject to large uncertainties. In particular, since the phase space for air-shower measurements can not be probed with human-made accelerators, significant model dependencies arise in the interpretation of the measured air-shower data (see section section 3.6).

In the following, an introduction to the underlying physics and important concepts in the context of air-shower development in the Earth’s atmosphere is given. Firstly, a short overview of the properties of the atmosphere, the medium that constitutes the calorimeter for high-energy cosmic ray detection, is presented in section 3.1. Secondly, in section 3.2, the evolution of air-showers in the atmosphere and the connection of the key observables to the properties of the primary cosmic-ray are discussed in a simplified model. Different EAS measurement techniques are described in section 3.5. Lastly, in section 3.6 modern air-shower simulation codes and connected uncertainties and deficiencies are discussed.

¹The amount of matter a cosmic ray has to cross until it reaches a particular observation level depends on the its inclination

3.1. Atmospheric density

As air showers propagate through the atmosphere, knowledge about the atmospheric properties is of great importance to understand their evolution. Since the atmosphere constitutes the target nuclei for interactions within the air shower, its density profile has a significant impact on the air-shower development. The key observables for the derivation of the atmospheric density are the temperature T and the pressure P . Using the ideal-gas approximation, the density is given as

$$\rho = \frac{\langle M_{\text{atm}} \rangle P}{RT}, \quad (3.1)$$

with the mean molecular weight of the atmosphere, $\langle M_{\text{atm}} \rangle$, and the gas constant R . In order to find an estimate of $\langle M_{\text{atm}} \rangle$, the composition of the Earth's atmosphere has to be measured.

For dry air, the majority of the atmosphere is comprised of nitrogen (78.08%) and oxygen (20.95%), with minor contributions of argon [47]². The given composition results in a mean molecular weight of $\langle M_{\text{atm}} \rangle = 28.97 \text{ g/mol}$. Up to $\sim 100 \text{ km}$, the atmospheric composition is approximately stable, with an average atomic number of $\langle A_{\text{atm}} \rangle = 14.5$ [48].

By integrating the atmospheric density above an altitude h , the total amount of matter that a particle traverses on a vertical path through the atmosphere can be obtained via

$$X_v(h) = \int_h^\infty \rho(h') dh'. \quad (3.2)$$

This quantity is often referred to as *vertical depth* or *mass overburden*. Multiplication of the vertical depth with the gravitational constant gives the atmospheric pressure $P = gX_v$, which can be combined with Eq. (3.1) and $\rho = -dX_v/dh$ (see Eq. (3.2)) [41] to

$$\frac{dX_v}{X_v} = -\frac{\langle M_{\text{atm}} \rangle g}{RT} dh. \quad (3.3)$$

Assuming a constant temperature, the simplified *isothermal model* for the atmospheric density profile can therefore be derived as

$$X_v(h) = X_0 e^{-\frac{h}{h_0}}, \quad (3.4)$$

where $h_0 = RT/\langle M_{\text{atm}} \rangle g \approx 6.4 \text{ km}$ and $X_0 \approx 1030 \text{ g/cm}^2$ are the scale height and vertical depth at sea level, respectively. Although significantly simplified, the isothermal model describes well the general trend of the atmospheric density as a function of altitude. However, for high altitudes, and particularly due to seasonal variations in the

²Only contributions above the 0.1% level are denoted here.

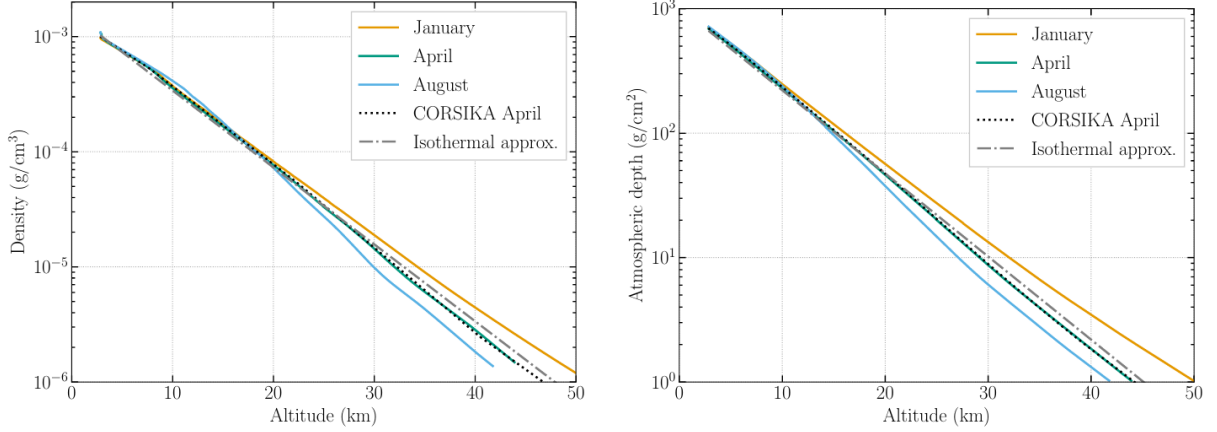


Figure 3.1.: Example profiles of the atmospheric density (left) and depth (right) as a function of the altitude. Profiles for different months are based on balloon and satellite measurements taken at the South Pole in 2013. Additionally, the profiles used within the CORSIKA simulations relevant for this work are shown as dotted black lines. For all profiles, a significant deviation from the isothermal model can be observed. Figure taken from [41].

temperature profile, deviations in the real density and atmospheric depth profiles are visible (see Fig. 3.1). Therefore, for a consistent EAS interpretation, a realistic model of the atmosphere above the detector is taken into account in detailed simulations of the shower development (see section 4.4).

For a particle traveling with an inclination relative to the vertical path, the concept of the vertical depth can be generalized to the *slant depth* X , where the integration is carried out along the trajectory l of the particle. If the particle arrives at a zenith angle θ , the h and X_v can be modified with a factor of $1/\cos\theta$ in order to obtain the corresponding quantities for the inclined track:

$$l = \frac{h}{\cos\theta} ; X = \frac{X_v}{\cos\theta} . \quad (3.5)$$

It should be noted that these relations are only valid in the approximation of a negligible curvature of the Earth, which is valid for zenith angles up to $\sim 60^\circ$ [48].

3.2. Air-shower development

A high-energy cosmic ray entering the Earth's atmosphere interacts with an air nucleus, producing secondary particles that, in turn, interact to produce more particles. Subsequently, a cascade develops along the initial direction of the primary cosmic ray. With each iteration, more particles are produced until the average particle energy falls below

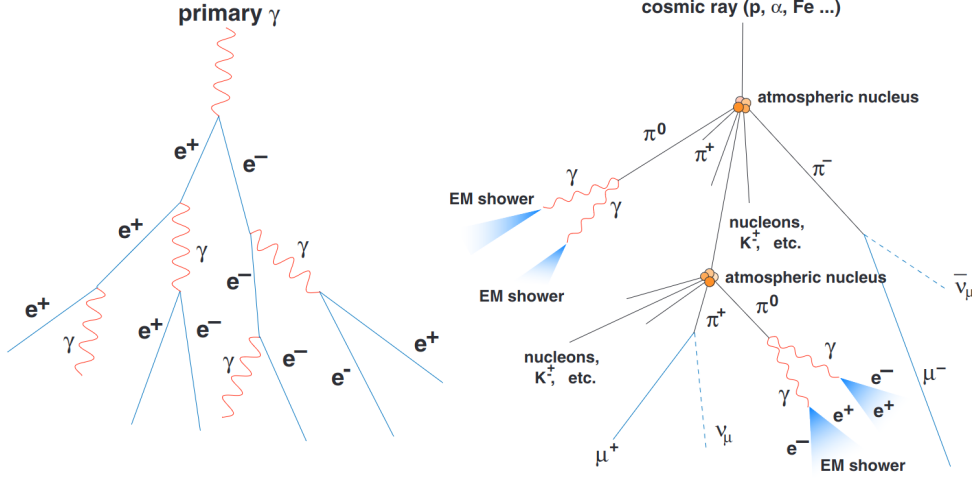


Figure 3.2.: Schematic illustration of an electromagnetically induced and a hadronically induced extensive air shower (left and right, respectively). Figure taken from [49].

the threshold for particle production. At this point, the *shower maximum*, the development stage at which the shower contains the maximum number of particles, is reached. After its maximum, the air shower attenuates, and the remaining particles reach the Earth's surface. A schematic of the first few interactions in the development of a photon- and hadron-induced air shower is shown in Fig. 3.2. While a photon-induced shower produces mainly electromagnetic (EM) particles (electrons, positrons, and photons), primary hadrons lead to three main components, a hadronic, EM, and muon component. Additionally, also neutrinos are produced and constitute a fraction of the energy of the cascade that is lost in the context of EAS measurement.

The development of the particle cascade can be described for each particle species by a set of coupled equations³ of form

$$\frac{dN_i(E_i, X)}{dX} = -\frac{N_i(E_i, X)}{\lambda_i} - \frac{N_i(E_i, X)}{d_i} + \sum_j \int_E^\infty \frac{F_{ji}(E_i, E_j)}{E_i} \frac{N_j(E_j, X)}{\lambda_j} dE_j, \quad (3.6)$$

where the flux of particles of type i within a given energy interval $[E, E + dE]$ is given by $N_i(E_i, X)dE_i$ at slant depth⁴ X [8]. The first two terms of Eq. (3.6) describe the particle loss from interaction with interaction length λ_i and from decay with decay length d_i within the slant depth element dX . λ_i , d_i , and X are expressed in units of g/cm^2 . The interaction length can be expressed as

$$\lambda_j = l_j \rho(h) = \frac{\rho(h)}{n_A \sigma_j^{\text{air}}} = \frac{A m_p}{\sigma_j^{\text{air}}}, \quad (3.7)$$

with the atmospheric density $\rho(h)$ as a function of altitude h , interaction length l_j in cm, local number density n_A , proton mass m_p , mean mass A of the atmosphere, and the

³The basis for these equations are applicable to many other settings, such as the cosmic-ray propagation and in astrophysical scenarios [8].

⁴The slant depth is measured along the direction of the primary particle.

nucleus-air cross section σ_j^{air} [8]. An important observation from Eq. (3.7) is that the interaction length does not depend on the density when expressed in g/cm^2 . Conversely, the decay length depends linearly on the density with

$$d_j = \rho(h)\gamma c\tau_j, \quad (3.8)$$

where γ is the Lorentz factor and the rest lifetime of the particle of type j is described by τ_j . This is an important feature for air-shower physics, as the ratio of particle decay and interaction changes throughout shower development and depending on the atmospheric density⁵. The last term of Eq. (3.6) describes the production of particles of type i by the decay or interaction of particles of type j with air nuclei. The particle yield of type i with energy $E_i < E_j$ from a particle j of energy E_j is given by $F_{ji}(E_i, E_j)$.

The description using cascade equations is enough to model the EAS development in great detail and derive particle fluxes and densities as well as the longitudinal development⁶. However, cascade equations usually only describe the average behavior of air showers. Therefore, to model the full complexity of EAS development in four dimensions and study shower-to-shower fluctuations, typically Monte Carlo (MC) methods are employed⁷ (see section 3.6). For a more intuitive understanding of the key properties of air showers, it is sufficient to describe them using the simplified models discussed in the following. However, before discussing the details of hadronic-induced showers, it is useful to have a closer look at the simplified development of EM cascades.

3.2.1. Electromagnetic cascades

EM cascades in the Earth's atmosphere can be produced by photons, electrons, or positrons. In the simple *Heitler model* [53], an EM particle with energy E_0 splits after a splitting length of $\lambda_e = \log(2)X_0$, where $X_0 \sim 37\text{g}/\text{cm}^2$ is the EM radiation length [52]. The splitting process produces two secondary particles that share the initial energy equally with $E_0/2$, and each undergoes another splitting after λ_e and so on⁸. A schematic view of this process is illustrated in Fig. 3.3 (left). Depending on the particle type, the splitting process can be understood differently. In the case of electrons/positrons (e^-, e^+), they undergo Bremsstrahlung, typically in the Coulomb field on an air nucleus, and produce a

⁵This is of particular importance for the production of muons which are produced in the decay of mesons.

⁶Examples for particle transport codes simulating air showers by numerically solving cascade equations are *CONEX* [50] and *MCEq* [51].

⁷It should be noted, that *CONEX* also allows for hybrid simulations where MC simulations of the first few interactions are the input to cascade equations to include the effects of shower-to-shower fluctuations.

⁸Note that, in this model, the radiation length of electrons/positrons and photons is assumed to be similar. In reality, the mean free path for photons is smaller compared to that of electrons/positrons by a factor of 7/9 [54] and is therefore only an approximation.

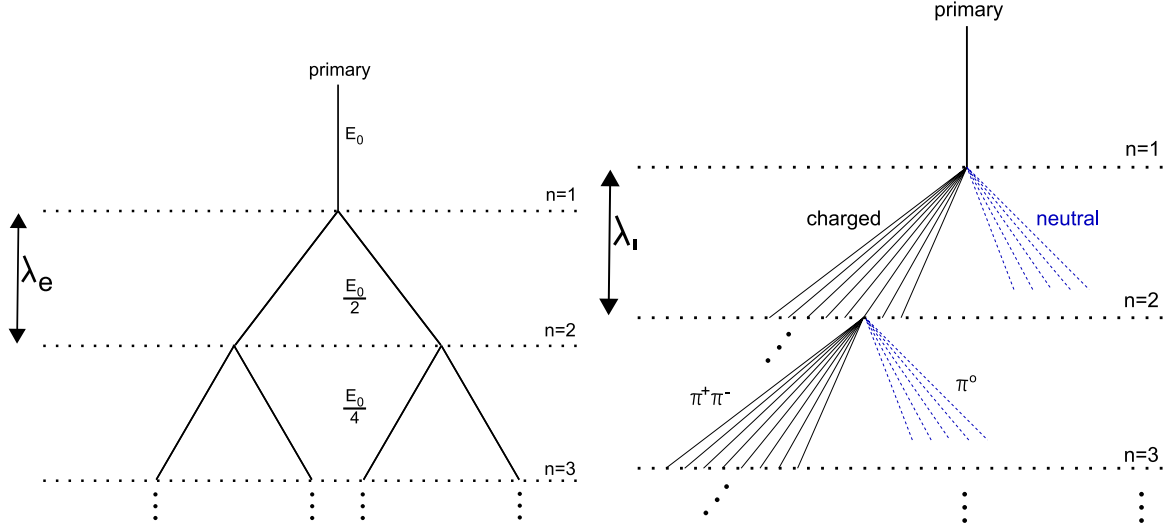


Figure 3.3.: Schematic illustration of the Heitler model of EM cascades (left) and the Heitler-Matthews model of pion cascades (right). Figure taken from [52].

photon via $e^\pm \rightarrow e^\pm + \gamma$. For photons, the splitting describes a pair production process $\gamma \rightarrow e^+e^-$. After each splitting length, the number of particles is therefore doubled:

$$N_n = 2^n, \quad (3.9)$$

where n is the generation number (number of λ_e the cascade has traversed along the primary direction) and can be expressed as $n = X/\lambda_e$. Due to the equal distribution of E_0 over all particles produced, the energy at n is given by

$$E_n = \frac{E_0}{N_n}. \quad (3.10)$$

The multiplication process continues until the particle energies fall below the *critical energy* E_c^{EM} (~ 85 MeV for air) below which energy loss processes (ionization or absorption) are larger than particle production (Bremsstrahlung or pair production). The maximum number of particles in the EM cascade, $N_{\text{max}}^{\text{EM}}$, and the depth at which this maximum is reached (*shower maximum*), $X_{\text{max}}^{\text{EM}}$, are then given as

$$\begin{aligned} N_{\text{max}}^{\text{EM}} &= \frac{E_0}{E_c^{\text{EM}}}, \\ X_{\text{max}}^{\text{EM}} &= \lambda_e n_c = \lambda_e \frac{\ln(E_0/E_c^{\text{EM}})}{\ln 2} \sim \lambda_e \ln E_0. \end{aligned} \quad (3.11)$$

Therefore, already from the simple Heitler model, two main features of air showers can be derived. Namely, that the number of particles scales linearly with the primary energy E_0 and the shower maximum is proportional to $\ln E_0$.

3.2.2. Hadronic cascades

The simple Heitler model for EM cascades was extended to the context of hadronic cascades by their approximation as a cascade of pions in the *Heitler-Matthews model* [55]. It is useful to first consider a primary proton initiating an air shower. In this model, a nucleon⁹ interacts after one interaction length λ_I and produces charged pions (π^- and π^+) and neutral pions, π^0 , with multiplicities rn_{tot} and cn_{tot} , respectively. For pions of $10 - 1000$ GeV in air, $\lambda_I \approx 120 \text{ g/cm}^2$ [8]. The so-called pion-charge ratio $c = 1 - r$ is typically assumed to be $1/3$, i.e., an equal number of $\pi^\pm$ and π^0 are produced. An important difference to the Heitler model is that one part of the cascade is excluded from the multiplication process. Namely, neutral pions instantly decay into a pair of photons ($\pi^0 \rightarrow 2\gamma$, branching fraction $\sim 98.8\%$ [56]) that in turn can produce an EM cascade, but are lost to the hadronic cascade. However, through this process, the hadronic cascade constantly transfers energy to the EM cascade. Setting the pion-charge ratio to $2/3$, the number of charged pions and the energy per pion can be obtained as

$$\begin{aligned} N_n^{\text{ch}} &= \left(\frac{2}{3} n_{\text{tot}} \right)^n, \\ E_n^\pi &= \frac{E_0}{(n_{\text{tot}})^n}. \end{aligned} \quad (3.12)$$

The multiplication process continues until the $\pi^\pm$ energy is low enough that their interaction length becomes larger than their decay length. At this point, they decay into muons and neutrinos. This characteristic energy E_{dec} therefore depends on the atmospheric density. Typical values of E_{dec} (referred to as the critical pion energy E_c^π in the following) are around $20 - 30$ GeV [8]. The generation number n needed to reach E_c^π is then given by

$$n_c = \frac{\ln(E_0/E_c^\pi)}{\ln n_{\text{tot}}}, \quad (3.13)$$

which has typical values of $4 - 7$ [57]. Under the approximation that all charged pions decay into muons and neutrinos ($\pi^\pm \rightarrow \mu^\pm + \overset{(-)}{\nu}_\mu$, branching ratio $\sim 99.99\%$ [58]) after reaching E_c^π , the number of muons can be deduced as¹⁰

$$\begin{aligned} N_\mu^{\text{p}} &= N_{n_c}^{\text{ch}} = \left(\frac{2}{3} n_{\text{tot}} \right)^{n_c} = \left(\frac{E_0}{E_c^\pi} \right)^\beta, \\ \beta &= \frac{\ln \left(\frac{2}{3} n_{\text{tot}} \right)}{\ln n_{\text{tot}}} = \frac{\ln \left(\frac{2}{3} \right)}{\ln n_{\text{tot}}} + 1, \end{aligned} \quad (3.14)$$

⁹For the description of this model, the index p is used generalized for any nucleon

¹⁰In reality, β has values around 0.9, the muon number therefore scales sub-linearly with the primary energy. This is a direct result of the energy transfer to the hadronic cascade [2]

and would be modified correspondingly for different values of r ¹¹ [52].

Due to the decay of π^0 , about 90% of the energy initially retained in the hadronic cascade is transferred to EM particles. Further, the number of EM particles at $X_{\max}$ can be estimated as

$$N_{\max}^{\text{EM,p}} = \frac{E_0 - N_{\mu}^{\text{p}} E_c^{\pi}}{E_c^{\text{EM}}}, \quad (3.15)$$

from the energy contained in the EM component. To account for the strong attenuation of EM particles within the atmosphere, a scale length $\Lambda \sim 65 \text{ g/cm}^2$ ¹² [52] can be introduced to describe the approximately exponential attenuation via

$$N_{\text{EM}}^{\text{p}} \sim N_{\max}^{\text{EM,p}} e^{-\frac{X_{\text{obs}} - X_{\max}}{\Lambda}}, \quad (3.16)$$

which is valid in the case $X_{\text{obs}} \gg X_{\max}$, where X_{obs} is the atmospheric depth at the observation level. When converting Eq. (3.16) into logarithmic scale:

$$\ln N_{\text{EM}}^{\text{p}} \sim \ln N_{\max}^{\text{EM,p}} - \frac{X_{\text{obs}} - X_{\max}}{\Lambda}, \quad (3.17)$$

it becomes clear that $\ln N_e$ depends linearly on $X_{\max}$ but only logarithmically on the number of EM particles at $X_{\max}$ (which depends on the hadron multiplicity and on the number of muons). Therefore, inferring dependencies of N_e on the hadronic interactions directly from the Heitler-Matthews model is not possible.

$X_{\max}$ can be derived by considering only the EM sub-showers produced by the first hadronic interaction¹³ via

$$X_{\max}^{\text{p}} \sim \lambda_{\text{I}} + X_{\max}^{\text{EM}}(E_0/(2n_{\text{tot}})) \approx \lambda_{\text{I}} + \lambda_{\text{e}} \ln \frac{E_0}{n_{\text{tot}} E_c^{\text{EM}}}, \quad (3.18)$$

where the additional factor 1/2 results from the production of two photons in the π^0 decay [41]. Therefore, $X_{\max}$ depends linearly on λ_{I} and logarithmically on the total number of particles. The structure of Eq. (3.18) does not change for the inclusion of higher generations of hadronic interactions [52].

In principle, shower-to-shower fluctuations are not directly included in the Heitler-Matthews model. However, on the basis of Eq. (3.18), fluctuations in $X_{\max}$ can be related to fluctuations in λ_{I} , i.e., of the first interaction, and to fluctuations in the multiplicity:

$$\text{Var}(X_{\max}) \propto \text{Var}(\lambda_{\text{I}}) + \lambda_{\text{EM}}^2 \text{Var}(\ln n_{\text{tot}}), \quad (3.19)$$

where the variance of the first interaction $\text{Var}(X_0) = \lambda_{\text{I}}^2 \propto 1/\sigma_{\text{I}}^2$ [52]. Therefore, the relative contribution of both sources of fluctuations depends on the size of the cross

¹¹In first order, a small change of Δr would modify the muon number as $\frac{\Delta N_{\mu}^{\text{p}}}{N_{\mu}^{\text{p}}} \approx n \frac{\Delta r}{r}$ [2]. Therefore, a 10% increase in r would result in a 50% increase in the muon number.

¹²The factor Λ is based on shower universality and is independent of the type of the primary particle.

¹³This is necessary as the Heitler-Matthews model does not describe the parallel development of the EM and hadronic cascades [52]. However, $X_{\max}$ is dominated by the EM sub-showers stemming from the hadronic interaction with the largest inelasticity, i.e., typically the first interaction [41].

section of the primary in the atmosphere. To draw further conclusions about the shower-to-shower fluctuations, more detailed simulations are needed.

3.2.3. Superposition model

The derivations obtained from the Heitler-Matthews model describe air-shower properties for single primary nucleons. Based on that, expressions for primary nuclei comprised of multiple nucleons can be derived with the *superposition model*. In this model, the particle cascade produced by a nucleus with mass number A and energy E_0 is approximated as A individual nucleons¹⁴ that interact independently, where each nucleon carries an equal amount of the total energy, E_0/A . The resulting particle cascade can then be described as a superposition of A single and simultaneous nucleon air-showers. The expressions for the shower maximum, the number of EM particles, and the number of muons are then modified as

$$X_{\max}^A = X_{\max}^{\text{p}}(E_0/A) \approx X_{\max}^{\text{p}} - \lambda_{\text{e}} \ln A, \quad (3.20)$$

$$N_{\max}^{\text{EM},A} = A N_{\max}^{\text{EM},\text{p}}(E_0/A E_c^{\text{EM}}) \approx N_{\max}^{\text{EM},\text{p}}(E_0), \quad (3.21)$$

$$N_{\mu}^A = A N_{\mu}^{\text{p}}(E_0/A) = A \left(\frac{E_0}{A E_c^{\pi}} \right)^{\beta} = A^{1-\beta} \left(\frac{E_0}{E_c^{\pi}} \right)^{\beta} = A^{1-\beta} N_{\mu}^{\text{p}}(E_0). \quad (3.22)$$

Therefore, the shower maximum depends on the primary mass and is linear in $\ln A$. Similarly, the number of muons depends on the mass, where $\ln N_{\mu}$ is proportional to $\ln A$. In the case of iron showers, which contain $\sim 40\%$ more muons than proton showers at EeV energies, the shower maximum is reached $80 - 100 \text{ g/cm}^2$ earlier [8]. In the superposition model, the number of EM particles at the shower maximum does not depend on the mass but only on the primary energy.

Generally, the superposition model can be used to estimate average shower characteristics, such as the average shower maximum and number of muons. However, there are many shortcomings connected to the assumptions in the Heitler/Heitler-Matthews model. Firstly, in reality, the energy is not shared equally between secondaries. In particular, particles produced in the forward direction typically carry the largest fraction of the initial energy (in the lab frame). The particle multiplicity and charge-ratio are therefore average quantities in the Heitler-Matthews model. Secondly, the weak energy dependencies of the particle multiplicity and λ_{I} are neglected. Further, due to the modeling of hadronic showers as pure pion cascades, other long-lived particles (kaons, protons, neutrons, etc.) are not taken into account. However, they have a significant impact on the energy fraction

¹⁴This holds in good approximation since the observed primary energies are much larger than the binding energy which, for the relevant nuclei, has maximum values of $\sim 8.8 \text{ MeV}$ per nucleon (Fe-56) [59].

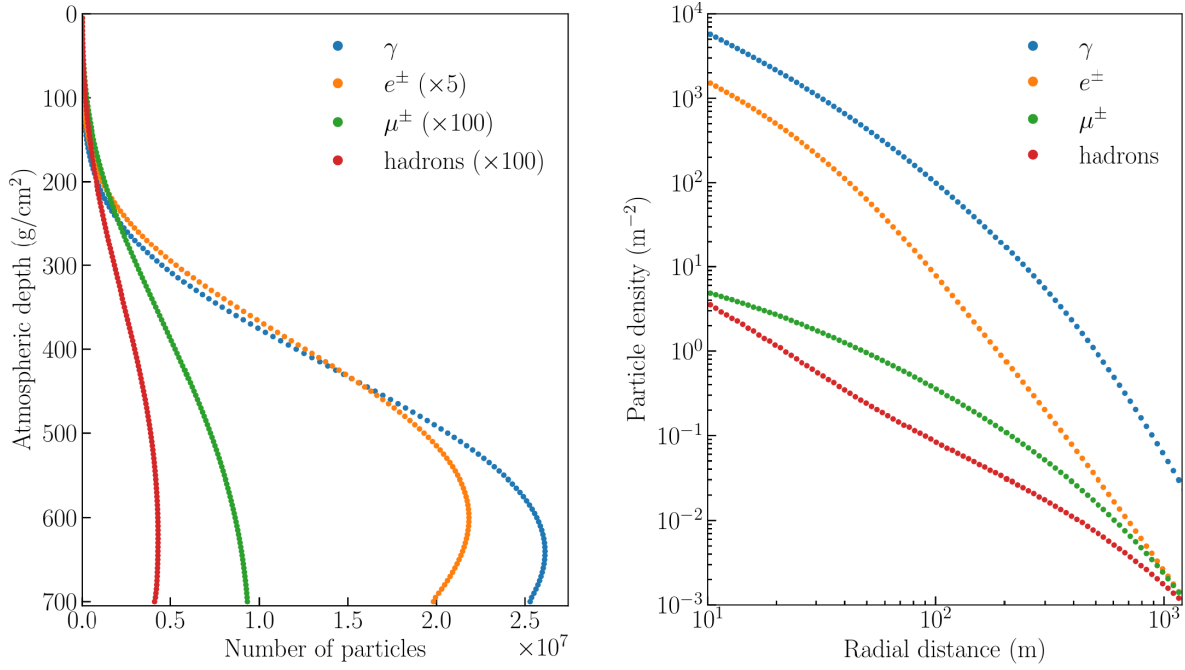


Figure 3.4.: Average longitudinal (left) and lateral (right) particle distribution for vertical air showers with a primary energy of 10 PeV produced with the high-energy hadronic interaction model Sibyll 2.1 [60]. The showers are simulated using realistic atmospheric conditions for the IceCube Neutrino Observatory and the lateral distribution is derived from the particle content at the respective observation level of 2835 m ($\approx 698 \text{ g/cm}^2$). Figure taken from [41].

that is contained in the hadronic cascade. Lastly, the critical energy, E_c^π , depends on the density and therefore on the atmospheric profile and the inclination of the primary.

3.3. Particle distributions

While the simplified models discussed so far are useful to derive a intuitive understanding of some air-shower characteristics, full MC simulations of the shower development are required to gain more detailed insights. For this purpose, the longitudinal and the lateral particle distributions derived from simulations are shown in Fig. 3.4. The number of EM particles increases until the shower maximum, beyond which the energy loss leads to a successive decrease. For muons as penetrating particles, the number of muons exhibits a nearly plateau-like structure with increasing slant depth. For depths much larger than the included range, the number of muons slightly declines mainly due to ionization losses, while muon decay is relevant only for low-energy muons in the sub-GeV range [61].

The general behavior for lateral particle distributions is the steep decline of the particle

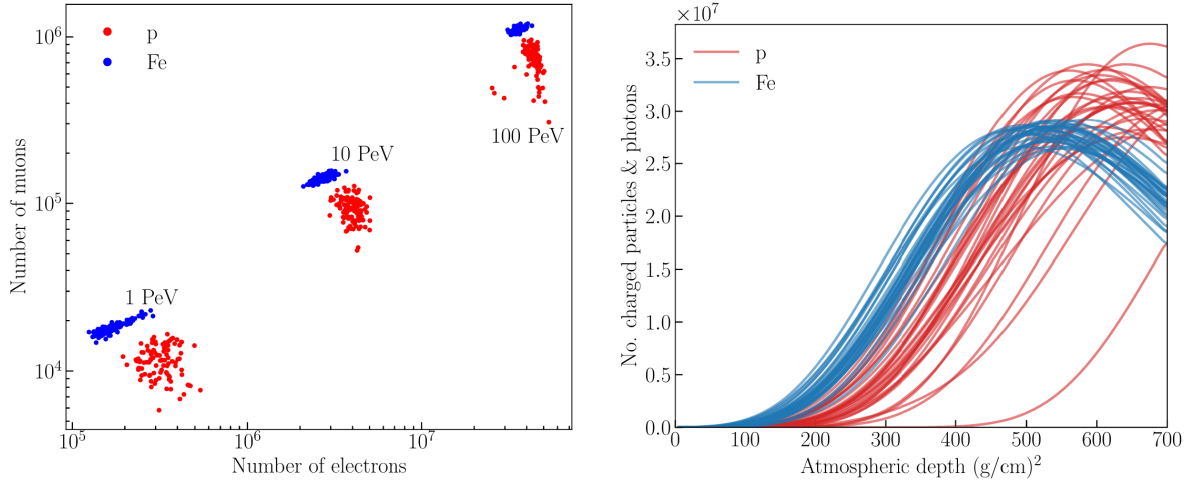


Figure 3.5.: Correlation between the number of muons and the number of electrons in 100 proton- and iron-initiated air showers for different primary energies (left). Longitudinal profile for 30 proton and iron showers at 10 PeV primary energy (right). Figure taken from [41].

density with increasing distance to the shower axis. Compared to the EM component, the hadron lateral distribution is significantly flatter. This is because of the comparably large average transverse momentum of secondary hadrons (350 – 400 MeV) that results in a large angular separation from the shower axis [62]. In contrast to that, the main contribution to the lateral spread of the EM component that stems from the decay of high energy π^0 comes from multiple Coulomb scattering. Only at large distances much larger than the Molière radius¹⁵, the EM particles from the decay of low energy π^0 dominate [65]. Since muons are produced mainly in the decay of low-energy charge pions [2] with significant angular spread with respect to the shower axis, the muon distribution is also flatter compared to the EM component.

In the superposition model, it is derived, that the shower maximum is linearly correlated to $\ln A$. Additionally, due to the mass dependence in the muon content, the number of electrons and muons at the observation level is a valuable quantity to estimate the cosmic-ray energy and mass. The correlation between both is illustrated in Fig. 3.5 (left). From the Heitler-Matthews model it is known that both quantities are correlated and grow linearly with the primary energy. However, due to the mass dependence in the shower maximum and the energy transfer from the hadronic to the EM component, the

¹⁵The Molière radius is a characteristic quantity describing the transverse spread of low-energy particles in air showers [62] and corresponds to the distance below which at least 90% of the ionizing shower particles are contained [63]. It is defined as $r_M = \lambda_e \frac{S_{MS}}{\rho E_c^{EM}} = \lambda_e \frac{21 \text{ MeV}}{\rho E_c^{EM}}$, where $E_{MS} = m_e c^2 \sqrt{4\pi/\alpha} \approx 21 \text{ MeV}$ describes the energy loss due to multiple Coulomb scattering and ρ is the air density [64]. The corresponding distance for the IceCube Observatory is $\sim 128 \text{ m}$.

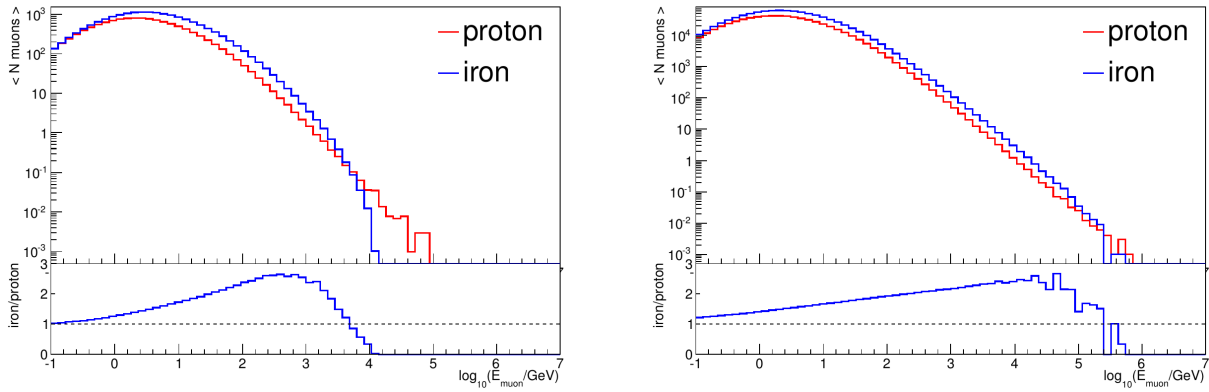


Figure 3.6.: Average muon energy spectrum for proton and iron primaries at 1 PeV (left) and 100 PeV (right) with zenith angles of $0.8 < \cos \theta < 1$ produced with Sibyll 2.1. The bottom panels show the ratio between iron and proton. Figure taken from [42].

number of electrons is larger for proton-initiated air showers while the number of muons is smaller as expected from the superposition model. Since the average $X_{\max}$ is reached earlier for iron compared to proton primaries, the EM component is attenuated further for iron. Fig. 3.5 (right) shows the longitudinal profile for proton- and iron-initiated air showers up to the observation level relevant for measurements with the IceCube Observatory. The rough estimation of the shower-to-shower fluctuations based on the Heitler-Matthews model (Eq. (3.19)) shows their relation to fluctuations in the first interaction. In fact, the different longitudinal profiles show large variations of the depth of the first interaction, in particular for proton primaries. This is connected to the differences in their cross section. In addition, fluctuations in the particle content are visible. Typically, the shower-to-shower fluctuations for heavy primaries are smaller compared to light primaries. This is expected from the superposition model, as the showers initiated by heavier nuclei are approximated as superposition of multiple sub-showers for each nucleon of the primary. Generally, shower-to-shower fluctuations have a significant impact on the shower observables and therefore pose a challenge for the reconstruction of air-shower properties on a single-event basis.

3.4. Muon energy spectrum

Since muons are only weakly affected by attenuation, most of the muons reach the observation level. Depending on the stage of the shower development, muons are produced with different energies. An example of a muon energy spectrum obtained at the observation level is shown in Fig. 3.6 for proton and iron primaries. Since muons in the sub-GeV energy range are more strongly affected by absorption and muon decay processes, the

energy spectrum decreases at the lowest energies. The bulk of the muons arriving at the observation level are in the GeV range. As expected from the superposition model, iron produces significantly more muons than proton. However, at muon energies $\gtrsim \text{TeV}$, the ratio between the muon energy spectra of iron and proton starts to decrease. This is because the energy in iron primaries is distributed among all nucleons. Muons that are produced at the early stages of the shower development can therefore exhibit significantly larger energies for proton primaries for the same primary energy. Therefore, iron primaries typically results in a higher muon multiplicity while protons produce muons with higher energies. Such high-energy muons¹⁶ can propagate deep into the ground after reaching the observation level and can be measured by underground detectors such as the IceCube Neutrino Observatory. Since the other shower particles are attenuated quickly in dense media, this *muon bundle*¹⁷ can be detected with comparably low background contamination.

One shortcoming of the Heitler-Matthews model is the assumption of a pure pion cascade. In reality, also the decay of kaons has a significant contribution to the muon production. The dominant channel for muon production in kaon decay is $K_L^0 \rightarrow \pi^\pm + \mu^\mp + \bar{\nu}_\mu^{(-)}$ with a branching fraction of $\sim 27\%$ [66]. Muons originating from the decay of pions and kaons are generally referred to as *conventional muons*. Since the critical energy scales linearly with mass [67], the relative contribution of heavier hadrons increases for increasing muon energy. Muons that stem from hadrons that have decay lengths of below 1 cm and therefore decay almost instantly are *prompt muons* [68]. The flux of prompt muons is dominated by decays of charmed mesons, e.g., $D^\pm \rightarrow \mu^\pm + X$ and $D^0 \rightarrow \mu^\pm + X$, and unflavored vector mesons such as $\eta \rightarrow \mu^+ + \mu^- + \gamma$. Here, X is used as generalized denotation to summarize the multitude of decay modes. It should be noted, that the production of charmed mesons is not included in the high-energy hadronic interaction models used in this thesis¹⁸. However, the influence of prompt muons is only important for highly energetic muons well beyond the 10 TeV scale and is therefore not relevant for this work.

3.5. Measurement techniques

With the information about the longitudinal and lateral distributions detailed in the previous section, different ways of measuring air showers can be discussed. Since the

¹⁶High-energy muons are a valuable probe of the first interactions in the air-shower development and of the connected hadronic physics.

¹⁷Since high-energy muons stem from the first interactions during the shower development, they exhibit only a small angular spread around the shower axis and are therefore highly collimated [41].

¹⁸Newer versions of the hadronic interaction model Sibyll (2.3c/d [69, 70]) include charm production. However, at the time of writing no simulations with these newer versions are available for the relevant data set.

Earth's atmosphere acts as a calorimeter, the energy deposit of the shower can be observed not only directly via the shower particles but also by measuring the EM radiation that is produced through the propagation of the EM component. The multitude of different detection channels is illustrated in Fig. 3.7. The gold standard for modern air-shower observatories is the utilization of multiple detection channels that provide complementary information. The primary objectives for air-shower measurements are the estimation of the primary energy, the direction of the osmic ray, and its mass. For this purpose, the main observables are the number of EM particles (or the energy contained within the EM component), the number of muons, and the shower maximum. The incident direction of cosmic rays is measured via the arrival time distributions of the air-shower particles.

Particle detection

One main detection channel are particle detectors, which are typically distributed over a large surface array in regular patterns. The sparsity of their arrangement and the altitude at which the detector array is located determine the threshold of the primary energies that can be measured. This is because each particle detector only samples the lateral distribution at a given distance, which limits the observable *shower size* (total number of particles at given observation level). Widely used particle detectors are water-Cherenkov tanks and scintillators¹⁹. Both measure the signals produced by charged particles that cross the sensitive detection volume and assign a corresponding time stamp. Air showers are then measured by means of time coincidences in the detected signals of neighboring detectors. Using the time distribution of the resulting charge *footprint* of a measured air-shower event, the arrival direction of the cosmic ray, i.e., the shower axis, can be triangulated. The *core position*, the point at which the shower axis crosses the plane in which the detector array is deployed, can in first order be determined by the center of gravity of the measured charge distribution. A more sophisticated method for the reconstruction of the shower geometry using the signal and time information involves their description with appropriate model functions as discussed in more detail in section 4.3.1

The shower size or primary energy is typically determined using a dedicated reference signal at a specific distance from the shower axis. Depending on the observation level of a given observatory, the relative contribution of muons to the measured signal distribution differs significantly. In principle, since the number of muons is almost linearly correlated with the primary energy, even a pure estimate of the muon number can be used to reconstruct the energy. However, the muon component is prone to large fluctuations and

¹⁹Scintillation detectors are typically thin panels in which only low-energy EM particles are fully stopped, while water-Cherenkov tank have a large volume and exhibit distinct charge deposits from muons that usually cross the entire tank, leading to an energy deposit along their full track.

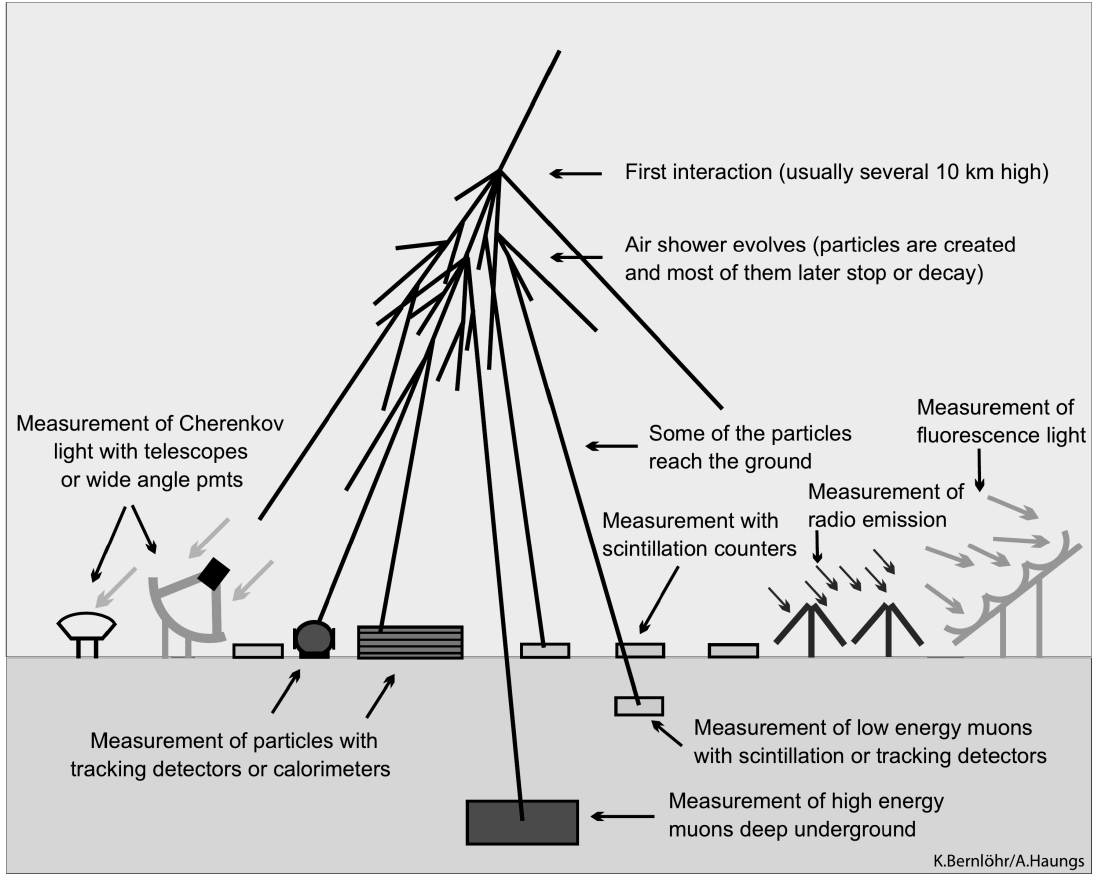


Figure 3.7.: Illustration of the different air-shower detection channels. Figure taken from [71].

systematic uncertainties due to its strong connection to the modeling of the hadronic component (see section 3.6.2 for a detailed discussion).

For particle detector arrays, the primary mass is usually estimated based on observables sensitive to the number of muons. Since the signal distributions are typically dominated by EM contribution, two main approaches are possible to derive information about the muon component. Firstly, dedicated muon detectors can be employed that utilize shielding to absorb EM particles. Examples for air-shower observatories using this approach are KASCADE [32]/KASCADE-Grande [33], AGASA [72], AMIGA [73], GRAPES-3 [74], LHAASO [20], and Yakutsk [75]. Secondly, if the signal waveforms are available in addition to the integrated signal, the rise time²⁰ as well as the distinct structure created by muons can be used to estimate the muon contribution. This is because muons typically arrive earliest and exhibit a smaller temporal spread compared to the EM component since they are less prone to attenuation and scattering. Examples of observatories using the signal waveforms to estimate the muon contribution are Haverah Park [76] and the Pierre Auger Observatory [77, 78].

²⁰Time duration during which the integrated signal rises from 10% to 50% of the total signal [76, 77].

Another way to obtain information about the primary mass is by studying the signal distribution as a function of the distance to the shower axis. Since heavy primaries, on average, develop earlier in the atmosphere compared to light primaries of the same energy and therefore feature a more shallow X_{max} , the resulting showers exhibit a larger spatial spread. In addition, the shower is attenuated further compared to lighter primaries, increasing the ratio of muon to EM contribution to measured signals. Overall, heavy primaries therefore feature a more flat lateral distribution of measured signals. The slope of the measured signal distribution was used, e.g., by the Volcano Ranch experiment [79]. Air-shower arrays can also comprise different detectors to utilize complementary information. For example, the GRAPES-3 experiment uses proportional counters in addition to scintillators to track the passage of muons [80]. The Tibet AS-gamma experiment uses a combination of scintillation detectors and emulsion chambers with *burst detectors* that measure high-energy particles in the core of air showers [81]. The KASCADE-Grande experiment used hadron calorimeters and multi-wire proportional chambers in addition to its scintillator array which allow the measurement of the hadronic core and muon tracks [82]. A prominent combination of air-shower arrays and deep underground detectors that measure high-energy muons produced in air showers. Examples for observatories featuring a deep underground detector are the IceCube Neutrino Observatory (see chapter 4 for a detailed overview), the EAS-TOP experiment that was located above the Gran Sasso National Laboratory in which the MACRO muon detector was deployed [83], and the SPASE air-shower array with the AMANDA detector [84].

Air-Cherenkov detection

Charged particles that are created in air showers can move faster than the speed of light in Earth's atmosphere and therefore produce Cherenkov radiation [85]. The refractive index n that determines the emission angle of the Cherenkov photons depends on the atmospheric density and therefore on the altitude. Most of the emission occurs in the ultra-violet region of the electromagnetic spectrum. Since the bulk of the charged shower particles that create Cherenkov emission are electrons/positrons, the measurement of Cherenkov emission is mainly a measure of the EM energy. The detection of Cherenkov light is possible via non-imaging and imaging Cherenkov telescopes (IACTs). While the former are typically large telescopes that are sensitive to small primary energies between 30 GeV – 100 TeV [42] but are limited toward large energies due to their limited effective area, the latter are distributed as ground arrays where they measure the lateral distribution of the emitted Cherenkov light. Due to the density-dependent emission angle and multiple scattering of the emitted radiation, photons from all shower stages can be measured, providing information about the longitudinal development [86]. The slope of the

measured lateral distribution is sensitive to the shower maximum and can therefore be used to estimate the primary mass [87]. In addition, for the measured wavelengths, the Cherenkov emission occurs incoherently which leads a relation between the light intensity and the shower energy [85].

Examples of IACTs are H.E.S.S. [88], MAGIC [89], and VERITAS [90], typically featuring a small field of view but very good angular resolution, which is beneficial for source observations. Experiments employing non-imaging Cherenkov telescopes are, e.g., Tunka-133 [91], EAS-TOP [92], and Yakutsk [93].

A disadvantage of air-Cherenkov measurements is the limited duty cycle around 10-20%, as clear and moonless nights are required [86].

Air-fluorescence detection

As air showers propagate through the atmosphere, mainly the EM shower particles can ionize surrounding atoms [94]. Due to their relative abundance, mostly nitrogen atoms are therefore excited and emit photons in the ultra-violet range [86]. For sufficient shower energy ($\gtrsim 100$ PeV [42]), this fluorescence light can be measured by ground telescopes and used to reconstruct the primary characteristics. An advantage of the fluorescence detection is the isotropic emission, which allows for the measurement from any direction. Fluorescence emission enables the measurement of the calorimetric energy [85] and the longitudinal profile [95], which can be used to reconstruct the shower maximum. This is achieved by sampling the longitudinal profile in bins of slant depth and modeling the resulting distribution via the Gaisser-Hillas function [96]

$$N(X) = N_{\max} \left(\frac{X - X_0}{X_{\max} - X_0} \right)^{\frac{X_{\max} - X_0}{\lambda}} e^{-\frac{X_{\max} - X}{\lambda}}, \quad (3.23)$$

where $N_{\max}$ describes the shower size at $X_{\max}$ and X_0 and λ are mass- and energy-dependent parameters that can be understood as the depth of first interaction (if $X_0 > 1$) and the average interaction length, respectively [42]. The integral of the distribution then is a measure of the total amount of deposited energy while the shower maximum is directly obtained from the fit.

Similarly to the air-Cherenkov observation, fluorescence measurements are limited to clear and dark nights, limiting the duty cycle to 10-20%. Examples for experiments using air-fluorescence detection are the Fly's Eye detector [97] and the successor experiment [98]. In combination with particle detector arrays, the Pierre Auger Observatory [99] and the Telescope Array [100] feature telescopes for air-fluorescence detection, where particle detectors enable the measurement of air showers with full duty cycle.

Radio detection

The propagation of the EM component through the Earth's atmosphere produces another type of electromagnetic radiation, radio emission. The main part of the radio emission is caused by the deflection of electrons and positrons in opposite direction due to the geomagnetic field. The resulting charge movement on a macroscopic level translates into a transverse electric current [85]. As the number of particles changes throughout the shower development, this current changes as a function of time and therefore leads to linearly polarized radio emission that depends on the Earth's magnetic field strength and is emitted orthogonal to the direction of the shower particles and to the local magnetic field [85, 8] analogously to a Hertz dipole. This emission is the *geomagnetic effect*. A second process, the so-called charge excess radiation or *Askaryan effect*, is an additional source of radio emission. It is based on the fact that a $\sim 20\%$ excess of electrons is present in air showers compared to positrons, caused by the ionization of atoms during shower development [8]. The electrons produced in ionization processes can propagate alongside the shower or annihilate with positrons. Both effects lead to a time-dependent negative net charge that is carried by the shower since the more massive ions produce a negative ion plasma behind the shower disc [101]. This net charge can be approximated as a point-like time-dependent charge leading to radially inward-polarized radio emission relative to the shower axis [85, 102]. The contribution of the Askaryan effect to the total radio signal is on the level of 10-15% [103].

Similarly to the air-Cherenkov radiation, radio emission is beamed in the forward direction [104]. However, due to its large wavelength, radio emission is coherent and the expected electric field is proportional to the electron number [8] and therefore to the primary energy. The radiated power is therefore quadratically proportional to the number of electrons and the primary energy. Due to the forward-focus of the radio signal, the spatial spread of the resulting lateral distribution is comparable to the emission of air-Cherenkov photons [8]. The slope of the lateral distribution is directly related to the shower maximum and can be used to infer the primary mass.

An advantage of radio detection is the nearly unlimited duty cycle [85] while featuring systematic uncertainties comparable for air-Cherenkov and -fluorescence detection [105]. Examples for air-shower experiments using radio detection are LOFAR [106] and AERA [107]. Additionally, the planned surface-array enhancement of the IceCube Neutrino Observatory [108] as well as the surface array of IceCube-Gen2 [109] (see section 4.5) will feature radio antennas that can provide information on the EM energy and the shower maximum and operate with a duty cycle of 100%.

3.6. Simulation

For the indirect observation of cosmic rays via the measurement of EASs, the development of the particle cascade through the Earth’s atmosphere has to be modeled as accurate as possible. This is because the measured data from air-shower observatories is interpreted by means of a comparison to the expectations from MC simulations. However, in particular the description of high-energy hadronic interactions during the shower development introduces large systematic uncertainties [62], since the interactions need to be modeled beyond the phase space reached by collider experiments and are therefore not well constrained. This makes the reconstruction of the cosmic-ray mass composition challenging, since the muon content in air showers, which is an important estimator for the mass of the primary, is directly linked to the hadronic cascade (see section 3.2).

In this section, the simulation of EASs and the connected challenges relevant for this work are discussed in more detail. Firstly, a short overview of the basic principle of the *COsmic Ray SIMulations for KAscade* (CORSIKA) [110], the most widely used tool for the simulation of EASs is presented in section 3.6.1. Further, different models for the description of hadronic interactions within the shower development and their influence on the prediction of different air-shower observables are introduced in section 3.6.2. Lastly, the most prominent discrepancy between measured air shower data and simulations, the *Muon Puzzle* is discussed in section 3.6.3.

3.6.1. CORSIKA

CORSIKA was initially developed in the context of the KASCADE experiment [32] but is now since more than 30 years the standard tool for the simulation of EASs. It can be used to inject particles with energies up to 10^{20} eV at the top of the atmosphere and simulate the development of the resulting particle cascade through the atmosphere down to a specified observation level, where the secondary particle distributions are saved, including spatial and temporal information as well as the particle type and energy.

CORSIKA allows for a variety of different input settings, such as the injection of different nuclei, the injection energy and inclination, and the atmospheric profile and interaction models used for the simulation of the shower development. During the shower propagation, the particles are tracked and processes like ionization, deflection in the Earth’s magnetic field, decays and hadronic interactions are taken into account. The latter are described using external hadronic interaction models, which are discussed in more detail in the next section. Additionally, also the production of Cherenkov radiation and neutrinos can be included [110]. The simulation of radio emission is possible via the embedded *CoREAS* [111].

As discussed in section 3.2, the atmosphere as the medium in which the particle cascade develops is of great importance for EAS simulations. In particular, the atmospheric density has a direct impact on interaction and decay lengths (Eqs. (3.7) and (3.8)) and is therefore of special importance for muon production. Therefore, the isothermal model introduced in section 3.2 with its exponential density profile is discarded in favor of a more realistic description of the atmospheric profile for the production of EAS simulations. The default atmosphere used in CORSIKA is described by five different layers in altitude. In the lower four layers, the atmospheric depth is described by an exponential function, while the fifth layer employs a linear decrease in the atmospheric depth as a function of height [42]. A more detailed discussion about the atmospheric model used for the production of EAS simulations used for the IceCube Neutrino Observatory is given in section 4.4. A more comprehensive overview of the technical details and implementation of air shower physics can be found in [110].

3.6.2. Hadronic interaction models

The development of EASs is dominated by hadronic collisions of air-shower particles and atmospheric nuclei involving low-momentum transfer. Since these interactions are in the non-perturbative regime of quantum chromodynamics (QCD), they cannot be calculated directly from first principles [2]. Instead, effective theories and phenomenology are used to derive the rates and secondary particle spectra produced in the hadronic interactions. For this purpose, dedicated software codes based on accelerator data, *hadronic interaction models* or *hadronic event generators* are employed to simulate the interactions (in the extrapolated phase space) and return the types and kinematics of the final-state particles, which are then further propagated with CORSIKA [68].

Depending on the energy regime of the hadronic interactions, either a high-energy or low-energy hadronic interaction model is used. The energy threshold used to define the transition between the two models is usually around 100 GeV [2]. The three low-energy hadronic interaction models applicable within CORSIKA are FLUKA [112], the *Ultrarelativistic Quantum Molecular Dynamics* (UrQMD) transport model [113], and GHEISHA [114], where the latter is disfavored [2]. The range of application of these models is typically limited to energies below TeV. Note that while low-energy hadronic interaction models have a significant impact on the muon lateral distribution [115, 116], their impact on the total muon yield is small compared to high-energy models. Since the differences between the simulation results of low-energy hadronic interaction models are small compared to those of high-energy models [86], only the differences between the latter are discussed in more detail in the following.

A necessity of high-energy hadronic interaction models used for EAS simulations is abil-

ity to describe a variety of projectiles, such as nuclei protons or charged pions, as well as different targets like nitrogen, oxygen, and argon which are important for EAS development. While for the use case of high-energy physics (HEP), production of heavy flavors and heavy bosons is important, it is largely discarded for the simulation of EASs [2]. As mentioned, high-energy models are required to describe hadronic interactions in the phase space beyond collider scales, which introduces large systematic uncertainties. This includes both the extrapolation to center-of-mass (cms) energies that is an order of magnitude larger compared to the LHC scale and to forward rapidities not well covered by the LHC²¹.

Examples for high-energy hadronic interaction models focused on the description of EASs are QGSJet [117, 118] and Sibyll [60, 69, 70]. Therefore, only physics relevant for EAS development is implemented using a limited set of parameters tuned on comparably small data sets [2], including mainly proton-proton collisions and final-state particles relevant for EASs [41]. Conversely, hadronic event generators like EPOS [119, 120] and DPMJet [121, 122] have a more general focus which includes heavy-ion collisions. The parameter sets for these more general models are roughly an order of magnitude larger ($\mathcal{O}(100)$ parameters) compared to models focused mainly on EAS simulations but are tuned on correspondingly larger data sets, which can include collider and fixed target data. The theoretical basis of the commonly used high-energy hadronic interaction models is Gribov-Regge field theory (GRFT) [123], which uses a unique amplitude for the exchange of *Pomerons*²² to link the inelastic cross-section to particle production [2]. An important concept is the *Pomeron amplitude*, which defines the energy and impact parameter scaling within GRFT models [2]. In this context, two different approaches are adapted. Firstly, the *soft+hard* approach defines the Pomeron amplitude as sum of a purely soft and purely hard Pomeron based on external parton distribution functions (PDFs). Secondly, in the *semi-hard* approach, Pomerons are described as convolutions of a soft and a hard component using DGLAP equations [125]. Since in the first approach one Pomeron is always connected to valence quarks, the elasticity²³ is constant, resulting in a more narrow pseudo-rapidity distribution compared to the semi-hard approach which is in better agreement with experimental data at TeV energies [126]. Further, the semi-hard approach allows for tuning of parameters to PDF data [2].

In the following, a short overview on the main differences between the high-energy hadronic

²¹The phase space important for air-shower development starts at around $\eta \gtrsim 2$, with the pseudo-rapidity $\eta = -\ln \tan \theta/2$ [86]. Here, θ defines the scattering angle (with respect to the beam axis)

²²Pomerons are theoretical constructs defined as color-neutral objects within GRFT that can be exchanged between partons and can be understood as trajectories in GRFT. They are used to describe soft hadronic interactions via multiple scattering processes in which each scattering event is mediated by Pomeron exchanges [123]. In this context, each Pomeron represents a microscopic parton cascade [124].

²³Defined as the energy fraction of the most energetic particle.

interaction models relevant for this work is presented. A more comprehensive description of the differences in the treatment of nuclear collisions, diffractive processes, and in the energy sharing of partons is presented in [2].

Sibyll 2.1

The hadronic event generator Sibyll 2.1 [60] is specialized in the description of EASs. Its theoretical basis is the *minijet model*, which describes particle jets with small transverse energies that can still be calculated within perturbative QCD [68]. For the description of soft hadronic interactions, Sibyll 2.1 uses the *dual-parton model* [127], in which collisions lead to fragmentation into a quark-diquark or quark-antiquark system [68]. Further, color strings are formed between opposite colors [128], which are then fragmented using the *Lund algorithm* where the number of strings does not depend on the energy [129] and determines the number of projectile nucleons that interacts in hadron-nucleus collisions [68]. For nucleus-nucleus interactions, Sibyll 2.1 uses the *semi-superposition* model [60]. Heavy hadrons and thus prompt leptons that are predominantly produced in decays of short-lived mesons are not included in Sibyll 2.1.

QGSJet-II-04

QGSJet-II-04 [130] utilizes GRFT to describe soft hadronic interactions, where the description of collisions is based on multiple scattering processes mediated by Pomeron exchanges and employs the semi-hard Pomeron approach. The Pomerons form strings that are cut to form two strings according to the *two-string* model, which are then fragmented using the Lund algorithm similar to Sibyll 2.1 but with some deviations in the initial momenta of the strings [68]. Collisions with high transverse momentum transfer are described using the minijet model.

While the decay of short-lived resonances is not explicitly modeled, their respective contribution is included in the stable secondary hadron spectra [68]. However, similar to Sibyll 2.1, heavy hadrons are not considered.

EPOS-LHC

The hadronic interaction model EPOS-LHC [131] is based on GRFT and employs the semi-hard Pomeron approach similar to QGSJet-II-04. However, the description of hadronization within EPOS-LHC goes beyond the two-string model. This is the result of a correc-

tion derived from *color-reconnection*²⁴ that is introduced due to the insufficient description of hadronization at high energies using simple two-string models [68]. EPOS-LHC employs the *core-corona* model, which leads to the formation of quark-gluon plasma (QGP) droplets through string merging at sufficiently high string densities, which hadronize via micro-canonical statistical decay [2]. With this procedure, a higher yield of baryons and strangeness can be produced. For lower string densities in the corona, string fragmentation is applied.

Another unique feature of EPOS-LHC is the consistent treatment of the energy sharing in the context of GRFT, where typically energy conservation is only considered at the level of particle production but not for cross-section calculations [133]. Compared to classical GRFT, EPOS-LHC is therefore able to better model the narrower particle multiplicity distribution observed in measured data [126], which is caused by the suppression of multiple parton interactions [2].

Similar to Sibyll 2.1 and QGSJet-II-04, EPOS-LHC does not include prompt lepton fluxes.

EPOS-LHC and QGSJet-II-04 are *post-LHC* models, as they are tuned to the results from the LHC, including mainly ATLAS [134], CMS [135], TOTEM [136], and LHCf [137], as well as fixed target data from experiments like NA61/SHINE [138]. While more recent versions of Sibyll (e.g., Sibyll 2.3c [69], 2.3d [70]) are released at the time of writing, no corresponding simulations are produced for the simulation set and measured data used in this work. Therefore, only the *pre-LHC* model Sibyll 2.1 is discussed here.

After the brief overview of the technical differences of the high-energy hadronic interaction models used for this work, their influence on the distributions of EAS observables can be studied. As motivated in section 3.2, the main parameters of interest are the interaction cross section, the depth of the shower maximum $X_{\max}$, and the muon multiplicity N_{μ} .

The nucleus-air cross section determines the probability of a cosmic ray to interact in the atmosphere. While for low energies, the cross section is reasonably well constraint by measurements, its uncertainty increases as a function of energy. Fig. 3.8 (left) illustrates the proton-air cross section predicted by EPOS-LHC, QGSJet-II-04, and Sibyll 2.1, compared to different measurements. At cms energies of up to ~ 40 GeV, the cross section rises approximately with $\ln E_{\text{cms}}^2$, while at higher energies the scaling is roughly proportional to $\ln^2 E_{\text{cms}}^2$ [8]. The cross section for Sibyll 2.1 decreases significantly after tuning with LHC data, which results in a better agreement with EPOS-LHC and QGSJet-II-04 [139]. At high energies, the cross section can be measured by air-shower observatories like the Telescope Array and the Pierre Auger Observatory, which is, however, related to comparably large uncertainties. Therefore, the *Run3* of the LHC which includes proton-oxygen collisions and is ongoing at the time of writing will be of special interest to derive

²⁴Describes the process of the dynamic rearrangement of the color fields of partons during hadronization [132].

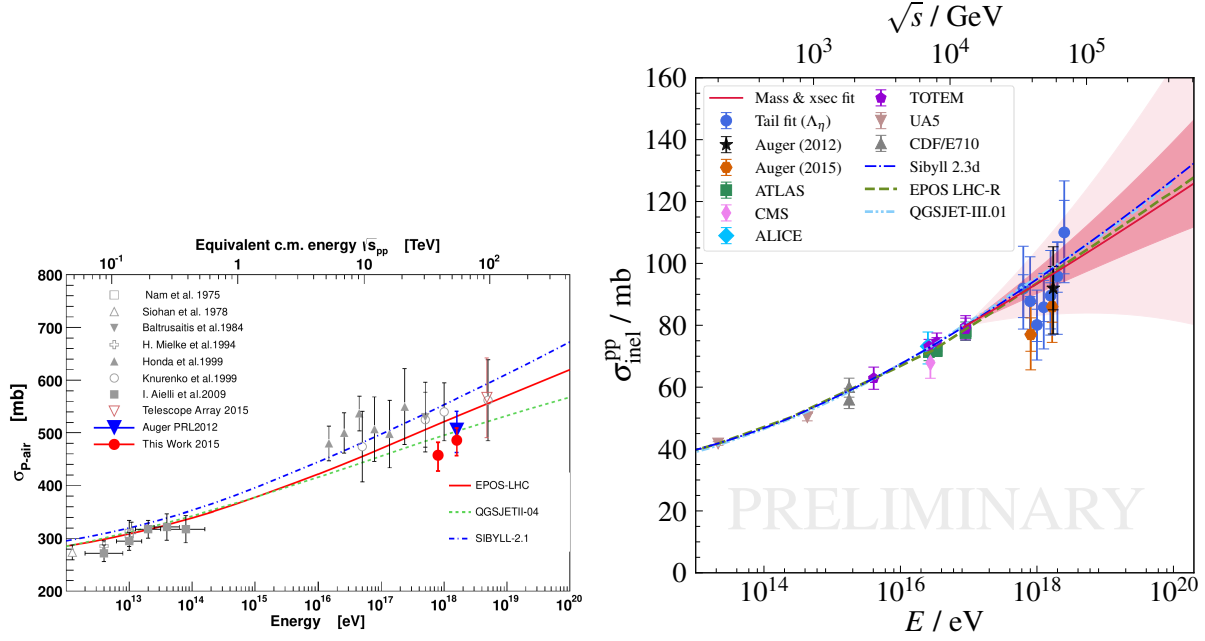


Figure 3.8.: Proton-air cross section predicted with different hadronic interaction models and including measured data from the Telescope Array and the Pierre Auger Observatory (left). Figure taken from [140]. Inelastic proton-proton cross section estimated from a combined fit of the mass composition, cross-section and shift in the X_{max} scale to data from the Pierre Auger Observatory (right). The dark and light shaded bands show the statistical and total uncertainty. Predictions from different hadronic interaction models are shown as lines. Figure taken from [141].

constraints based on high-precision data.

In Eq. (3.7), the link between the cross section and the interaction length is given. With increasing mass of the primary, the cross section increases as well which can be understood in a naive picture from the increasing nuclear radius. For example, for a primary proton of 1 PeV, the interaction length becomes $\sim 60 \text{ g/cm}^2$, while it is around $\sim 10 - 12 \text{ g/cm}^2$ for iron of the same energy [42]. Consequently, at 1 PeV, proton and iron primaries, on average, interact around 20 km/30 km above sea level, respectively. However, since the atmospheric density is roughly exponential, the distribution of the depth of the first interaction exhibits a large tail toward high altitudes. Therefore, typically, cross-section measurements of air-shower observatories assume a proton-like composition for fits of the tail of the measured X_{max} distributions, including a systematic uncertainty to account for a contribution of primary helium [142]. More refined methods of the measurement of proton-proton cross sections are currently developed using a combined fit of the cross section, mass composition, and X_{max} scale with data from the Pierre Auger Observatory [141]. The resulting proton-proton cross section as a function of primary energy is shown in Fig. 3.8 (right), including uncertainty bands of the combined fit and compared to

various accelerator measurements and predictions from different post-LHC models. The combined fit is consistent with the model predictions within the uncertainties involved. Although the large systematic uncertainties in the proton-proton cross section were visible for pre-LHC models [140], the agreement between various models is improved significantly through the addition of LHC data.

From Eq. (3.18), it is clear that the cross section largely determines the position of $X_{\max}$, while the dependence on the total number of particles is logarithmic. Since $X_{\max}$ determines the age of an observed shower, also the number of EM particles at the observation level is influenced. Also the elasticity influences the position of $X_{\max}$. Due to the insufficient detector coverage in colliders in the forward direction, the elasticity is not well constraint. Among the post-LHC models, Sibyll 2.3 has the largest elasticity, which is likely due to its lower particle multiplicity [126].

Fig. 3.9 (left) shows the distribution of the average value of $X_{\max}$ as a function of primary energy for different post-LHC models and compared to EAS measurements. For reference, also the more recent hadronic interaction model, EPOS-LHC-R [143], is shown, which is tuned to a larger data set and includes an improved treatment of collective hadronization and hadronic re-scattering. The latter are motivated by the deficiency of high-energy hadronic interaction models in describing the muon yield in EASs at high energies, as will be discussed in detail in section 3.6.3. It allows for breaking of the isospin symmetry in string fragmentation by means of a higher production of ρ^0 mesons compared to charged $\rho^\pm$, resulting in an increased number of muons since ρ^0 decay into charged pions ($\rho^0 \rightarrow \pi^+ + \pi^-$), retaining energy in the hadronic shower component. Note, that the isospin symmetry breaking is theoretically and experimentally motivated [143]. In addition, hadrons can scatter off each other after their initial production before the system fully expands. This is important mainly for the regime in which particles are close and slow enough to interact, and is therefore mostly relevant for the mid-rapidity region [144]. For this reason, an increase in the fraction of ρ^0 in the forward direction can be produced without causing tensions with accelerator data in the mid-rapidity region.

The EPOS-LHC-R model predicts the largest average value of $X_{\max}$ among the post-LHC models and EPOS-LHC the lowest. It should be mentioned, that this is only true for QGSJet-III, while QGSJet-II-04 which is relevant for this work predicts lower values of $X_{\max}$ compared to EPOS-LHC. Note, that EPOS-LHC-R results in an interpretation of the measured $X_{\max}$ values that is compatible with iron at the highest energies. A comparison of the $X_{\max}$ prediction with the pre-LHC model Sibyll 2.1 is shown in Fig. 3.9 (right). Compared to Sibyll 2.1, the post-LHC models predict slightly deeper $X_{\max}$ by about 20 g/cm^2 for ultra-high energy cosmic-rays, resulting in an increase in the average mass composition.

Fig. 3.10 (left) shows the muon multiplicity at the observation level for different post-LHC models as a function of primary energy. As motivated, EPOS-LHC-R produces the high-

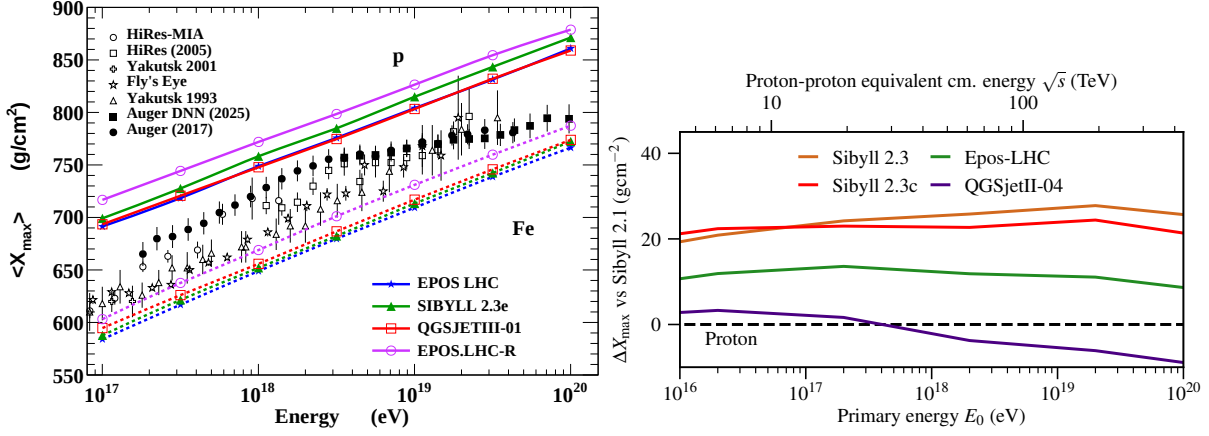


Figure 3.9.: Predictions of the average value of $X_{\max}$ for proton and iron primaries as a function of primary energy compared to measured data from various experiments (left). Figure taken from [144]. Ratio of $X_{\max}$ predicted by different hadronic interaction models to Sibyll 2.1 as a function of primary energy (right). Figure taken from [145].

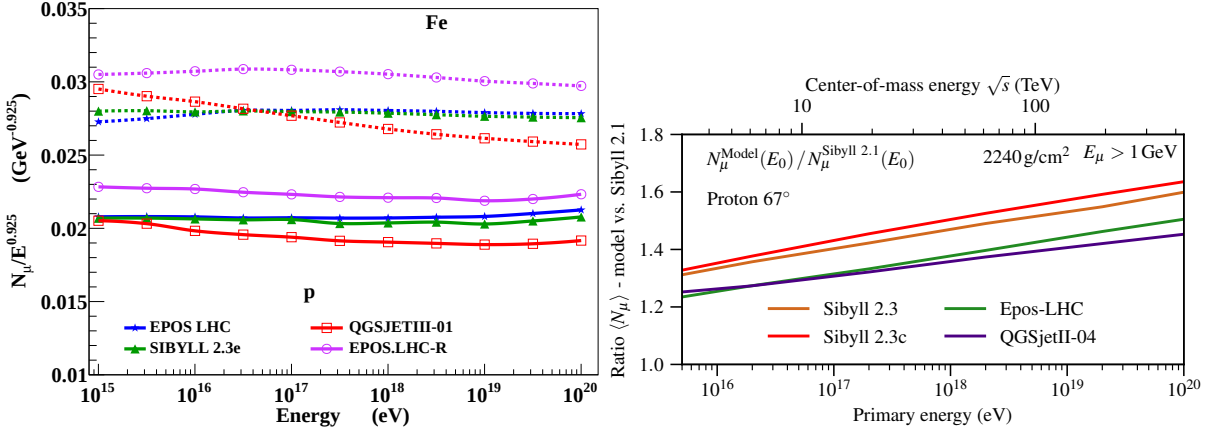


Figure 3.10.: Normalized number of muons as a function of primary energy predicted by different high-energy hadronic interaction models (left). Proton and iron primaries are shown as solid and dashed lines, respectively. Figure taken from [144]. Ratio of the muon multiplicity N_{μ} predicted by different hadronic interaction models to Sibyll 2.1 as a function of primary energy (right). Figure taken from [145].

est number of muons among all models. Generally, for post-LHC models, the number of muons is increased compared to pre-LHC models. This is visualized with a comparison of the muon yield predicted in post-LHC models compared to Sibyll 2.1 in Fig. 3.10 (right). Compared to Sibyll 2.1, an increase by a factor of ~ 1.35 and ~ 1.6 for energies of 10^{16} eV and 10^{20} eV , respectively, is visible [145] where the post-LHC versions of Sibyll predict the highest number of muons. The differences in muon yield between these models are discussed further in section 9.1, as the results of this thesis are interpreted in the context of different hadronic interaction models.

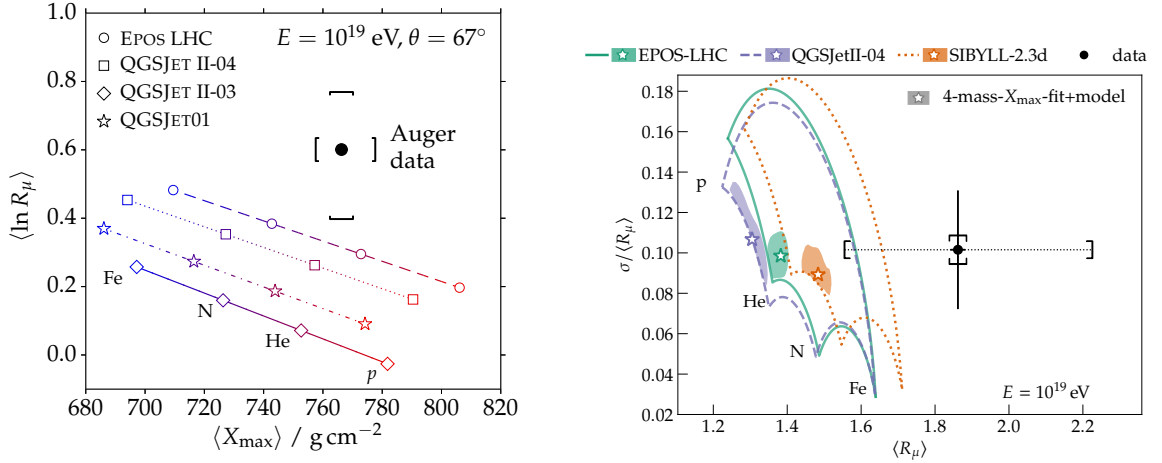


Figure 3.11.: Normalized muon number R_μ for inclined showers of $\sim 67^\circ$ at 10^{19} eV vs $X_{\max}$ measured by the Pierre Auger Observatory (left). Additionally shown are corresponding predictions for different hadronic interaction models for different primary mass. Figure taken from [148]. Measurement of the fluctuations of the average number of muons performed by the Pierre Auger Observatory compared to possible mixtures of four primary mass components, proton, helium, nitrogen, and iron, illustrated as colored contours (right). Shaded areas show the ranges allowed by $X_{\max}$ measurements. Figure taken from [149].

3.6.3. Muon Puzzle

As mentioned, a significant discrepancy in the predictions of the muon yield in air showers between measured data and simulations is observed for the current versions of hadronic interaction models. Discrepancies were first reported by HiRes-MIA [146] and NEVOD-DECOR [147], which was further established in a near-model independent measurement by the Pierre Auger Observatory in [148]. The result is shown in Fig. 3.11 (left) compared to predictions of different hadronic interaction models. A clear discrepancy is visible, showing a significantly larger muon content observed in the measurement compared to all model predictions. Conversely, fluctuations of the number of muons measured for the first time by the Pierre Auger Observatory shows no large discrepancies compared to the model predictions [149] (see Fig. 3.11 (right)), suggesting a non-exotic scenario that leads to the discrepancy in the muon content [2]. Several follow-up measurements were performed after the initial publication, which were combined in a meta-analysis by the *Working group on Hadronic Interactions and Shower Physics* (WHISP), showing an excess of the measured muon content by a variety of different experiments with an 8σ significance. To combine the different measurements, an abstract muon scale is defined independent of differences in the muon energy threshold and the zenith angles included in different measurements,

the co-called *z-scale* or *z-value*

$$z = \frac{\ln\langle N_\mu \rangle - \ln\langle N_\mu \rangle_{\text{H}}}{\ln\langle N_\mu \rangle_{\text{Fe}} - \ln\langle N_\mu \rangle_{\text{H}}}, \quad (3.24)$$

which interprets the average number of muons (or any quantity proportional to it) that is obtained in measured data in the context of the proton-iron difference of the same quantity obtained from simulations. Eq. (3.24) has the advantage of being insensitive to potential mistakes in estimating the reconstruction resolution and cancels biases present in different experiments [150]. From a physical perspective, therefore, only values between 0 and 1 should be obtained, since proton and iron mark the extreme scenarios for the cosmic-ray composition. Since the energy scale differs between different experiments, a cross-calibration is conducted, assuming the observed offsets in measured cosmic-ray fluxes from different experiments stem entirely from differences in their respective energy scale [2]. Note, that this calibration only removes relative offsets. A global offset cannot be excluded but is estimated at around 10% [151]. The results of the meta-analysis compared for different hadronic interaction models and after cross-calibration are shown in Fig. 3.12. While post-LHC models like EPOS-LHC and QGSJet-II-04 result in a better agreement with the measured data compared to pre-LHC models, a systematic upward trend is visible as a function of primary energy for all models. Since the muon number is closely related to the cosmic-ray mass, the *z*-values follow the average mass composition indicated by the X_{max} measurements and the flux models. To remove this modulation, the difference $\Delta z = z - z_{\text{mass}}$ is calculated, where z_{mass} describes the average mass composition given by GSF. The resulting distributions are shown in Fig. 3.13 for EPOS-LHC and QGSJet-II-04. A significant positive slope is found from fits to Δz obtained from different experiments, showing a logarithmic increase as a function of primary energy. The observed deviation starts to become significant around 40 PeV (~ 8 TeV cms energy) and is known as the *Muon Puzzle*. In this thesis, the Muon Puzzle is investigated in the energy range of a few PeV to 100 PeV by measurements of low-energy ($\sim$ GeV) muons with IceCube at an observation level of ~ 2835 m.

It should be mentioned, that while the Muon Puzzle specifically refers to the mismatch in the measured and predicted number of muons (the bulk of muons are in the low-energy (GeV) region and are produced at later stages of the hadronic cascade), other discrepancies, for instance, in the attenuation of muons with zenith angle and mass overburden [153, 154] have been reported.

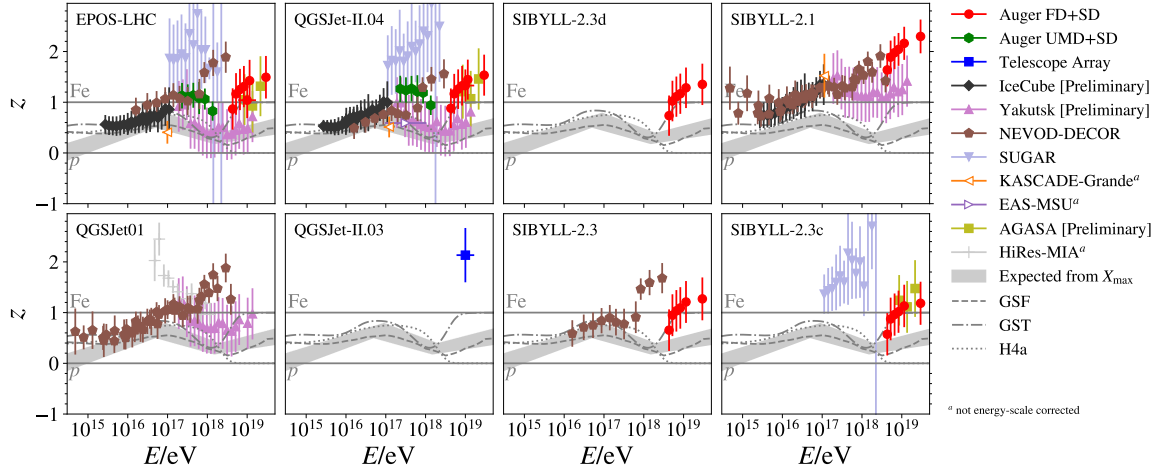


Figure 3.12.: Comparison of a variety of different measurements expressed as z -values (Eq. (3.24)) for different hadronic interaction models. For comparison, the predictions from different cosmic-ray composition models as well as the expectations from $X_{\max}$ measurements are shown as gray lines and band, respectively. Figure taken from [152].

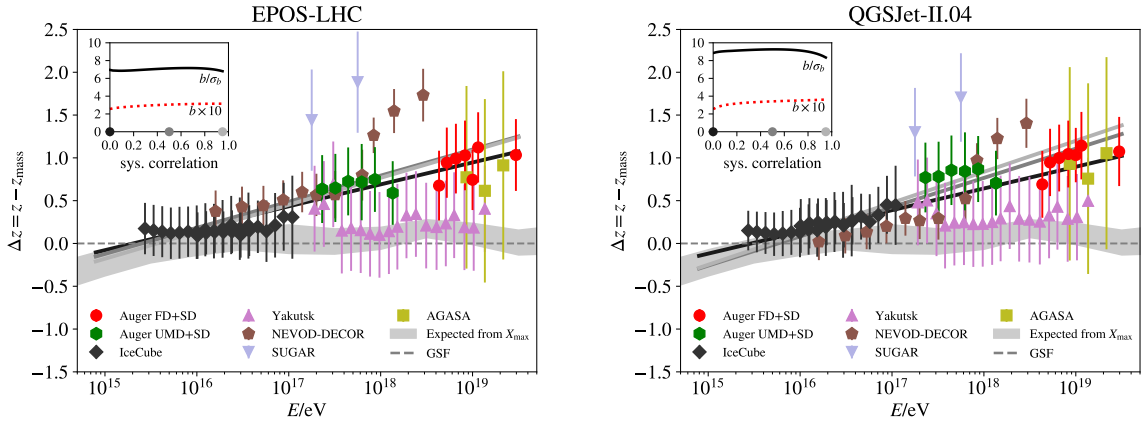


Figure 3.13.: Distribution of the z -values subtracted by the average mass composition z_{mass} given by GSF. Different lines indicate fits to the data with different underlying assumptions about the correlations of the systematic uncertainties of the data. Figures taken from [152].

Impact of hadronic interaction features and possible solutions to the Muon Puzzle

To derive possible solutions to the Muon Puzzle, the impact of changes in hadronic interaction features should be discussed in more detail in the context of air-shower observables. The muon deficit increases logarithmically with primary energy similar to the number of steps in the hadronic cascade (see Eq. (3.13)), suggesting a compounding effect with

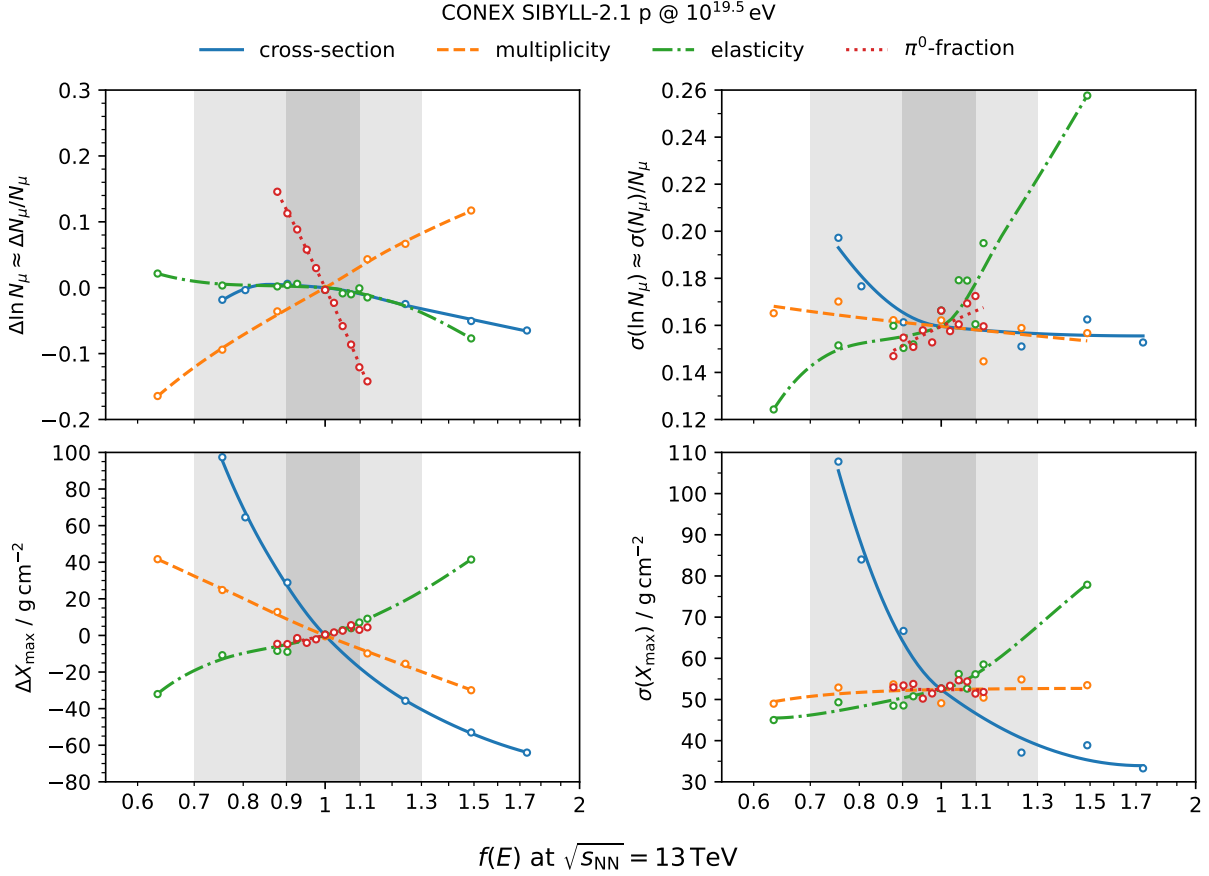


Figure 3.14.: Influence of changes in hadronic interaction features on the mean and standard deviation of the muon number (top left and right) and $X_{\max}$ (bottom left and right) for a proton-initiated shower of $10^{19.5}$ eV produced with CONEX using Sibyll 2.1. Lines indicate fits to the data points, the dark and light shaded bands illustrate the $\pm 10\%$ and $\pm 30\%$ modification regions, respectively. Figure taken from [2].

a small change in the hadronic interaction features that increases the muon yield after multiple steps rather than a drastic change in one of the first stages of the hadronic cascade. The parameters of interest that have a large impact on the shower development, therefore, are the inelastic hadronic cross-section, the secondary particle multiplicity, the elasticity, and the energy ratio of short-lived hadrons (mainly π^0) to long-lived hadrons [2]. Fig. 3.14 shows the impact of these parameters obtained from ad hoc changes during the simulation of EASs using Sibyll 2.1 as presented in [155] for the LHC energy scale. In this study, the parameters are modified by an energy dependent factor $f(E)$ starting at 1 PeV, motivated by the start of the increase of the linear fit in Fig. 3.14. In this context, a factor of $f(E) = 1$ corresponds to unchanged parameter values in the EAS simulations.

It is clear, that a modification of the number of π^0 relative to the one of long-lived hadrons (i.e., the fraction of energy lost to the EM component with each step in the cascade development) has the largest impact on the number of muons produced in EASs

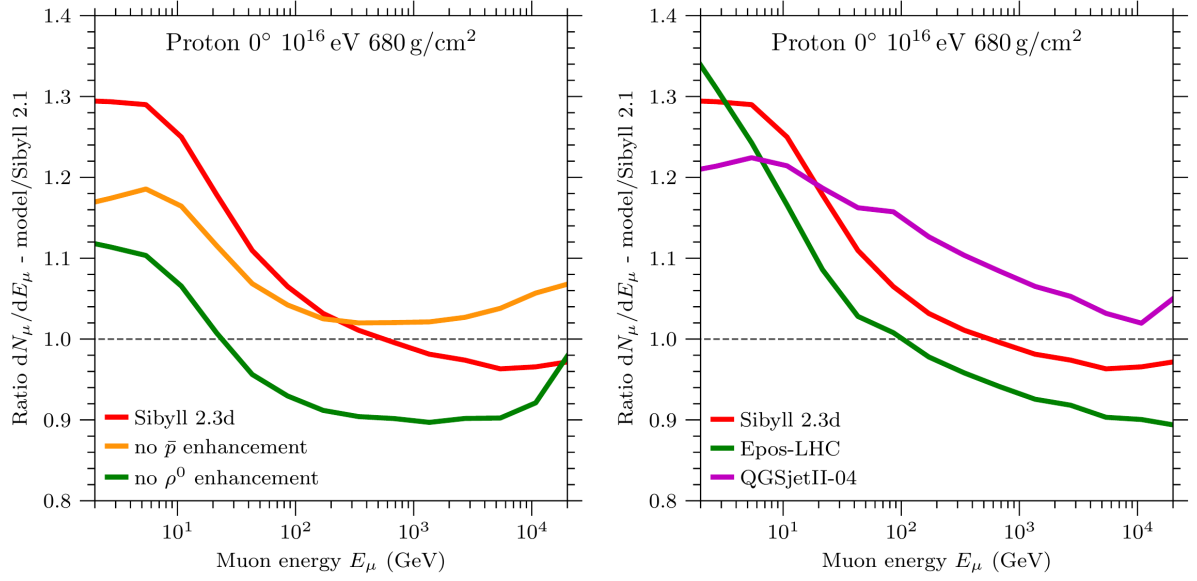


Figure 3.15.: Comparison of the muon energy spectrum of Sibyll 2.3d with switched off ρ^0 and baryon enhancement (left) and of different post-LHC models (right) to Sibyll 2.1. Figures taken from [41].

without a large change in $X_{\max}$. The latter is of great importance, as no discrepancy is found in measurements of $X_{\max}$. This is emphasized in Fig. 3.16 (left), which shows the influence of changes in the hadron multiplicity and energy ratio R of the EM to hadronic energy on the muon number and $X_{\max}$ compared to a measurement from the Pierre Auger Observatory. Only an increase in R results in a shift in the model predictions toward the data point, indicating a change in R as a possible solution for the Muon Puzzle.

As mentioned, the new hadronic model EPOS-LHC-R leads to an increase in the muon yield through an increased production of ρ^0 , which is in better agreement with air-shower measurements at high energies. However, further studies are required with data from observatories that operate at lower primary energies to test its validity. In addition to the ρ^0 enhancement, also an enhancement of the baryon-pair production results in a higher muon yield. A visualization of the impact of both effects on the muon energy spectrum for proton-initiated showers produced with Sibyll 2.3d compared to Sibyll 2.1 is shown in Fig. 3.15. Note, that the muon energy spectrum differs significantly between different hadronic interaction models. This is a strong motivation for studies of the muon energy spectrum in data to derive constraints on hadronic interaction models (see chapters 6 and 8 for a further discussion).

More recent studies additionally suggest the need for a deeper $X_{\max}$ scale [156], which would result in a heavier mass composition derived from $X_{\max}$ measurements. The impact of a constant shift in the $X_{\max}$ scale as estimated in [157] on the muon number is shown in Fig. 3.16 (right) for different hadronic interaction models. Based on this shift,

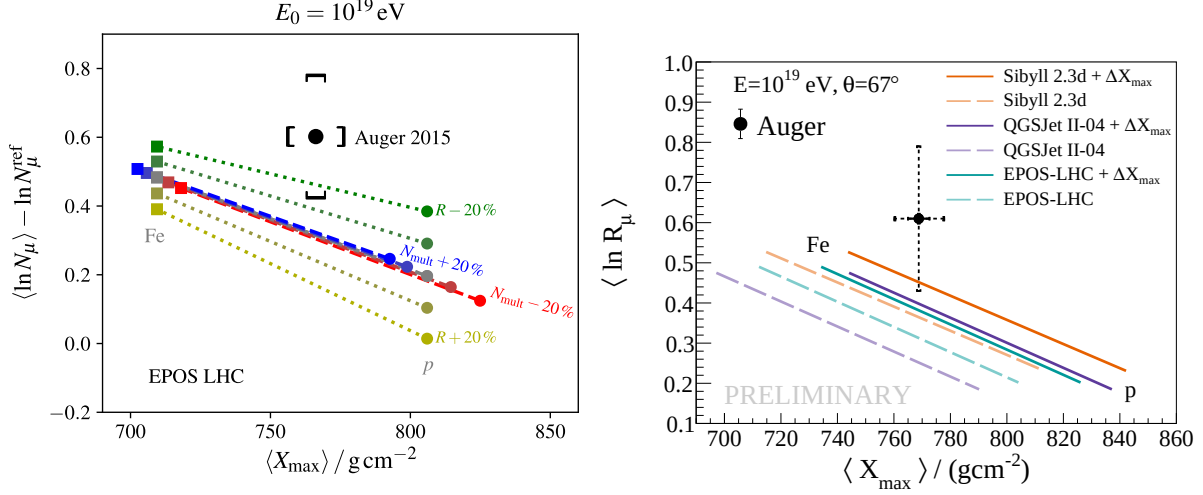


Figure 3.16.: Influence of a modification of the average hadron multiplicity, N_{mult} and the ratio of the EM to hadronic energy, R , on X_{max} and N_μ for EPOS-LHC and compared to data from the Pierre Auger Observatory (left). Figure taken from [2]. Muon scale, R_μ , vs X_{max} measured by the Pierre Auger Observatory compared to predictions for proton and iron primaries for different hadronic interaction models with and without a shift in the X_{max} scale (right). Figure taken from [156].

a reduction of the muon deficit at the 10 EeV scale to the level of 15 – 25% is observed.

One possible part of a solution of the Muon Puzzle is the baryon and universal strangeness enhancement reported by the ALICE (at LHC) collaboration [158], which is observed in different collision systems at mid rapidity. This increase in the production of strange hadrons as a function of multiplicity can lead to a significant increase in the muon yield. However, corresponding high-precision measurements in the forward region, e.g. by LHCb [34], have to be performed to test if this enhancement is also present in the phase space relevant for air showers.

Further measurements relevant for the solution of the Muon Puzzle include the hadron multiplicity over a wide rapidity range, the inelastic and diffractive cross-sections, charged particle spectra, and the measurement of the forward energy flow [2]. A comprehensive overview of all collider and fixed-target experiments that can conduct measurements of particular relevance for air-shower physics and the connected Muon Puzzle is presented in [2].

The most promising insights are expected to be gained by the LHC Run3 which includes collision systems that are of direct relevance for air showers, namely proton-oxygen and oxygen-oxygen. Since a large part of the uncertainties introduced by hadronic interaction models stems from the extrapolation from proton-proton measurements to collision systems occurring in air showers [2].

While the understanding about the physics related to the Muon Puzzle has improved

since it was first established in 2015, a large amount of information is still missing to solve the discrepancy between data and simulations. In this context, additional data specifically in the phase space relevant for air showers is needed. Additionally, further validation tests of hadronic interaction models from different air-shower experiments are of great importance. The IceCube Neutrino Observatory measured air showers up to the energy range in which the muon deficit in simulations becomes significant (see Figs. 3.12 and 3.13 and therefore air-shower measurements with the IceCube surface array, IceTop, have a strong impact on the significance of the linear increase in Fig. 3.13. A unique feature of the IceCube Neutrino Observatory is its capability to measure low- ($\sim \text{GeV}$) and high-energy ($\gtrsim 400 \text{ GeV}$) muons (see chapter 4) in coincidence for the same air-shower events, which probes hadronic interactions at two vastly different energy regimes. As shown in Fig. 3.15 (right), the muon-energy spectrum differs significantly between different hadronic interaction models and can therefore be tested with IceCube. However, for this purpose, event-by-event information is needed of the low- and high-energy muon yields to study their correlations. This is a strong motivation for this work, which aims to develop an event-by-event reconstruction of the muon content in air showers, discussed in detail in chapters 6 to 9.

4

IceCube

With a average thickness of around 2.1 km [159], the antarctic continent constitutes the largest ice mass on Earth [160]. In combination with the excellent optical properties of the deep antarctic ice [161], this enables a unique three-dimensional detector set-up with optical detectors for the measurement of neutrinos and high-energy muons produced in EASs. The IceCube Neutrino Observatory (IceCube) employs a combination of a deep in-ice and a surface detector for the measurement of astrophysical neutrinos and EASs. The observatory is located at the geographic South Pole, near the Amundsen-Scott Station. Its in-ice detector array comprises one cubic kilometer equipped with photo-multipliers for the measurement of Cherenkov light. The surface component, IceTop, follows the footprint of the in-ice array and employs ice-Cherenkov tanks distributed over an area of one square kilometer. While the science goals for measurements with the in-ice array include astrophysical neutrinos, neutrino oscillations, and beyond standard model physics, IceTop is a stand-alone cosmic-ray detector that measures EASs in the primary energy range between a few hundred TeV and EeV and is also used to study coincident surface and in-ice information produced by EASs.

In this chapter, the design and detection principle of the IceCube Neutrino Observatory is introduced, with a focus on EAS physics. For this purpose, first, the basic detection principle of IceCube is discussed in section 4.1. Further, the design of IceTop and the in-ice array is detailed in section 4.2. The basis for the reconstruction of EASs measured with IceTop and the in-ice array are discussed in section 4.3. This includes a detailed overview of the standard processing of IceCube, which is used for the reconstruction of air-shower quantities. In addition, previous cosmic-ray analyses relevant for this work are discussed. Moreover, the details of the simulated dataset used for the analyses presented in this work are summarized in section 4.4. Lastly, a short overview of the ongoing enhancement of IceCube, as well as the next-generation experiment, IceCube-Gen2, is given in section 4.5.

4.1. Detection principle

A charged particle propagating through a dielectric medium polarizes the molecules in the vicinity of its track. The polarization leads to a charge asymmetry, resulting in a dipole field along its track [162] that leads to the emission of electromagnetic waves. If the particles move at a velocity $v = \beta c$ faster than the phase velocity of light in the medium, the emission is coherent, and a wavefront is created analogously to a sonic boom. The basic principle of the creation of such a *Cherenkov cone* is illustrated in Fig. 4.1. The forward angle of the Cherenkov cone, i.e., the angle of constructive interference, is characterized by θ and can be defined as

$$\cos \theta = \frac{c/n(\lambda)}{\beta c} = \frac{1}{\beta n(\lambda)}, \quad (4.1)$$

where $n(\lambda)$ is the refractive index of the dielectric medium, which depends on the wavelength λ , and $c/n(\lambda)$ classifies the speed of light in the medium. Typically, Cherenkov radiation is measured in media such as water or ice, which have a refractive index of $\sim 1.31 - 1.33$ for wavelengths of $300 - 600$ nm [42]. These are also the wavelengths relevant for the measurements of IceCube (see sections 4.2.1 and 4.2.2), as ice constitutes the detection medium for both its in-ice and surface component. Moreover, from Eq. (4.1), θ can be estimated to be $\sim 41^\circ$ for the case of IceCube. The spectrum of emitted Cherenkov photons is given by the *Frank-Tamm* formula [163]

$$\frac{d^2 N}{dx d\lambda} = \frac{2\pi\alpha Z^2}{\lambda^2} \left(1 - \frac{1}{\beta^2 n^2(\lambda)} \right), \quad (4.2)$$

which describes the number of photons emitted for a given track segment and wavelength, with the fine structure constant α and the charge of the particle Z . Thus, the number of Cherenkov photons depends mainly on λ and the charge of the particle, and not its energy.

Particle propagation in matter

Charged particles propagating through a medium undergo various energy-loss processes. Of special relevance for IceCube and this work is the propagation of charged leptons through matter. The mean rate of energy loss for a charged particle of energy E that travels the distance X is also referred to as the *stopping power* [165]. Note that the energy loss through Cherenkov emission is $\mathcal{O}(\text{keVcm}^{-1})$ [162] and is therefore small compared to other loss processes.

Firstly, charged particles that propagate through matter can ionize (and excite) the medium through interactions with the electrons of the medium. Ionization is a continuous energy loss process and can be described by the *Bethe formula* [166]. The mean

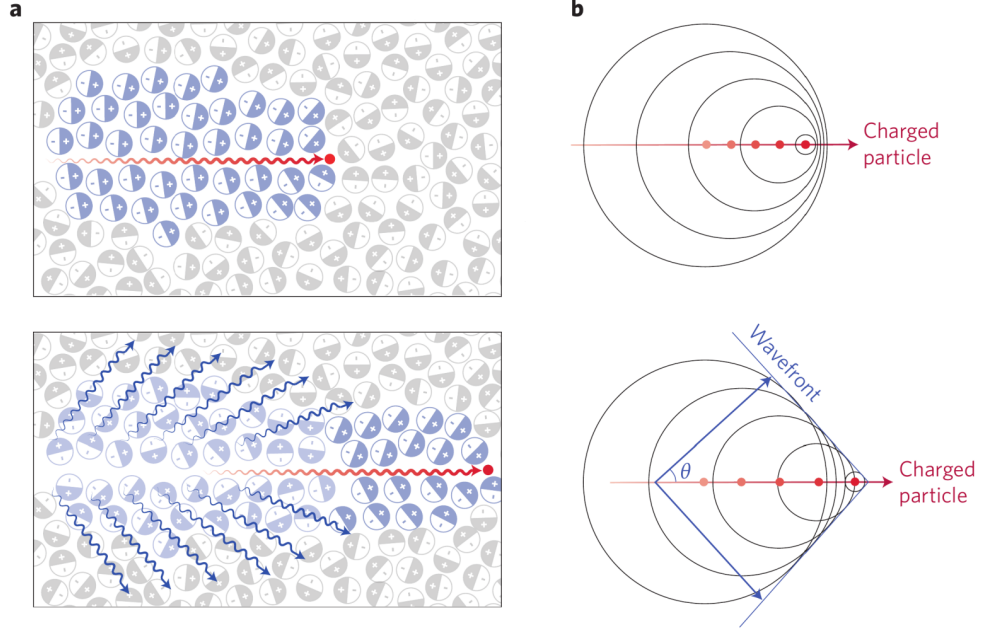


Figure 4.1.: Charged particle propagates with $v < c$ (a, top) and $v > c$ (a, bottom) through a dielectric medium and polarizes it (top). After returning back to the ground state, electromagnetic waves are created, which are coherent if $v > c$ and can be observed as a Cherenkov cone with a characteristic angle θ (b, bottom). Figure taken from [164].

ionization loss of muons in ice is shown in Fig. 4.2. Charged particles in the energy range within the minimum of the ionization curve are *minimum ionizing particles* (MIPs). This is the case for muons of $\lesssim 1$ GeV. Note that ionization loss is the dominant energy loss process for muons of energies below ~ 500 GeV.

In addition to ionization losses, charged particles can also undergo radiative losses. These include *Bremsstrahlung*, pair-production, and photo-nuclear interactions. Radiative losses become important at high particle energies and dominate the total energy loss above ~ 1 TeV for muons. However, radiative losses are subject to large fluctuations and therefore do not occur continuously. For this reason, they are often referred to as *catastrophic* energy losses.

Bremsstrahlung is typically produced by the sudden deceleration of a charged particle in the electromagnetic field of an atomic nucleus¹. However, the dominant contribution to radiative losses is the production of e^+e^- pairs in the field of a nucleus. Photo-nuclear interactions describe the inelastic scattering of a charged lepton with an atomic nucleus within the medium and have the smallest contribution to radiative losses. All processes can induce particle cascades in the medium, which can have sufficient energies to produce Cherenkov emission and can therefore contribute to the measured signal.

¹Note that Bremsstrahlung is suppressed for muons compared to electrons by the mass-squared factor $(m_e/m_\mu)^2$ due to the inverse mass-squared factor in its cross section [8].

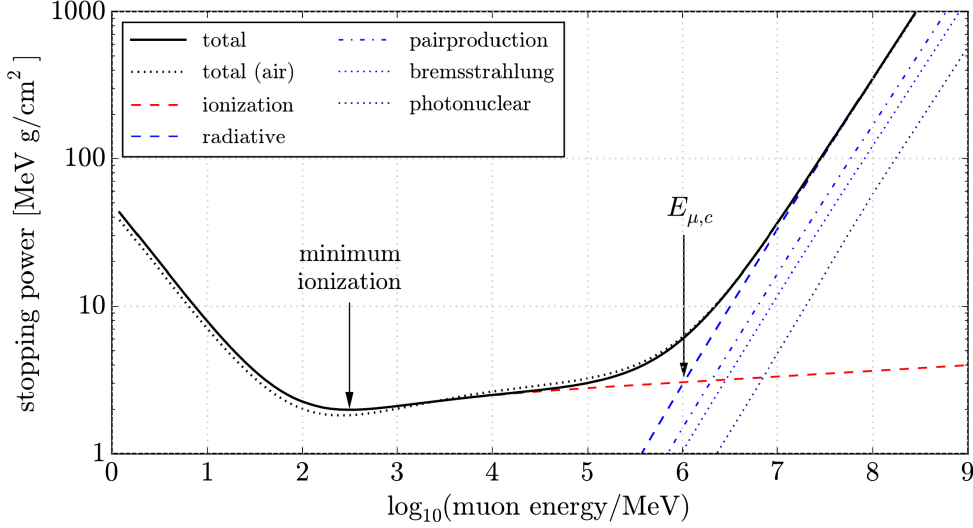


Figure 4.2.: Visualization of the all components of the mean energy loss of muons in ice. Red and blue indicate ionization and radiative losses, respectively. Figure taken from [68].

The mean energy loss of muons is often described as

$$\left\langle -\frac{dE}{dX} \right\rangle = a(E) + b(E) \cdot E, \quad (4.3)$$

where E is the muon energy and the parameters $a(E)$ and $b(E) = b_{\text{Br}}(E) + b_{\text{pair}}(E) + b_{\text{had}}(E)$ describe ionization and radiative losses (Bremsstrahlung, pair production, and photo-nuclear interaction), respectively [8]. For muons in ice, $a = 0.249 \text{ GeV/mwe}$ and $b = 0.422 \cdot 10^{-3} \text{ mwe}^{-1}$ [167], where mwe (*meter water equivalent*) normalizes the traversed amount of matter to an equivalent amount of water². The mean muon energy after traversing a depth of X in a medium can be determined by solving Eq. (4.3):

$$\langle E(X) \rangle = \left(E_0 + \frac{a}{b} \right) \cdot e^{-bX} - \frac{a}{b}, \quad (4.4)$$

and can be used to estimate a muon energy threshold to reach a detector deployed at a particular depth. In the case of the IceCube in-ice array that is deployed at a depth of $\sim 1450 \text{ m}$ (with an ice density of $\approx 0.92 \text{ gcm}^{-3}$) below the Antarctic surface, an energy threshold of $\sim 446 \text{ GeV}$ is obtained [41]. However, note that while this value roughly estimates the mean muon energy required to reach the in-ice detector, the threshold is subject to fluctuations in the energy losses. In addition to the energy-loss processes described above, charged particles can interact with the atomic nuclei of the medium by means of repeated elastic Coulomb scattering. Although the energy loss of these interactions is negligible assuming a large target mass compared to the charged lepton, such *multiple scattering* processes can lead to an angular deflection of the incident particle. Since multiple scattering scales with the inverse of the particle momentum and with the

²Since the density of water $\approx 1 \text{ g/cm}^3$, 1 mwe corresponds to $X = 100 \text{ g/cm}^2$.

density of the medium, the angular deflection within the atmosphere is negligible for high-energy muons ($\sim \text{TeV}$). However, it can have a significant impact on their propagation through the ice to the in-ice detector of IceCube. For low-energy muons in the multiple GeV range and below, multiple scattering is of significant impact for their angular deflection during the development of EASs (see chapter 6 for a more detailed discussion). For a more comprehensive overview, see [168, 169].

4.2. Detector components

The IceCube Neutrino Observatory is located at the geographic South Pole and is comprised of a deep in-ice array and a surface component, IceTop. A schematic overview of all components is shown in Fig. 4.3. The IceCube Laboratory (ICL) is situated roughly in the center of IceTop and contains the hardware for the data acquisition (DAQ).

For the detection of Cherenkov radiation produced by charged particles traversing the sensitive detector volume, both the in-ice array and IceTop use photo-multiplier modules, *Digital Optical Modules* (DOMs). The DOMs employ a photo-multiplier tube (PMT) for the collection of Cherenkov light. In addition to the PMT, the DOMs contain an on-board digitization system to perform the first steps of the data acquisition. A schematic overview of a DOM and the functionality of its electronic components is shown in Fig. 4.4. The DOM itself is encapsulated in a 13 inch glass sphere with a thickness of 0.5 inches to withstand the high pressure conditions in the deep Antarctic ice. On top of each DOM, a penetrator allows for the connection of three pairs of wires for the power supply and connection to ICL, as well as the connection to the neighboring DOMs to search for coincidences. To ensure an optical coupling between the PMT and the glass sphere, a silicone gel layer is employed. The glass sphere is made of borosilicate glass, which has low natural radioactivity and provides good optical transmission for the wavelength range relevant to the Cherenkov spectrum in ice. Each PMT is housed in a mu-metal grid, which reduces the influence of the Earth magnetic field on the light collection efficiency. The PMT used in IceCube are Hamamatsu R7081-02 PMTs³ and operate optimally in the wavelength range of 300 – 650 nm, with a maximum quantum efficiency⁴ of $\sim 25\%$ at 390 nm [171]. PMTs measure photons that hit the photocathode via the creation of *photoelectrons* (PEs). Subsequently, the PEs are directed toward a set of dynodes. At each dynode, they detach more PEs, leading to a cascade of PEs that is measured as a signal at the anode. Standard IceCube DOMs have a signal gain of $\sim 10^7$, leading to

³DOMs deployed in the DeepCore sub-array use Hamamatsu R7081MOD PMTs, which have a higher quantum efficiency of $\sim 65\%$ around 390 nm.

⁴The quantum efficiency is defined as the number of photoelectrons that are emitted from the photocathode of the PMT to the total number of incident photons [170].

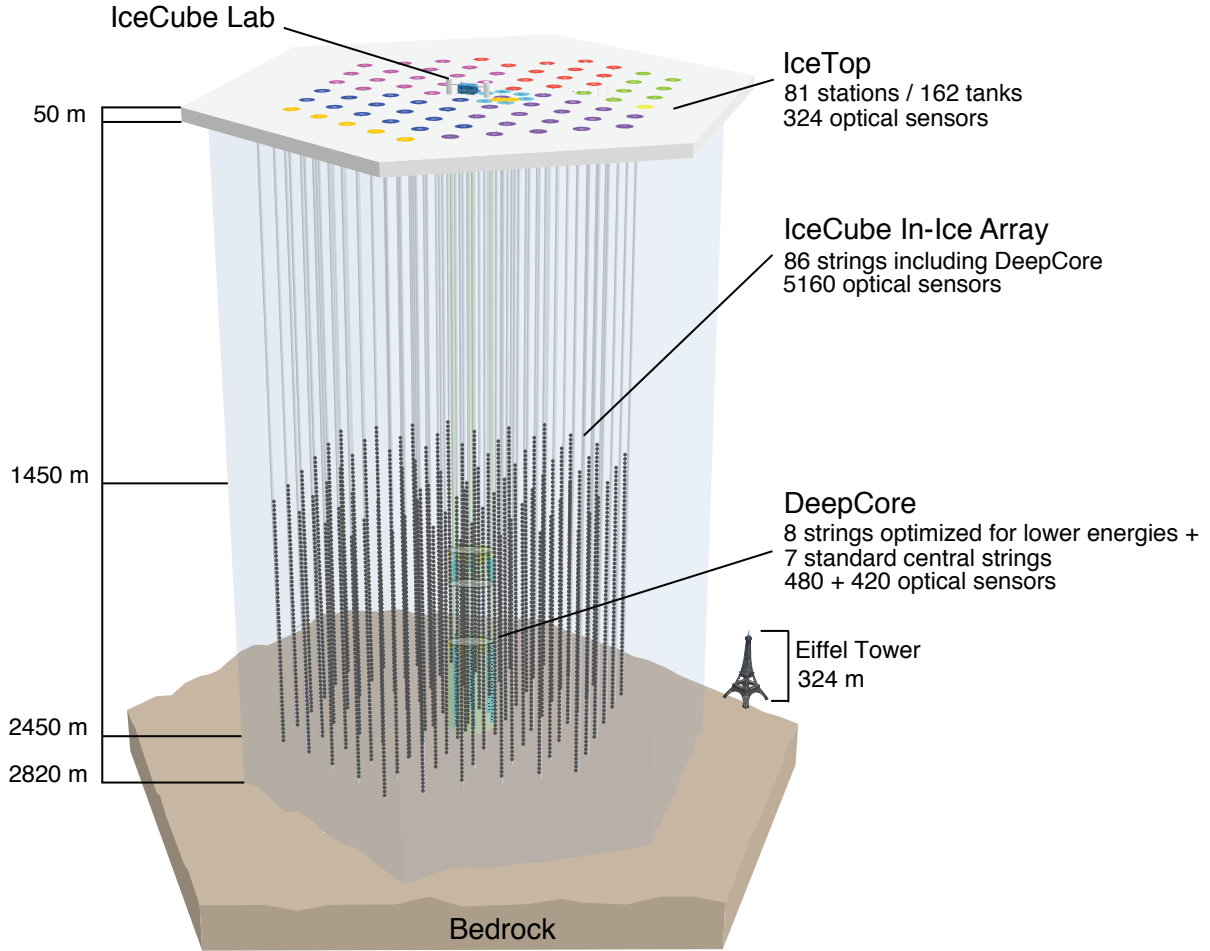


Figure 4.3.: Schematic view of the IceCube Neutrino Observatory, comprising the deep in-ice array with its dense sub-array DeepCore, and the surface component IceTop. Figure taken from [172].

PMT waveforms of $\sim 0.001 - 2$ V [171]. Note that for IceTop, the DOMs are operated at two different gains of 10^5 (*low-gain* (LG)) and $5 \cdot 10^6$ (*high-gain* (HG)). The PMT signals are linearly correlated to the measured charge. However, linearity is lost upon saturation. The main component of the onboard DAQ is the main board, which, among others, contains the *Field Programmable Gate Array* (FPGA), preamplifier, and digitizers. The time stamp of the signals is determined by a 20 MHz oscillator on the main board that is calibrated regularly with a master clock in the ICL. In addition, an LED on the main board is used for calibration purposes. A detailed discussion of all components of the DOMs can be found in [173].

If the peak voltage of the measured PMT signals surpasses a *discriminator* threshold, it is recorded by the DOM electronics. In this case, the signals are sent to a custom-made integrated circuit, the *Analog Transient Waveform Digitizer* (ATWD) [174], which samples the signals in 128 bins with a width of 3.33 ns (corresponding to 427 ns total sampling

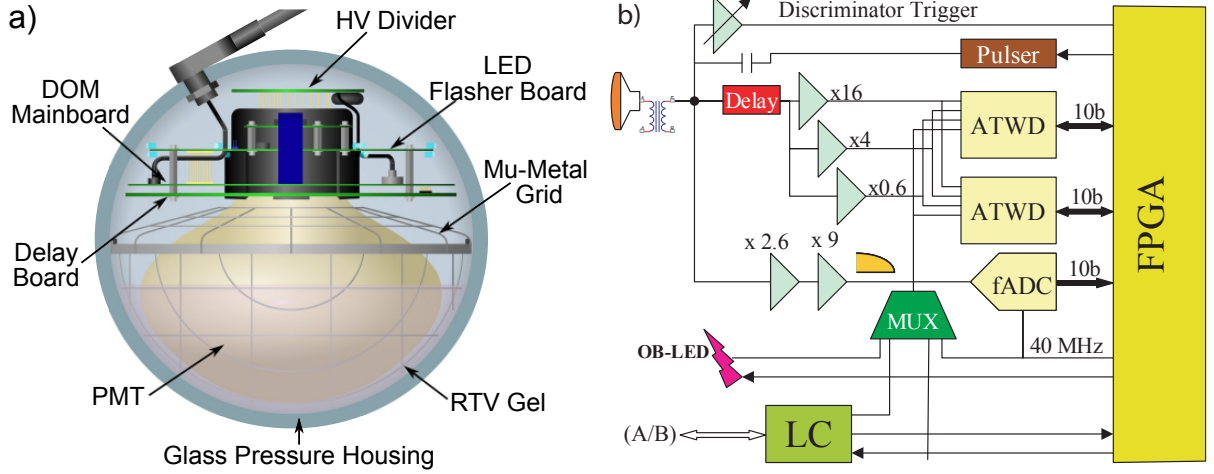


Figure 4.4.: Schematic view of the IceCube Digital Optical Module (DOM) (a) and the main components and connections of the Data Acquisition System (DAQ). Figures taken from [171].

time) [171]. The signals are then delayed by 75 ns by a Delay board to allow for a trigger decision. For the recording of waveforms, the ATWD features three channels with different gains to increase the dynamic range. To minimize the dead-time, each DOM is equipped with two ATWD chips that are used alternately. After analog sampling, a *fast-Analog-to-Digital Converter* (fADC) digitizes the three channels of the ATWD chip sequentially. After the fADC launch, the *hit* information is saved for one second, since the information that is sent to transmitted to the ICL depends on coincidence conditions. The coincidence requirements differ for IceCube and IceTop and are described in more detail in section 4.2.3.

4.2.1. In-ice detector

Overall, the IceCube in-ice array for the detection of high-energy neutrinos comprises 86 strings, each equipped with 60 DOMs. Of the 86 strings, 78 strings are arranged in a hexagonal grid with a string spacing of 125 m. The DOMs are deployed 17 m apart from each other at depths of 1450 m to 2450 m below the surface. The total number of DOMs therefore is 4680.

For the measurement of neutrinos with lower energies (10 – 100 GeV) relevant for studies of, e.g., atmospheric and supernova neutrinos, an additional, more dense sub-array, *DeepCore*, is deployed in the center of IceCube in depths of 2100 m to 2450 m. DeepCore strings have spacings in the range of 41 – 105 m and a DOM separation of 7 m on each string. In addition, 10 more DOMs with a spacing of 10 m at depths of 2000 m, which are used as a veto for atmospheric muons and are needed due to the presence of a large dust

layer between depths of 2000 – 2100 m.

Since the Antarctic ice constitutes the detection medium, a detailed knowledge of its properties is crucial for the measurements of IceCube. For this reason, the scattering and absorption lengths of photons in the ice are subject to extensive studies. Effective scattering coefficients are derived from dedicated flasher runs, in which the LEDs of certain DOMs are lit. The South Pole ice model *SPICE* [161] used within IceCube is studied and developed through the maximum illumination of all LEDs on string 63. Based on the light information collected in the neighboring strings, the scattering and absorption coefficients are fitted. The ice model typically used for IceCube analyses is the *SPICE-Mie* model, which is based on the Mie scattering [175], describing the collision of an electromagnetic plane wave with a homogeneous sphere [42].

It should be mentioned that while air bubbles can only be found above depths of 1400 m, dust is present throughout the in-ice array. The largest dust layer is observed at depths of 2000 – 2100 m and causes an increase in the absorption coefficients by roughly one order of magnitude. During the deployment of the IceCube, hot-water drilling was used to insert individual strings. The refrozen *hole ice* with a diameter of ~ 30 cm has different optical properties due to a higher concentration of air bubbles compared to the surrounding ice, which leads to a decrease in the local scattering length by ~ 50 cm [161]. Further features such as tilting, anisotropy, and movement of ice layers have been reported over the years. Improvements in the description of the ice properties are the subject of ongoing work and are crucial to reducing the systematic uncertainties introduced by ice models.

4.2.2. IceTop

The surface component of IceCube, IceTop, is situated at the surface of Antarctica at an elevation of ~ 2835 m⁵ above sea level (~ 690 g/cm²). It comprises 81 stations with two ice-Cherenkov tanks each, distributed over one square kilometer. The IceTop stations follow the footprint of the in-ice array, where each station is located in ~ 25 m distance from a string. Therefore, IceTop features an inter station distance of ~ 125 m. However, an additional three stations are deployed close to the DeepCore strings, resulting in a denser *in-fill* array that lowers the threshold for the measurement of EASs to a few hundred TeV, while the main array of IceTop operates in the energy range of PeV – EeV. An overview of the geometry of IceTop is shown in Fig. 4.5 (left).

The neighboring tanks (Tank A & Tank B) of each station are separated by ~ 10 m. A schematic view of an ice-Cherenkov tank is shown in Fig. 4.6. Each tank is a polyethylene cylinder with a radius of 0.91 m and a height of 1.3 m. The fill height of the ice is 0.9 m,

⁵Note that the surface exhibits a slope, which results in a variation of the elevation of tanks between 1944.54 m to 1950.08 m above the center of IceCube [42].

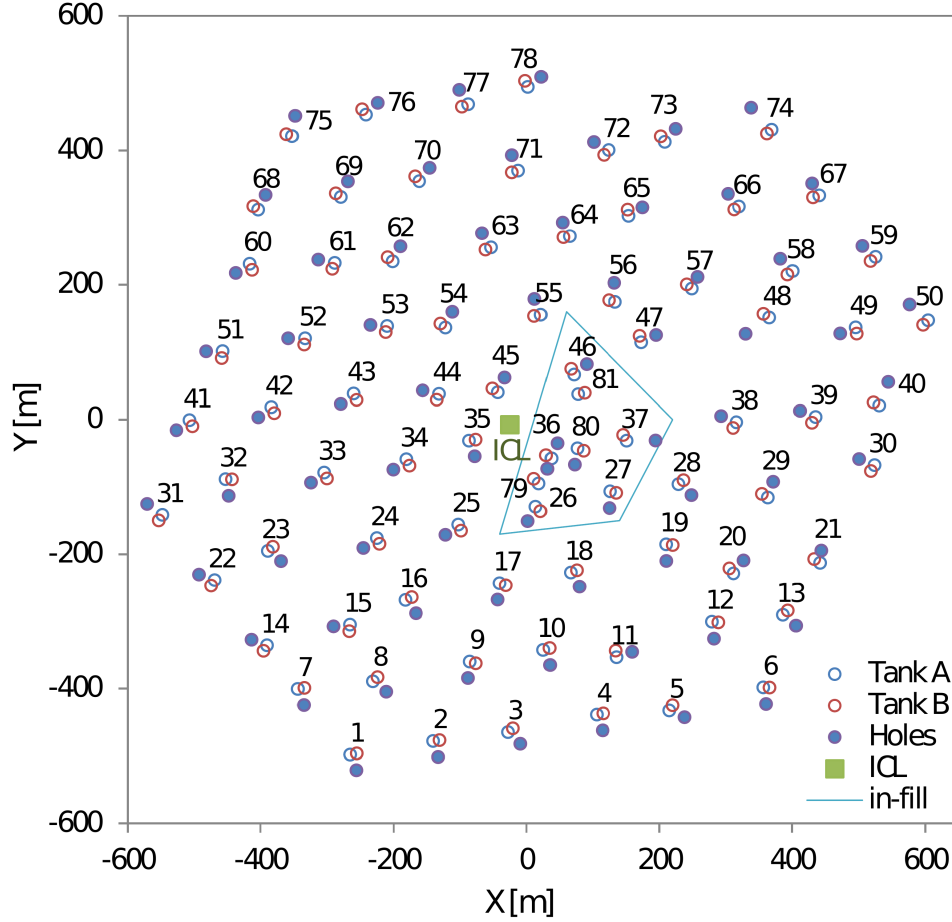


Figure 4.5.: Bird's eye view of IceTop with xy -coordinates relative to the IceCube center. Positions of the in-ice strings and IceTop tanks are shown as filled and open circles, respectively. Figure taken from [171].

where two DOMs are placed in the ice downward facing. The height of the ice volume roughly corresponds to two radiation lengths. Therefore, most of the photons produced in EASs that enter the tanks produce Cherenkov radiation via the production of e^+e^- pairs. Charged hadrons produced in EASs can directly produce Cherenkov radiation if their kinetic energy is sufficiently high ($\gtrsim 475$ MeV and $\gtrsim 70$ MeV for protons and pions in water/ice, respectively [86]) and indirectly via the production of secondary particles. The top 0.4 m above the ice volume is filled with a mixture of air and perlite for insulation and light tightness. The distance between the PMT centers is ~ 0.58 m. The tank is coated with an extra layer of insulation foam to minimize temperature variations inside the tank. The temperature stability is further enhanced as the tanks are inserted into trenches that are filled again after the deployment, such that the lids are aligned with the surrounding surface level. An illustration of the deployment of the IceTop tanks is shown in Fig. 4.7. The inside of most tanks is coated with a layer of zirconium dioxide powder, which maximizes the reflectivity for Cherenkov photons. However, a total of 12 tanks

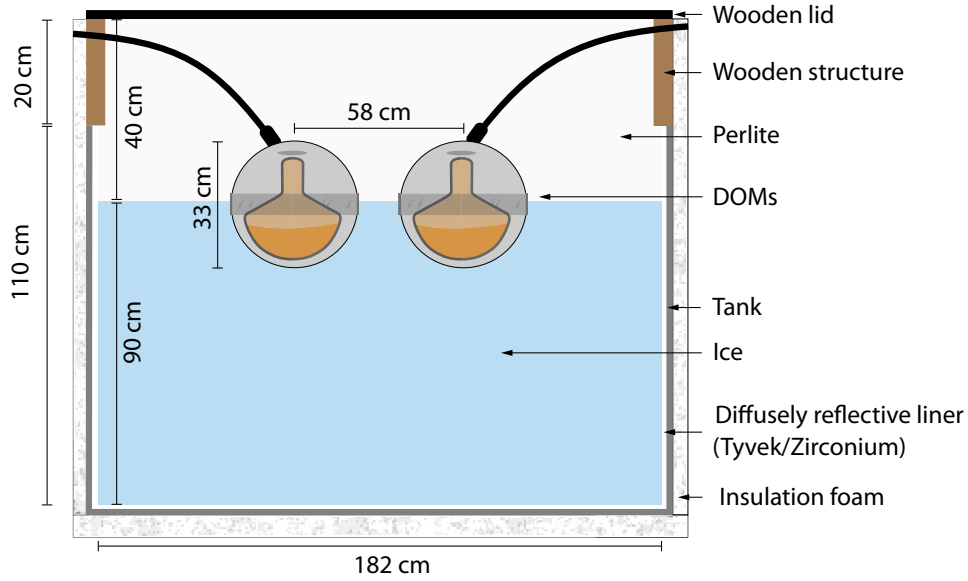


Figure 4.6.: Schematic view of the cross section of an IceTop tank. Figure taken from [171].

use Tyvek bags instead, out of which 8 tanks (station 21, 29, 30, and 39) have higher reflectivities compared to the other tanks [171].

Due to strong winds at the South Pole, the IceTop tanks are covered with increasing amounts of snow over the years. The rate of the snow accumulation is roughly 20 cm per year. However, the snow accumulation is not uniform across the array, but is influence, among others, by the surrounding terrain and the presence of buildings. Since the snow accumulation can lead to a significant attenuation of mainly the EM component of EASs, the snow heights of each tank are measured twice per year. The snow heights relevant for this work were measured in October 2012 and are illustrated in Fig. 4.8. The snow heights in this year exhibit moderate values of ~ 1 m on average, with only a few tanks having snow height above 2 m. However, already these snow levels have a significant impact on the measurement of EASs with IceTop, as discussed in detail in section 4.3.1 and chapter 4.



Figure 4.7.: Images of one IceTop station during (left) and right after deployment (right).

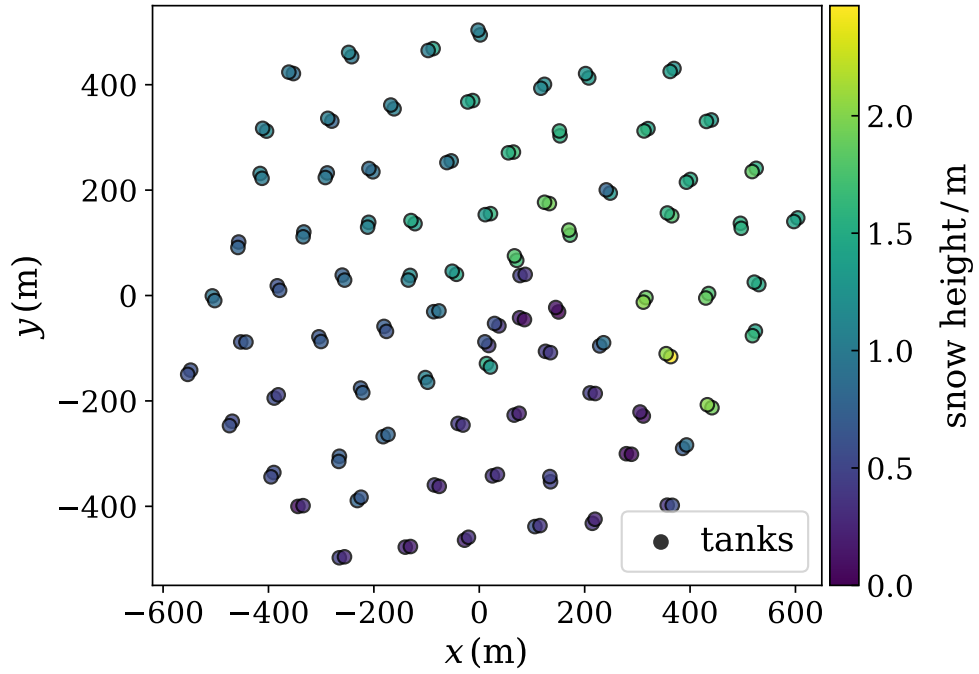


Figure 4.8.: Snow accumulation on top of IceTop tanks measured on 21st of October illustrated as color code.

4.2.3. Data acquisition

The first steps of the data acquisition are performed directly at the South Pole and are discussed in the following. More sophisticated cleaning, selection, and reconstruction algorithms are applied offline after the data is sent to the North via satellite (see section 4.3.1).

Based on the data collected in the DOMs by the ATWDs and fADCs, the DAQ process is initiated. Via a pair of cables, each DOM is connected to the *DOMHubs* in the ICL, which are responsible for the readout of the DOM signals. As mentioned, dedicated wire

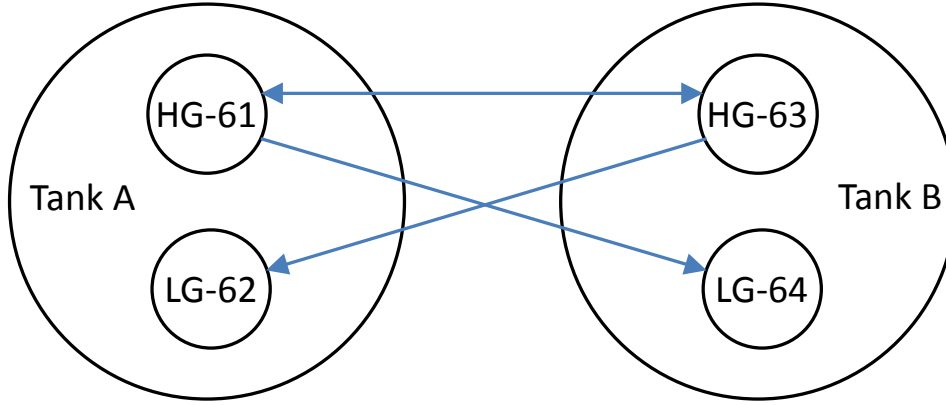


Figure 4.9.: Illustration of the LC cables within one IceTop station. Figure taken from [171].

pairs connected between the DOMs are used to test for a *local coincidence* (LC). This is because, typically, the noise rate of IceCube DOMs is of the order of 560 Hz and 780 Hz for standard and DeepCore DOMs, respectively [172]. Therefore, a coincident signal of a neighboring DOM is required to save and transfer the full waveform information to the ICL, which reduces the amount of data. For the DOMs of the in-ice array, a LC is fulfilled if one of the nearest or next-to-nearest DOMs exhibits a discriminator trigger (set to 0.25 PEs) within a time window of $\pm 1 \mu\text{s}$. The full waveform information is saved in this case and the hits are referred to as *hard local coincidence* (HLC). If no LC is found, no digitization is performed and the ATWD is reset, minimizing the dead-time of the DOM [42]. For these *soft local coincidences* (SLCs), only the total charge and time stamp of the signal are saved.

In the case of IceTop, LCs are determined on a station basis. If both tanks in one station exhibit a discriminator trigger (set to 23 PEs and 270 PEs for HG and LG, respectively) within a time window of $\pm 1 \mu\text{s}$, the station, i.e., both tanks, is classified as HLC. If only one tank in a station records a hit, it is classified as an SLC. For SLCs, the total charge and the time stamp are collected from the ATWD traces. In the case of HLCs, the full waveform information is saved. An overview of the LC cables connected between the IceTop DOMs of one station is shown in Fig. 4.9⁶. Naturally, the LC is mainly determined by the more sensitive HG DOMs.

The *StringHubs* that run on the DOMHubs collect the data and pass it to the SubTrigger system. The latter runs all IceCube triggers, which feature different requirements and readout windows. The most important trigger types for this work are the *Simple Multiplicity Triggers* (SMTs). For the in-ice array, the standard SMT trigger requires 8 HLC DOMs within a time window of 5 s. In the case of IceTop, six HLC DOMs within 6 s

⁶Note that an additional connection between the LG DOMs exists, which is useful due to the higher dead-time of HG DOMs and can be utilized when the HG DOM dies [171]. In this case, the LG DOM would be operated as HG DOM.

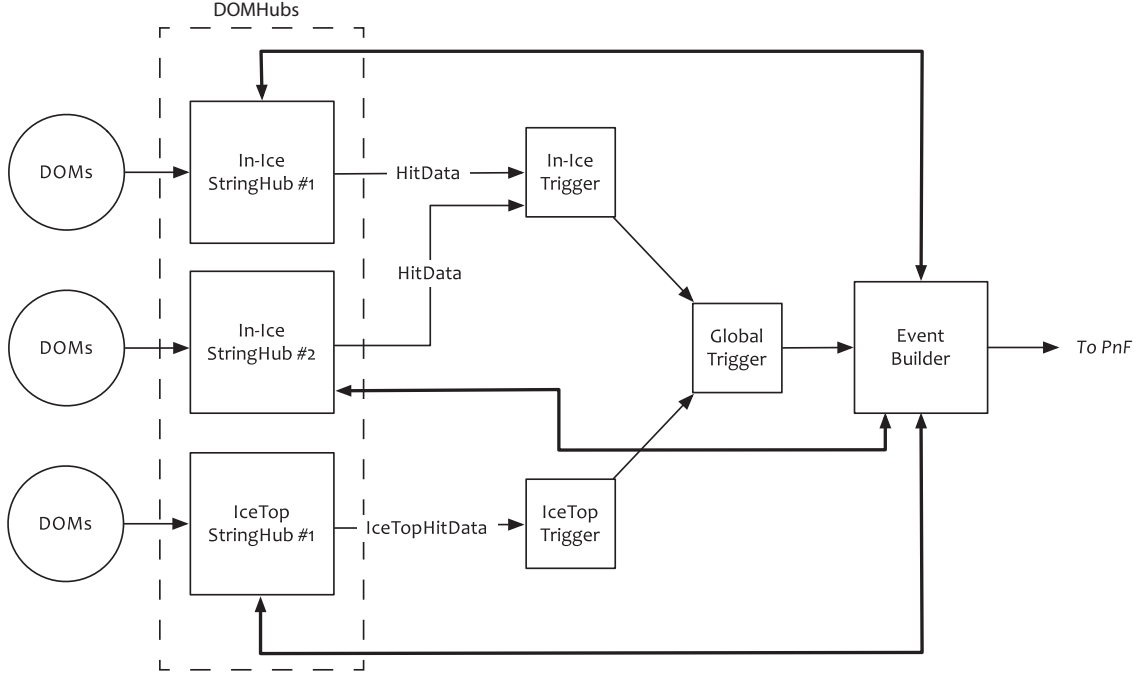


Figure 4.10.: Schematic view of the data flow within the IceCube DAQ system. Figure taken from [171].

are required. For the SMT trigger, the start time and end times, and consequently the trigger length, are determined by the first and last HLC hits, respectively. The last HLC is defined as the last hit after which no more hits are recorded within 5 s. However, an extra readout margin around the trigger window is added. In addition, in case an IceCube/IceTop SMT trigger is passed, also the IceTop/IceCube detector is read out within a specified time window around the trigger window. Overall, the resulting trigger rates are 2100 Hz and 25 Hz for the IceCube and IceTop SMT trigger, respectively [42].

Such individual sub-triggers are passed to the *global trigger*, which gathers the information of all sub-triggers and merges the corresponding trigger windows into a global readout window. The resulting data are formed into one *DAQ event* by the *event builder*. A schematic overview of the triggering system is shown in Fig. 4.10. Each DAQ event is sent to the *Processing and Filtering* (PnF) system, which selects interesting events based on calibration and rudimentary reconstruction algorithms.

Firstly, in charge calibration, the digitized signal is converted to the number of measured PEs. For this purpose, the ambient dark noise, mainly corresponding to one PE, is used to calibrate the PMT gain and voltage. The gain manifests in the single PE (SPE) peak position of the charge histogram comprising all waveforms. Details of this *DOMCal* procedure can be found in [172]. The DOMCal is performed on a yearly/monthly basis for IceCube/IceTop DOMs.

Furthermore, the DAQ is calibrated to determine the pedestal⁷ and gain for each digitizer of the main board. For this purpose, *beacon hits* are used, which describe forced triggers that are performed during data taking at a rate of 1.2 Hz/4.8 Hz for each IceCube/IceTop DOM [172] for which the entire waveform information is saved.

Therefore, continuous monitoring of the gain of the PMT and digitizer as well as the pedestals is enabled during normal data taking.

In addition to the charge calibration, also the signal times are calibrated. Within the *Reciprocal Active Pulsing Calibration* (RAPCal) procedure, the individual DOM clocks are compared to the master clock in the ICL to derive a common time base with $\mathcal{O}(\text{ns})$ accuracy. In between data transmission, a pulse is sent to each DOM via the power/communication cable and back to match both times. The RAPCal times are then converted to UTC.

The calibration of IceTop hits to physical units of *Vertical Equivalent Muons* (VEMs) as well as initial and more sophisticated reconstruction algorithms that are performed online and offline are discussed in detail in section 4.3.1.

4.3. Cosmic-ray analyses

The unique feature of the IceCube Neutrino Observatory is the combination of a surface array for the detection of air showers with a deep in-ice array. In chapter 3, it is shown that the measurement of the EM component in combination with the number of muons provides valuable insights into the characteristics of cosmic rays. While IceTop is sensitive to the EM component of air showers as well as low-energy muons, the deep in-ice array can measure the high-energy muon content. The observation of, both, the low- and high-energy muon content for the same air showers provides unique information about the underlying hadronic physics at two different energy scales. This constitutes a unique setup to test the validity of hadronic interaction models and derive constraints.

4.3.1. Standard processing

Measured EAS events undergo a complex processing chain that contains filter and reconstruction algorithms ensuring sufficient event quality to be used in cosmic-ray analyses. The standard processing for air-shower events measured with IceTop, and possibly in coincidence with the in-ice detector, that is used for analyses is the *Level3 (L3) processing*.

⁷The pedestal describes the counts at zero input voltage and needs to be subtracted from the waveform [42].

Level3 events can be used directly for analyses and for comparison and interpretation with simulations, or further filter and reconstruction steps may be applied depending on the specific requirements of an analysis. All steps of the Level3 processing relevant for the analyses presented in this section and for analysis presented in this work are discussed in the following. For a detailed overview of all steps of the processing chain see [42].

Level1

The first stage of the processing (*Level1*) is performed online by the PnF system (see section 4.2.3) at the South Pole which splits the data into interesting physics events and applies a first set of filters. In the online processing, DOMs that are flagged as unreliable during a specific run are removed from further processing. The remaining data are calibrated via the procedure detailed in section 4.2.3 to units of PEs. However, since HLCs contain the full waveform information while for SLCs only the charge and time stamp are known, this procedure is slightly different depending on the pulse type.

For HLCs in IceTop, the waveform is used to perform a proper baseline subtraction and subsequently fit a distribution of SPE signals that is used to convert the measured mV to PEs. The pulse time is determined by using the rise time of the first peak in the waveform. For this purpose, the leading edge of the first peak is fit between 10% and 90% of its maximum value. The fit is then extrapolated to the baseline, where the crossing point defines the start time (see Fig. 4.11). In the case of SLCs, the measured counts are converted to mV by means of average gain and baseline correction values via the DOM firmware. Using the the SPE peak charge, the total charge in mV is then divided to obtain the charge in PEs. Since this procedure is less accurate compared to the HLC charge calibration, SLCs are re-calibrated in the L3 processing. The pulse time for SLCs is determined by the time of the launch time of the DOM. [176]

If both DOMs in one tank are triggered, the information is merged into one tank pulse. Generally, the HG DOM is more sensitive and the respective charge and time are therefore used default pulse. However, in case the HG DOM is saturated, the LG DOM charge is used instead⁸.

To separate the measured pulses in the global readout window (see section 4.2.3) into interesting physics events to use for analyses, the HLC pulses are cleaned based on the pulse times. In order to find correlations between hits and remove most of the background and noise, the pulses are time-ordered and time coincidences are tested by $\Delta t < \Delta r/c + 200 \text{ ns}$ ⁹, where Δr is the spatial distance between the tanks and an ad-

⁸This is only the case if the time separation of the LG pulse is less than 40 ns relative to the HG pulse [42]. When no corresponding LG pulse is available, the tank pulse is removed from processing.

⁹Here, t describes the pulse time obtained in Fig. 4.11.

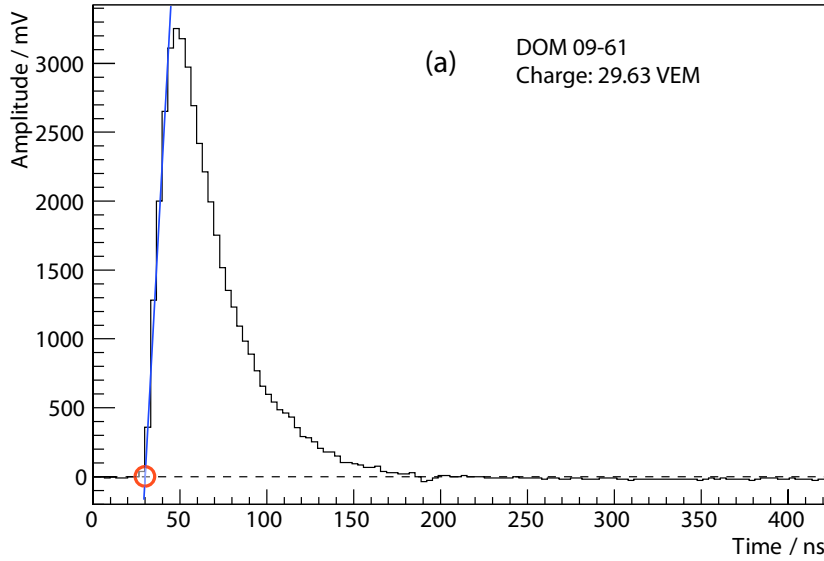


Figure 4.11.: Example of an IceTop waveform, typically featuring a steep rise and one peak, as well as an exponential tail. To determine the start time of the corresponding pulse, the leading edge is fit and extrapolated down to the baseline. Figure taken from [171].

ditional time tolerance of 200 ns is added. Afterwards, the cosmic-ray filters discussed in the following are applied to the separated events. The calibrated pulses of the in-ice detector (see [176] for a detailed overview) undergo a splitting procedure at Level3 (see section 4.3.1).

VEM Calibration

Due to slight differences in the response of individual DOMs, a similar energy deposit in a detector slightly differs for each tank. Therefore, tank pulses are calibrated into physical units of *Vertical Equivalent Muons* (VEM) to obtain a generalized charge unit. When calibrated to units of VEM, the details of each tank do not have to be simulated but a typical tank characteristic can be used for all tanks in simulation. For this purpose, atmospheric muons from low-energy showers are used to determine the charge equivalent to one VEM. Dedicated VEMCal launches are triggered with a rate of 0.2 Hz to provide continuous calibration of the VEM unit [171]. Since the measured muons have average energies of 2 – 2.5 GeV [171], they are minimum ionizing and lead to a distinct narrow signal response that depends on the track length¹⁰ of the muon inside the sensitive volume

¹⁰Note that Cherenkov light is emitted either by the muons themselves or by secondary electrons along their track. The intensity of Cherenkov photons is proportional to the energy deposit and therefore to the muon track length [171].

and can be used for calibration. It should be noted that, because of the dependence on the muon track length, the resulting charge histogram depends on the angular distribution of muons. An example charge distribution obtained from VEMCal launches on the 15th of April 2012 is shown in Fig. 4.12 (left). The distinct peak at around 140 PEs is caused mainly by vertical muons. However, fluctuations in the number of produced Cherenkov photons, the optical properties of a given tank, and the DOM electronics cause a smearing of the peak [171]. Due to the angular distribution of muons, smaller signal deposits can be caused by muons that traverse the tank on inclined tracks and only slip the edge of the detector, leading to a decreased track length. The peak at low charge values is mainly caused by EM contribution. To convert PEs to VEM, the distribution is fit with an empirical model, including the EM contribution, vertical muons, and muons that only clip the edge of the detector:

$$f(x) = p_0 \left(L(x; p_1, p_2) + \frac{1.85}{p_1 \left(\exp\left(\frac{x-p_1}{p_2}\right) + 1 \right)} \right) + p_3 \exp(p_4 x), \quad (4.5)$$

where the first part describes the muon contribution and the second part the EM background [171]. $L(x; p_1, p_2)$ describes the vertical muon contribution via a normalized Landau distribution, while the second part of the muon contribution accounts for edge clipping muons by means of a Fermi-like function. The EM contribution is modeled by an exponential function. The parameters p are free parameters of the fit.

The fit of Eq. (4.5) to the charge distribution determines the position of the muon peak in terms of PEs. The 1 VEM unit is then defined as the charge value at 95% of the muon peak. This is because a dedicated measurement with tagged vertical muons¹¹ resulted in a muon peak position that is 5% lower [171]. This 5% shift of the measured charges is applied for data and simulations and therefore does not affect the physics results. For most HG DOMs, 1 VEM corresponds to roughly 125 PEs. However, it is found, that 1 VEM corresponds to higher values of PEs in HG DOMs compared to LG DOMs (see Fig. 4.12 (right)). This origin of this systematic shift is not fully understood, but is accounted for via a cross-calibration of the LG DOMs [171]. While the charge spectra are modeled only for the HG DOMs, the signal ratio of the HG and LG DOM can be assumed to be constant in the overlap region between them where no saturation occurs, since the light yield per particle should be on average proportional for both DOMs. The relative difference between LG and HG signals is shown in Fig. 4.12 (right). Until the HG saturation regime, the differences are, on average, constant. Both, the constant region and the increase of the differences for high LG charges are taken into account by means of a

¹¹To tag vertical muons, a portable scintillator-based muon telescope was placed on top of an IceTop tank in the polar 2005/2006 season [177]. The resulting charge distribution vertical muons only results in a slightly lower muon peak as the accepted muon zenith distribution of a normal VEMCal launch is larger, leading to an increased average track length.

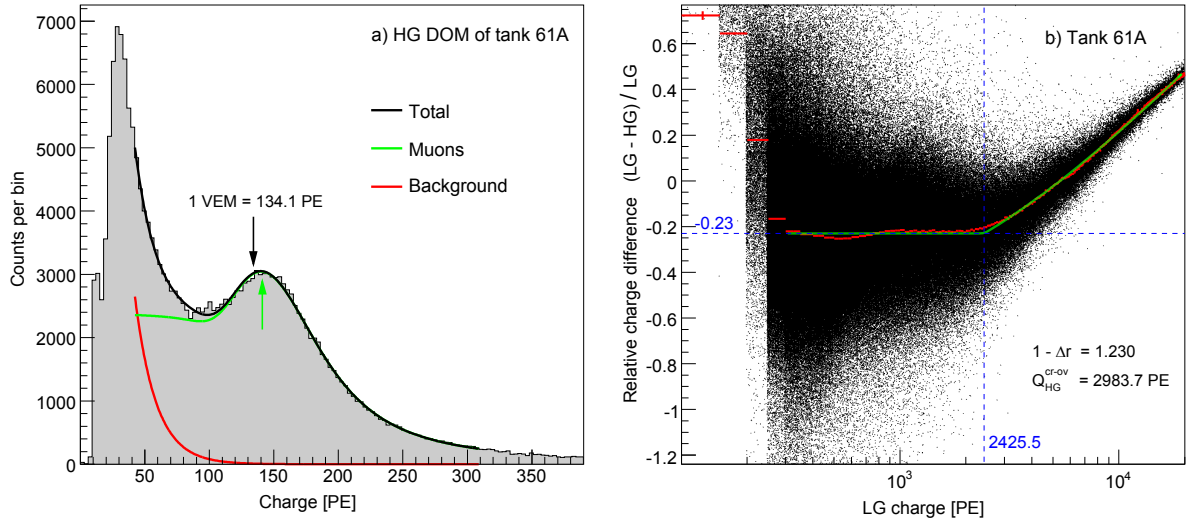


Figure 4.12.: Example charge spectrum obtain from VEMCal launches for the HG DOM of tank 61A (left). Fits to the EM contribution and to the muon peak are shown in red and green, respectively. The black total fit (Eq. (4.5)) is illustrated as black line. Relative difference between the charges measured with HG and LG DOMs of the same tank as a function of LG charge (right). Average values are indicated in red, fits to the average values are shown as green lines. Figures taken from [171].

fit (green lines) to the average values. The cross over point of the linear to the increasing behavior determines the HG-LG cross over.

For continuous monitoring of the VEM calibration, the VEM value is determined by combining the VEMCal distributions on a biweekly basis. With this procedure, maximum variations of $\sim \pm 10\%$ with a RMS of 3% are observed between consecutive calibrations [171]. Initially, the variations in the VEMCal were taken into account soon after the data transfer. However, since this led to undesired behavior, the correct calibration is now applied, after verification [42], during the Level3 processing.

Cosmic-ray filters

To select interesting physics events, dedicated filters are applied on the triggered data by the PnF system (see Fig. 4.10). The applied filters select events based on simple conditions or basic reconstructions that can be tested with minimal computation time. All filters relevant for the cosmic-ray analyses are discussed in the following.

For IceTop, two event filters that require simple trigger multiplicity thresholds are applied, the *IceTopSTA3* and *IceTopSTA5* filters. These filters are passed if at least three or five HLC stations are triggered, respectively. If an event passes the *IceTopSTA3* filter (energy threshold ~ 300 TeV [41]), the *IceTopSTA5* and *IceTop_InFill_STA3* filters are applied. The latter is focused on the selection of low-energy events around 100 TeV and requires at least three triggered HLC stations in the infill area. Most of the IceTop analyzes use

events that pass the *IceTopSTA5* filter, since the standard IceTop reconstruction requires 5 HLC stations.

Level2

At *Level2* of the processing chain, information that is removed at Level1 to save bandwidth for the transmission from the South Pole to the North is recovered. Depending on which event filter is passed, either the full waveform information or a compressed¹² version of the pulses are sent to North. In case the compressed information was sent, the pulses are uncompressed, re-combined into tank charges, calibrated to units of VEM, and the event splitting is redone similarly to Level1 [42]. Additionally, an initial selection of in-ice pulses that coincide with IceTop pulses is performed. At this level, the data can be monitored and potential issues can be resolved.

Level3

To improve on the Level2 event quality, another processing step is applied which improves on it in several ways. In particular, the changing IceTop conditions need to be measured and verified since they are not monitored continuously, and are then properly taken into account at Level3. Mainly, this includes the changing snow accumulation on top of the IceTop tanks and the surface temperature. The Level3 processing also incorporates more sophisticated cleaning and reconstruction algorithms. Before the reconstructions are performed, a first noise cleaning procedure is employed. The subsequent reconstruction is then used to perform a more advanced cleaning.

After removing unnecessary information from Level2 (mostly in-ice information that is not part of or connected to potential physics events) and unifying the naming scheme within the data files, the cosmic-ray filters are revisited. If only three or four HLC stations were triggered (*IceTopSTA3* or *IceTop_InFill_STA3*), the event is tested for spatial coincidence, requiring all stations to be next to each other. Otherwise, the event is discarded. Further, the corresponding *Geometry*, *Calibration* and *Detector-status* (GCD) files for each run are updated with the correct snow heights and verified VEMCal values (position of the VEM peak in PEs and HG-LG cross-over point) [42].

¹²For this purpose, the compressing tool *super Data Storage and Transfer* (sDST) is used. The sDST format only requires $\sim 9\%$ of the bandwidth of the original pulse series [42]. For more information see [172].

SLC calibration

Since the calibration of SLCs is less accurate compared to HLCs due to the missing waveform information, it is revisited at Level3 of the processing chain. The correction of the gain and baseline that is performed for HLCs using the individual waveforms, is carried out by means of a fixed baseline and gain for SLCs. Therefore, the effect of seasonal variations is not included in the calibration procedure. For a correct calibration, HLCs are re-processed as SLC hits (i.e., the waveform information is ignored and the total charge stamp and the DOM launch time are used to determine the charge and time, respectively), and the resulting pulses are compared to derive proper SLC calibration constants [178]. The relation between the resulting charges of these fake SLCs and the HLCs is characterized as a linear function, for which the exact parametrization changes for each DOM, and for each ATWD chip and channel. Thus, for each DOM, a set of six calibration functions is derived and saved for each run. This procedure for the correction of the SLC charges is only possible if the events passed the *IceTopSTA5* or *IceTop_InFill_STA3* filters, for which the necessary information about which ATWD chip and channel are used is always saved [42]. Events that only pass filters for which this information is lost have to be treated separately¹³. However, for the purpose of this work, only events that pass the *IceTopSTA5* filter are used.

For the correction of the SLC time stamp, the time offset between the HLCs and the fake SLCs is analyzed [180]. The observed average differences are of the order of 10–18 ns, and depend marginally on the measured charge values. Additionally, the derived correlation does not exhibit a time dependence [42]. The SLC times are then corrected for by the average shift obtained to match the HLC times.

SeededRT cleaning

To improve the simple cleaning procedures applied during the Level1 and Level2 processing, another cleaning is implemented at Level3. Until Level3, a simple time coincidence condition requiring hits to be within $1\,\mu\text{s}$ from each other is applied [42]. This leads to significant pollution due to after pulses that occur $\sim 1\,\mu\text{s}$ after the hit. Additionally, noise hits and uncorrelated muons and air showers that are within the required time frame but not spatially correlated with the physics hits of the main event are still included. For this reason, the *Seeded RT* cleaning is applied. The starting point of this algorithm is to search for a cluster of three HLC hits within a given radius and time. Subsequently, HLC hits are selected within a radius of $R = 180\,\text{m}$ and within a time of $T = 450\,\text{ns}$ with respect to the initial cluster [42]. This procedure is repeated for two further iterations and effectively removes the bulk of the noise hits. These cleaned pulses are the starting point for the standard reconstruction applied in the Level3 processing.

¹³A new SLC calibration procedure for such events was developed within [179].

Standard reconstruction

The goal of the standard reconstruction is the estimation of the shower geometry, i.e., the shower core location and the primary direction, as well as the reconstruction of the primary energy (and mass). The energy and mass can be related to the measured shower size and slope of the lateral distribution, respectively (see section 3.5). In the standard reconstruction, only HLC hits are included. This is sufficient for the reconstruction of the shower geometry and energy, as HLCs are by construction dominated by electromagnetic contribution due to their vicinity to the shower axis. However, SLCs are more sensitive to the muon contribution and therefore provide valuable information about the primary mass. For this reason, a more advanced reconstruction algorithm incorporating SLC hits is developed within this work and applied to reconstruct EASs with IceTop.

All parameters of interest of the standard reconstruction can be estimated using a negative log-likelihood minimization procedure that employs model functions for the description of the lateral distributions of measured signal strengths and arrival times. Since such procedures are sensitive to the choice of initial parameter seeds, first guesses are derived based on analytical calculations using the signal and time distributions.

Since the particle density is largest close to the shower axis, the shower core location can be related to the signal center-of-gravity (COG) of the measured distribution. For this purpose, the HLC tanks that observed the highest charges are used to calculate the COG:

$$\vec{x}_{\text{COG}} = \frac{\sum_i \vec{x}_i \sqrt{S_i}}{\sum_i S_i}, \quad (4.6)$$

where S_i is the signal measured in tank i and the number of tanks included in the calculation is seven [181]. Eq. (4.6) can therefore be understood as signal-weighted position. Note, that this procedure only performs reasonably well if the true core location is located inside the IceTop array (IceTop contained)¹⁴. For the purpose of this work, however, only IceTop contained events are included (see section 6.3).

As a first estimation of the primary direction, the shower front can be approximated as a plane. The curvature of the shower front can then be taken into account in the log-likelihood procedure. The difference between the measured times, t_i^{obs} , and the expected

¹⁴The reconstruction of IceTop uncontained events is more complex as the IceTop alone can not be used to obtain an accurate estimation of the shower geometry. However, for events with a coincident in-ice signal, the high-energy muon track reconstructed with IceCube can be used to determine the shower geometry with sufficient accuracy. With this combined information, the reconstruction of uncontained events can therefore be performed. Preliminary studies are discussed in [182, 183, 184]

times of the plane wave, t_i^{plane} , can be minimized using the χ^2 over all HLC hits

$$\chi_{\text{plane}}^2 = \sum_i \left(\frac{t_i^{\text{obs}} - t_i^{\text{plane}}}{\sigma_t} \right)^2, \quad (4.7)$$

where a first guess of the time fluctuations, σ_t , of 5 ns is applied [42]. Assuming speed of light propagation of the shower front, the expected time of a hit with position (x_i, y_i, z_i) is given by

$$t_i^{\text{plane}} = t_0 - \frac{ux_i + vy_i}{c}, \quad (4.8)$$

with the arrival time of the shower core, t_0 , and the direction vector $\vec{n}$ defined by u and v [42]:

$$\vec{n} = (u, v, -\sqrt{1 - u^2 - v^2}). \quad (4.9)$$

The minimization of Eq. (4.7), $\vec{\nabla} \chi_{\text{plane}}^2 = \vec{0}$, results in a set of three linear equations that can be solved analytically. The z position of the detectors is included in a second iteration.

Using the obtained initial values for the core position and primary direction, the negative log-likelihood minimization can be applied. This procedure includes a total of seven free parameters. Namely, three parameters to describe the core position, $\vec{x}_c = (x_c, y_c, z_c)^T$, two parameters for the primary direction, i.e., the direction vector $\vec{n}$, and two parameters to describe the signal lateral distribution. The latter is achieved by means of a lateral distribution function (LDF)¹⁵. To provide sufficient multiplicity to derive all seven parameters, a minimum of 5 HLC stations, i.e., 10 waveform measurements, are required for the standard reconstruction.

The likelihood function for the measured signals can be described using a log-normal distribution. The log likelihood is therefore given by

$$\mathcal{L}_{\text{sig}} = - \sum_i \left(\frac{\log_{10} S_i - \log_{10} S_i^{\text{exp}}}{\sqrt{2} \sigma_{\log_{10} S}(S_i^{\text{exp}})} \right)^2 - \sum_i \ln \left(\sigma_{\log_{10} S}^2(S_i^{\text{exp}}) \right), \quad (4.10)$$

where all HLC hits with lateral distances above 5 m are included [171]. This is because very close to the shower axis the LDF can exhibit unphysical behavior with the chosen parametrization (Eq. (4.11)). The LDF employed in the standard reconstruction is the *Double Logarithmic Parabola* (DLP) function

$$S_{\text{DLP}}(r) = S_{\text{ref}} \left(\frac{r}{R_{\text{ref}}} \right)^{-\beta - \kappa \log_{10} \left(\frac{r}{R_{\text{ref}}} \right)}, \quad (4.11)$$

with the signal strength S_{ref} at the reference distance R_{ref} . Eq. (4.11) defines a parabola in double logarithmic space with a shape that is described by β (slope) and κ (curvature of

¹⁵For a detailed discussion see section 6.1.

the parabola). While β is a free parameter of the reconstruction, κ is fixed at a value of ≈ 0.303 as it is found to not influence the result significantly [171]. The reference signal S_{ref} is the shower size parameter and is used as energy proxy. The optimal reference signal is obtained for a combination of a minimal shower size fluctuation and a minimal dependence on the primary mass¹⁶. For a reference distance of $R_{\text{ref}} = 125$ m, this condition is fulfilled, as the LDF slope and the shower size are minimally correlated at this distance [185]. For standard analyses, S_{125} is therefore used to reconstruct the primary energy. To account for the snow accumulation on top of the IceTop tanks, the expectation signal is modified during the reconstruction procedure assuming exponential attenuation:

$$S_i^{\text{exp}} = S_i e^{\frac{d_i^{\text{snow}}}{\lambda_{\text{snow}} \cos \theta}}, \quad (4.12)$$

where the snow height d_i^{snow} is given for each detector and the effective track length through the snow scales with $1/\cos \theta$. The strength of the attenuation is defined by the attenuation length λ_{snow} and can be understood as an effective quantity, as the snow affects EM particles and muons differently. Since the snow accumulation increases with time, λ_{snow} changes throughout the years. For the year 2010, the ideal value for λ_{snow} is determined to be 2.1 m based on studies of S_{125} spectra for different subsets of the IceTop array featuring different average snow heights [186]. In the case of measured data from 2012/2013 which is used in this work, λ_{snow} takes a value of 2.25 m [187]. It should be noted, that for increasing snow accumulation the exponential attenuation model becomes less accurate [188]. This is because, in practice, the attenuation depends on the lateral distance and the shower size, since they influence the energy spectrum of EM particles at a given location. Both quantities also affect the relative fraction of weakly attenuating muons¹⁷. However, for the data set used for this work, the exponential approximation of the attenuation performs reasonably well [188] and a corresponding systematic uncertainty is taken into account for the reconstruction (see chapter 8).

To estimate the uncertainty, $\sigma_{\log_{10} S}$, of the log signal, the signal fluctuations can be studied by comparing the tank signals in neighboring IceTop tanks within HLC stations. This is because the distance between the tanks in one station (~ 10 m) is small enough to be considered a double measurement at the same lateral distance and therefore of the same signal expectation value (see section 7.3.3 for a more detailed discussion). However, this is only approximately true at distances not too close to the shower core, since the steep falloff of the lateral distribution results in a significantly different signal expectation

¹⁶From the superposition model it is known, that X_{max} and therefore the slope of the lateral distribution at the observation level depends on the primary mass.

¹⁷A new *RA*d*i*us-*DE*pendent (RADE) snow model is developed in [188] that incorporates an attenuation factor as a function of lateral distance and S_{125} and employs a separate treatment of the expected EM and muon contributions to the measured signals. With this new model, better agreement of energy spectra throughout many different years is achieved. For the inclusion of more recent data sets, the snow attenuation should therefore be taken into account through the RADE model.

value for neighboring tanks. As the tanks in one station are almost never exactly at the same lateral distance which can bias the quantification of the signal uncertainty, a dedicated simulation study is performed using special simulations of a ring-like detector geometry. In this study, IceTop tanks are placed in rings with different radius around a center point. Then, vertical air showers are simulated and injected at the center of the geometry, resulting in all tanks of a ring having the same lateral distance. The difference in the measured signals in tanks of the same lateral distance for a specific signal expectation value can be modeled via a Gaussian fit, where the corresponding standard deviation is used as a measure of the signal uncertainty. The resulting signal uncertainty as a function of the signal expectation value can be parametrized as

$$\sigma_{\log_{10} S} = \begin{cases} -0.5519 - 0.078 \log_{10} S & , \log_{10} S < 0.340 \\ -0.373 - 0.658 \log_{10} S + 0.158 \log_{10}^2 S & , 0.340 \leq \log_{10} S < 2.077 \\ -1.058 & , 2.077 \leq \log_{10} S, \end{cases} \quad (4.13)$$

using a combination of a polynomial of 1st and 2nd order in double logarithmic space [189, 190].

To reconstruct the arrival direction, the deviation, Δt , from the plane front approximation (Eq. (4.8)) of HLCs is modeled via the sum of a parabola and a Gaussian function:

$$\Delta t(r) = ar^2 + b \left(1 - e^{-\frac{r^2}{2\sigma^2}} \right). \quad (4.14)$$

Here, the parameters $a = 4.823 \cdot 10^{-4} \text{ ns/m}^2$, $b = 19.41 \text{ ns}$, and $\sigma = 83.5 \text{ m}$ are fixed parameters of the reconstruction [171]. Eq. (4.14) is derived specifically for IceTop where the Gaussian part models a feature close to the shower axis for arrival time distributions observed with IceTop which could be caused by high-energy muons that arrive early. The likelihood function for the time fit is given by a Gaussian distribution. The log likelihood can be written as

$$\mathcal{L}_t = - \sum_i \left(\frac{t_i - t_i^{\text{exp}}(r_i)}{\sqrt{2}\sigma_t(r_i)} \right)^2 - \sum_i \ln(\sigma_t(r_i)), \quad (4.15)$$

where the expected times are given by the sum of the plane wave approximation and Eq. (4.14), $t_i^{\text{exp}}(r) = t_i^{\text{plane}}(r) + \Delta t(r)$. The time fluctuation, $\sigma_t(r)$, is obtained from measured data as a function of lateral distance [189]:

$$\sigma_t(r) = 2.92 \text{ ns} + 2.77 \cdot 10^{-4} \cdot r_i^2. \quad (4.16)$$

If an IceTop tank is saturated, it can be modeled via a dedicated saturation likelihood, which accounts for the probability of a given detector to observe a signal above the saturation threshold given an expectation signal. The saturation threshold for LG DOMs

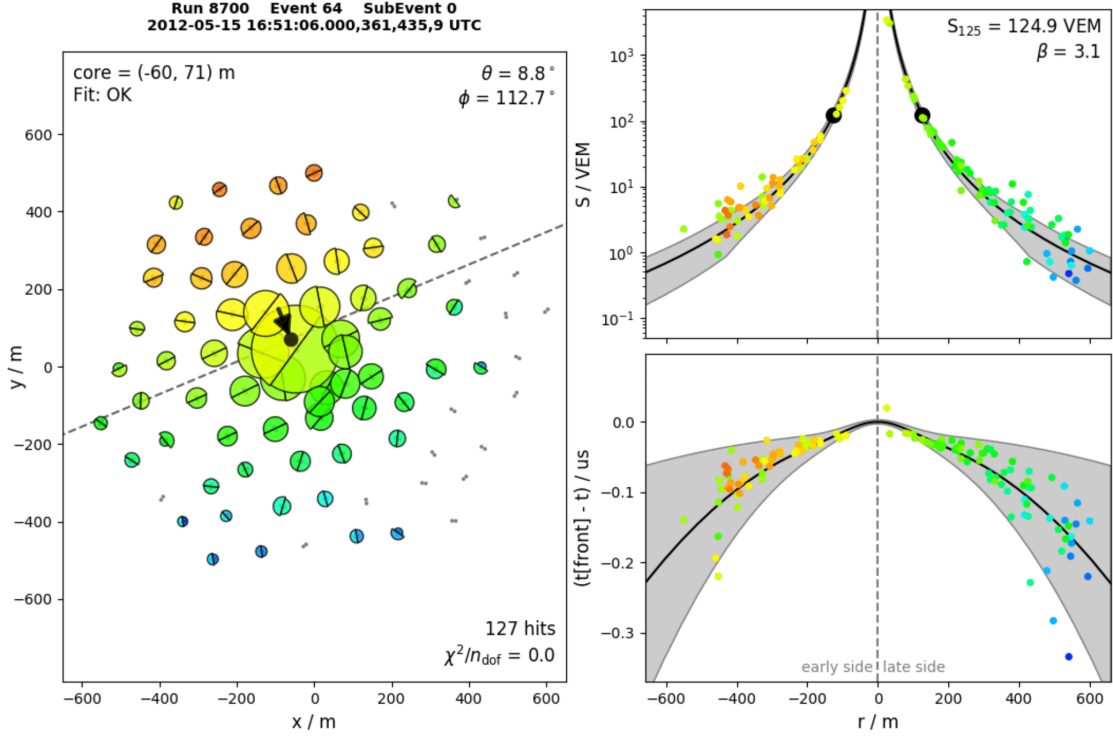


Figure 4.13.: Event display of a single simulated proton-induced air shower ($E_{\text{true}} = 97 \text{ PeV}$, $\theta_{\text{true}} = 9.0^\circ$, $\phi_{\text{true}} = 113.4^\circ$, $x_{c,\text{true}} = (-60 \text{ m}, 68 \text{ m})$ reconstructed with the standard reconstruction. Shower footprint with triggered HLCs shown as colored half-circles which are rotated according to the station orientation (left). The size of the half-circles corresponds to the measured signal strength, while the color code illustrates early hits in red and late hits in blue. The projection of the shower direction on the ground is drawn as arrow, the core position as black circle. The LDF fit (Eq. (4.11)) to the lateral distribution and time front fit (Eq. (4.14)) to the time delay relative to the plane wave are shown in the upper and lower panel of the right figure, respectively. Both, the early and late side of the shower determined by the shower geometry are shown. However, they are not treated separately in the reconstruction as this becomes important only for very inclined EAS. Figure taken from [41].

is around 90000 PEs [42]. Since tank signals are modeled via a log-normal distribution, the saturation probability is given by

$$p_{\text{sat},i} = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}\sigma_{\log_{10} S}(S_i^{\text{exp}})} e^{\left(-\frac{\log_{10} S_i - \log_{10} S_i^{\text{exp}}}{\sqrt{2}\sigma_{\log_{10} S}(S_i^{\text{exp}})}\right)^2} d \log_{10} S_i. \quad (4.17)$$

In addition, HLCs that do not have a trigger are important information that is included in the reconstruction. For this purpose, the probability of a detector being *silent* (not triggered) is described by the cumulative distribution function of the log-normal distribu-

tion:

$$p_{\text{sil},i} = \int_{-\infty}^{s_{\text{thr}}} \frac{1}{\sqrt{2\pi}\sigma_{\log_{10} S}(S_i^{\text{exp}})} e^{\left(-\frac{\log_{10} S_i - \log_{10} S_i^{\text{exp}}}{\sqrt{2}\sigma_{\log_{10} S}(S_i^{\text{exp}})}\right)^2} d\log_{10} S_i, \quad (4.18)$$

where the integral is evaluated up to the threshold signal $s_{\text{thr}} = 0.1657 \text{ VEM}$. Since only HLCs are included in the standard reconstruction, only full silent HLC stations are observed. The silent probability is therefore determined on a station basis to account for the coincident absence of a trigger in two neighboring detectors. Thus, the lateral distance used for the derivation of the signal expectation S_i^{exp} corresponds to the center of a silent HLC station. The silent probability of a full station is then given by $p_{\text{sil}}^{\text{sta}} = 1 - p_{\text{hit}}^2$, where the hit probability $p_{\text{hit}} = 1 - p_{\text{sil}}$.

The full log likelihood which is minimized in the reconstruction procedure can be summarized as

$$\mathcal{L} = \mathcal{L}_{\text{sig}} + \mathcal{L}_{\text{t}} + \sum_i \log p_{\text{sat},i} + \sum_i \log p_{\text{sil},i}^{\text{sta}}. \quad (4.19)$$

After the calculation of the first-guess parameters for the shower geometry, a rough estimation of S_{125} is derived using the observed tank signals at around 125 m distance from the first guess of the shower axis. The initial value for β is set to 2.6. For events that pass the IceTopSTA5 filter (at least 5 triggered HLCs) which are relevant for this work, the minimization of the log likelihood is performed iterative in a three step procedure. An example single event fit obtained after the third reconstruction step is shown in Fig. 4.13. In the first step, the direction is fixed while only the core position and the LDF parameters are varied. To ensure reasonable behavior of the core position estimation, it is varied within a box of 400 m diameter relative to the initial core position. In the second step, the direction is fit via the shower front function Eq. (4.14) along with the LDF Eq. (4.11) and the core position. The relative bounds for the latter are more tightly constrained in this step. Lastly, in the third step, once again only the core position and the LDF parameters are varied. All steps are optimized for events with core position inside the IceTop array and for zenith angles up to 40° [181] and are discussed in more detail in section 6.3.

Track-based cleaning

The high quality of the standard reconstruction can be utilized for a further pulse cleaning algorithm based on the reconstructed shower geometry [191]. For this purpose, the initial uncleaned pulses are used and selected based on their arrival time relative to the plane-wave approximation obtained from the full standard reconstruction. This is of particular importance for this work, because, in contrast to the SeededRT cleaning, this procedure can be applied not only for HLCs which are typically spatially clustered but also for SLCs that can occur far from the shower axis while still being physically related to an

event. The default time window applied in the track-based cleaning has a size of 1 s and comprises arrival times between +200 ns and −800 ns with respect to the plane wave. The resulting cleaned HLC pulses are used for the novel reconstruction algorithm developed in this work. In contrast to the standard reconstruction, this novel approach also includes SLC hits (see chapter 6). However, for the purpose of this work, a narrower time window of 0.5 s is used to select SLCs with arrival times between 0 ns and −500 ns relative to the plane wave. This time window is chosen to reduce the number of selected random background hits, predominately produced by uncorrelated muons, that are present in measured data but cannot be properly modeled in simulations (see section 8.1 for a more detailed discussion). In principle, in a more accurate track-based cleaning, the shower front curvature as a function of lateral distance could be included in the derivation of a cleaning time window. Studies in this direction are currently under investigation [192].

RockBottom

In contrast to previously published IceTop analyzes performed in the *Laputop* framework, the reconstruction used for this work is implemented in a new multi-detector EAS reconstruction framework, *RockBottom*, developed within [193, 182, 183]. Using the RockBottom framework, likelihood functions for different detector arrays can be combined in a global minimization procedure, including individual parameter spaces [183]. Different model functions for the description of the respective signal strength and arrival time distributions can be employed on the basis of underlying probability distributions. The parameters of the model functions can be fully adjusted with user-defined values. In addition to the surface array of IceTop and scintillation detectors and radio antennas of the IceTop-enhancement and the future Gen2 surface array, also the in-ice array can be included. For the latter, the energy loss $dE_{\mu,B}/dX$ of high-energy muon bundle can be reconstructed, e.g., using single-photo-electron (SPE) or multi-photo-electron (MPE) PDFs for the calculation of the in-ice likelihoods $\mathcal{L}_{\text{SPE}}^{\text{InIce}}$ and $\mathcal{L}_{\text{MPE}}^{\text{InIce}}$, respectively. For a more detailed discussion about the in-ice reconstruction see [176].

Individual likelihood functions and models are part of the same base class, allowing a straightforward implementation of additional detectors and reconstruction methods [194]. Since all likelihoods require information about the shower geometry, the corresponding hypothesis is passed to each likelihood. The information flow through the different software components is visualized in Fig. 4.14. The purpose of the main components can be summarized as

- **Likelihood Services:** Provide likelihood descriptions of the signal and time hypotheses for IceTop or other detector arrays, as well as for the in-ice array.
- **Signal Models:** Build the basis for the evaluation of the likelihood functions

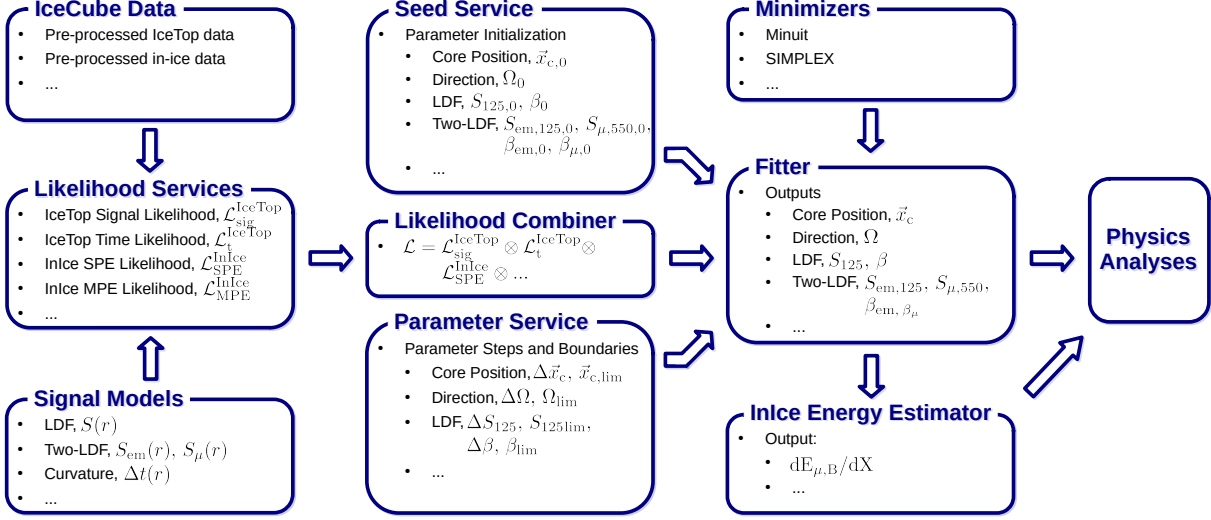


Figure 4.14.: Flowchart of the key software components of the RockBottom framework. Figure adapted from [182].

through the definition of model functions for the description of the signal and arrival time distributions measured with different detector arrays. In the case of IceTop, these distributions are described by Eq. (4.11) and Eq. (4.14), respectively.

- **Likelihood Combiner:** Constructs the global likelihood by combining all likelihoods that are part of a reconstruction procedure. No constraint on the number of likelihood functions is applied. Therefore, an arbitrary number of additional observables and detector arrays can be included for a reconstruction [182].
- **Seed/Parameter Service:** Initializes parameters and constructs bounds and step sizes for the minimization procedure.
- **Minimizer/Fitter:** Collects the information from the services and performs the minimization of the global likelihood (Eq. (4.19) in the case of the standard reconstruction) on the basis of a specified minimization algorithm, e.g., Minuit or SIMPLEX [195, 196].
- **In-ice Energy Estimator:** Reconstructs the energy loss profile of muons traversing the in-ice detector through the reconstructed muon track information and employing the IceCube reconstruction *Millipede* [176].

For the purpose of this work, the application of multiple model functions for the signal distribution observed with IceTop is of particular importance. In the context of the *two-component LDF*, or *two-LDF*, for which the RockBottom framework was initially developed [197] and which was first presented in [193] in an early state, two separate LDFs can be employed and fit to the lateral distribution of IceTop using different underlying signal models. This approach is further developed within this work and is used for the separation of the EM and muon components in air showers observed with IceTop (see

chapters 5 and 6 for a detailed discussion of the technical details and implementation). The standard reconstruction used in this work is implemented within the RockBottom framework. Its reconstruction performance is compared to the two-component LDF reconstruction developed in this thesis in chapter 7.

The inclusion of an in-ice likelihood is of particular interest for the reconstruction of events with core position outside of IceTop (IceTop-uncontained) that feature a coincident in-ice track produced by high-energy muons of the same shower, as it would significantly increase the aperture for cosmic-ray analyses. Due to the small angular separation of high-energy muons relative to the shower axis, the in-ice track can then be used to reconstruct the shower geometry and improve the reconstruction performance of IceTop. Preliminary studies are presented in [182, 183, 184].

4.3.2. Relevant results

To put the results obtained in this work into a more global context, some relevant results are selected from the variety of cosmic-ray analyses published by the IceCube Collaboration. The corresponding analyses are briefly introduced within the following sections.

Energy spectrum and composition

IceTop has measured the all-particle cosmic-ray energy spectrum for energies between 2.5 PeV and 1.3 EeV for contained events with zenith angles $\lesssim 37^\circ$ (see [186]). The energy reconstruction is based on the conversion of S_{125} as a function of the true MC energy to the reconstructed energy via a linear calibration fit in bins of the zenith angle (with a bin width of 0.05 in $\cos \theta$). The analysis was performed on an incomplete configuration of the IceTop array with 73 ice-Cherenkov stations. In [187], the analysis is repeated with three years of data. The results are shown in Fig. 4.15 and clearly show a double knee structure. Using the IceTop infill array, the spectrum was further extended toward low energies (250 TeV) in a dedicated analysis presented in [198].

Through the inclusion of both IceTop and in-ice information, the cosmic-ray composition is also analyzed in [187] and separated into four mass groups (proton, helium, oxygen, and iron). While the main observable for the energy reconstruction is S_{125} obtained in the standard processing (see section 4.3.1), the main observable for the derivation of the composition is the energy loss parameter dE/dX_{1500} (see section 8.3.2) of the accompanying high-energy muon bundle that is produced in EASs and measured with the in-ice detector. These observables, along with the zenith angle reconstructed with IceTop and two parameters related to the stochastic energy loss of high-energy muons

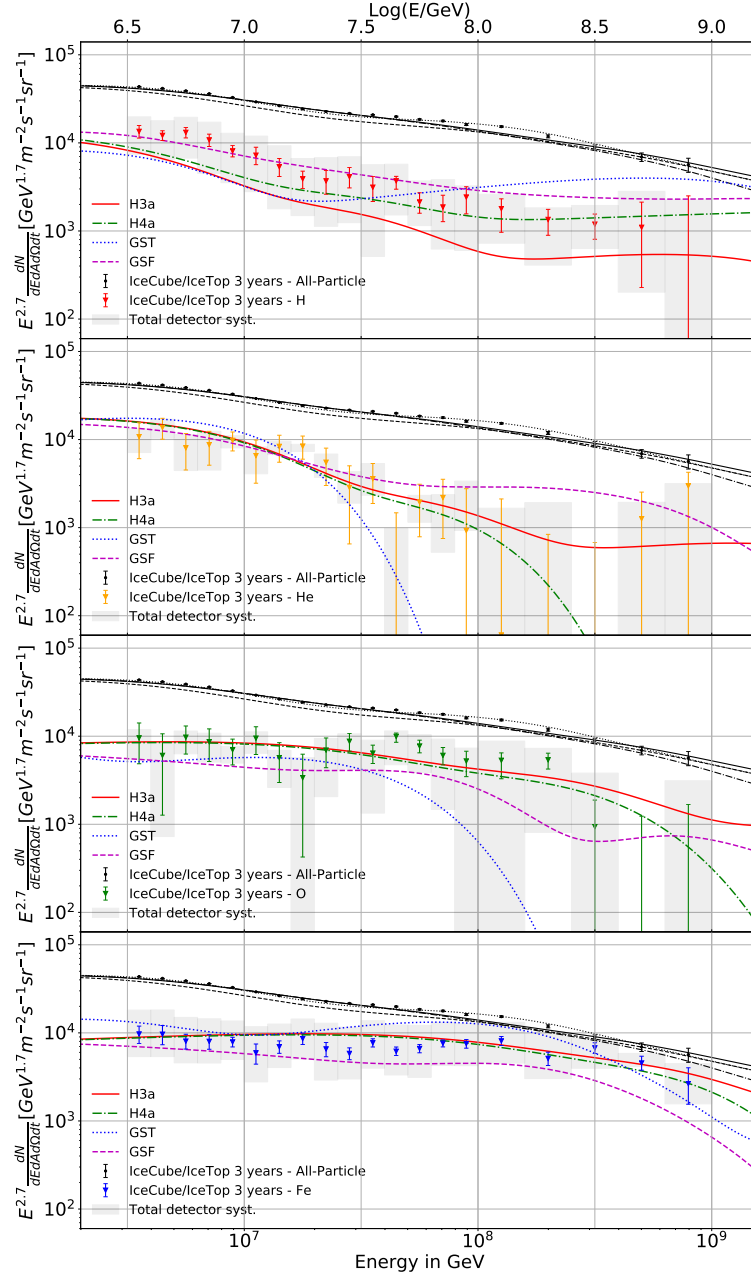


Figure 4.15.: Individual mass contributions to the energy spectrum in the PeV to EeV range obtained for Sibyll 2.1. Protons, helium, oxygen, and iron are illustrated in red, yellow, green, and blue, respectively. Systematic and statistical uncertainties are shown as boxes and error bars. For comparison, the expectations of different cosmic-ray flux models (see section 2.4) are drawn. Figure taken from [187].

in the in-ice detector, are combined in a neural network that was trained to reconstruct the primary energy and mass. The resulting fractional mass contribution to the energy spectrum is shown in Fig. 4.15. The systematic uncertainties include contributions of the uncertainty in the VEM calibration, the description of the attenuation of EAS particles

through the snow accumulation on top of the IceTop tanks, and the ice model used in simulations.

As expected from the discussion in section 2.3, the results show an increasingly heavy composition between the knee and the second knee.

Note, however, that the results of the mass composition are strongly dependent on the hadronic interaction model used for the analysis [187], in this case Sibyll 2.1. This is because of the differences in the muon content between different hadronic interaction models (see section 3.6.2), which cause mainly global shifts in the average composition.

For this reason, the work presented in this thesis uses multiple simulation sets produced with different hadronic interaction models (see section 4.4).

GeV muon density at large lateral distances

One main purpose of the analysis presented in this work is the reconstruction of the muon content on single-event basis for air showers measured with IceTop. The density of low-energy (~ 1 GeV) muons at large lateral distances has been measured for near-vertical showers ($\theta \lesssim 18^\circ$) between 2.5 PeV and 100 PeV in primary energy based on a statistical analysis in [199]. The analysis includes both HLC and SLC hits observed with IceTop. Since HLCs occur closer to the shower axis, they are dominated by the contribution of the EM component. Conversely, SLCs exhibit a larger relative contribution of muons as they are typically located far from the shower axis. Since single muons usually produce signals around one VEM, a peak-like feature can be observed in the signal distribution at large lateral distances. Fig. 4.16 (left) shows the lateral distribution of HLCs and SLCs for near-vertical showers of $\sim 10 - 12.5$ PeV in primary energy. The feature that appears at around 1 VEM is the *muon thumb*, produced by the contribution of muons far from the shower axis. However, since the inclusion of SLCs is prone to the contribution of accidental coincidences produced mainly by single muons from low-energy showers, which are not accounted for in simulations, this analysis employs an ad hoc injection of coincident hits with a successive reassignment of the local coincidences (see section 8.2 for more details) to account for their influence on the reconstruction. The settings for the simulation of coincident hits are based on measured data, where an injection rate of 1470 Hz is applied. The HLC and SLC hits used for this analysis are obtained from the track-based cleaning. All hits must be within a time window of -4 s and $+0.5$ μ s with respect to the reconstructed shower front. To account for the uncertainty of the VEM calibration procedure described in this section, a Gaussian smearing with a width of 0.05 VEM and 0.1 VEM is applied on the simulated HLC and SLC pulses, respectively. Fig. 4.16 (right) shows the signal distribution of HLC and SLC hits for an example bin in lateral distance (~ 646 m). The clear double-peak structure is caused by the contribution of the electromagnetic and

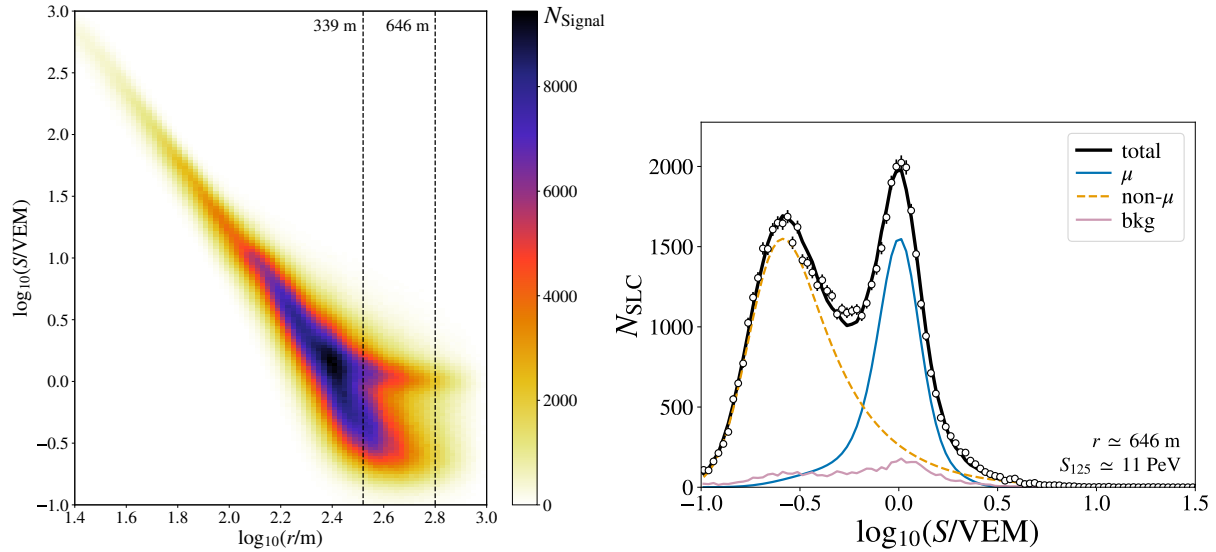


Figure 4.16.: Lateral distribution of HLC and SLC signals for showers with reconstructed energies of 10 – 12.5 PeV and zenith angles $\theta < 18^\circ$ (right). The feature around 1 VEM is produced by the muons at large lateral distances and is referred to as the *muon thumb*. The signal distribution of a vertical slice of the left figure for lateral distances of 646 m are shown on the right including fits of the signal models for the electromagnetic and muon contribution, illustrated as dashed orange line and solid blue line, respectively. The pink solid line shows the distribution of accidental signals. Figures taken from [199].

muon component. Such distributions can be obtained for different bins in lateral distance and in the energy proxy of the standard reconstruction, S_{125} . Using individual signal models for the electromagnetic and muon contribution, as well as a small accidental background component, the signal distributions can be described analytically. While the electromagnetic contribution is modeled using a power law with an additional systematic uncertainty to account for a possible small deviation from a power law, the muon signal model is based on a semi-analytical approach motivated by the fact that the muon signal distribution is, in first order, a function of the detector geometry (see chapter 5 for a detailed discussion). Since the latter depends on the average expected muon number, the density of muons can be obtained from the fit to the signal distribution in each bin. From this, the muon density at distances of 600 m and 800 m from the shower axis is reconstructed as a function of S_{125} , which is converted to the reconstructed primary energy using the calibration function derived in [186].

Since the reconstruction involves mass-dependent biases, correction factors are used to correct the raw reconstruction results. These correction factors are derived for each studied hadronic interaction model separately based on the ratio of the reconstructed and true average muon density as obtained from simulations. By describing the resulting ratio in bins of the reconstructed energy via a linear fit, an energy-dependent correction factor

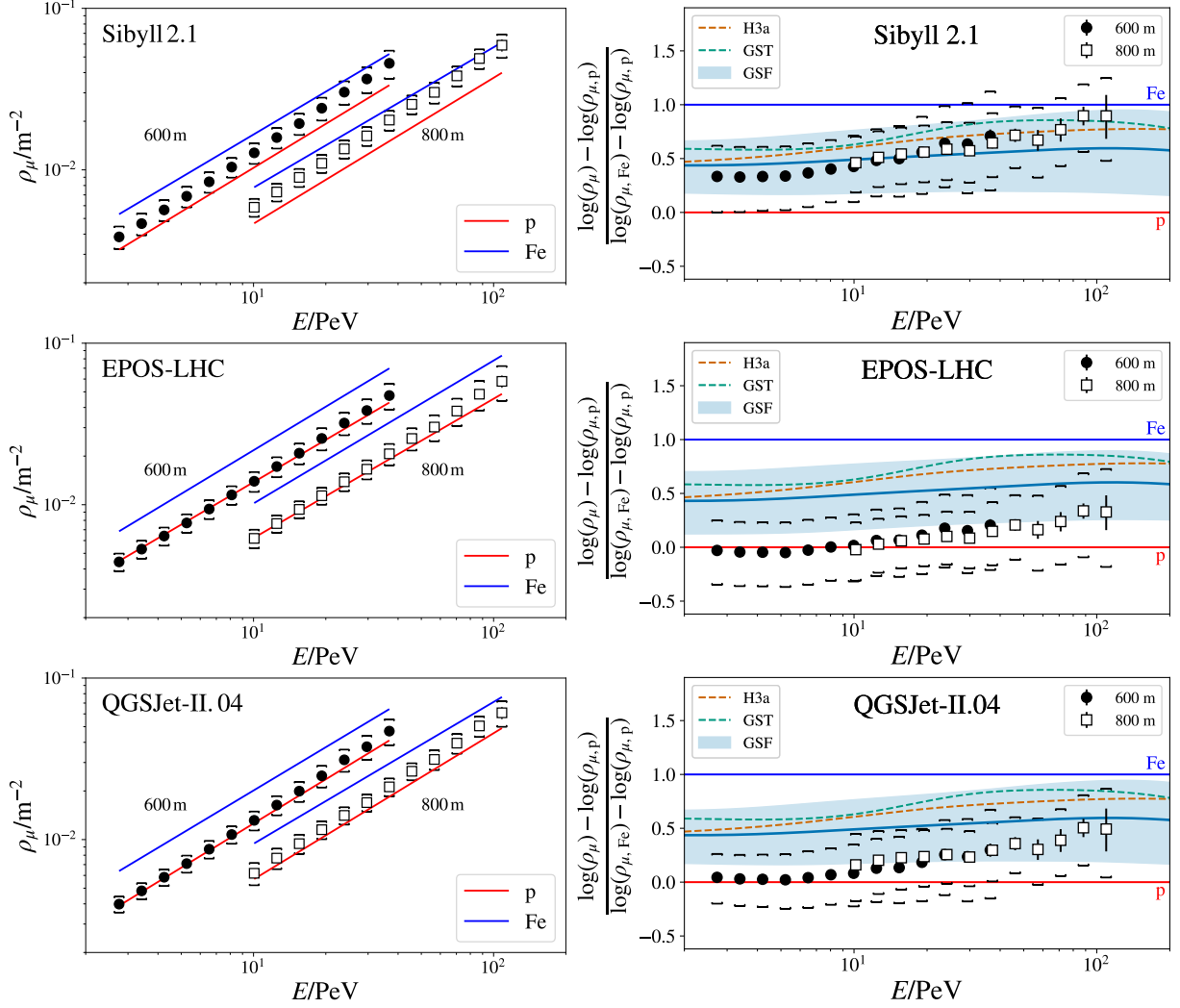


Figure 4.17.: Reconstructed muon density at lateral distances of 600 m and 800 m after application of the average correction factor for near-vertical showers and as a function of primary energy compared to MC expectations for the hadronic interaction models Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 (left). Systematic uncertainties are illustrated as brackets. Reconstructed muon densities expressed as z-values (Eq. (3.24)) and compared to the modern flux models H4a, GST, and GSF (right). Figures taken from [199].

is derived. Due to the mass-dependent reconstruction bias, these correction factors also depend on the mass and are determined from the average between a pure proton and iron flux assumption. The mass dependence is then taken into account by means of a systematic uncertainty assigned to each average correction factor.

The resulting corrected muon density at lateral distances of 600 m and 800 m as a function of primary energy are shown in Fig. 4.17 for the hadronic interaction models Sibyll 2.1, EPOS-LHC, and QGSJet-II-04. The right column also shows the results converted to the z-scale and compared to the modern flux models H4a, GST, and GSF (see section 2.4). The systematic uncertainties are shown in brackets and include the systematic

uncertainty of the correction factors, detector uncertainties, and the uncertainty on the energy scale. While for Sibyll 2.1 as a pre-LHC model the results are well compatible with the flux models, the post-LHC models EPOS-LHC and QGSJet-II-04 are both compatible with a mass composition that is pure proton or even lighter than proton for energies below ~ 10 PeV. The results of the muon density reconstruction are further discussed in section 9.6.

TeV muon multiplicity

In addition to the low-energy muon content, IceCube has also measured the high-energy muon multiplicity above 500 GeV for near-vertical showers ($\theta \lesssim 18^\circ$) between 2.5 PeV and 100 PeV in primary energy using coincident air-shower events, for which both IceTop and in-ice information is available. Muons above this energy threshold have a high probability of traversing the ice sheet between the surface and the in-ice detector and can produce an in-ice signal. The energy loss profile observed with the in-ice detector can be passed as an input vector to a neural network that relates the in-ice information to the number of high-energy muons on the surface [200]. An illustration of the construction of an energy-loss vector is shown in Fig. 4.18. The neural network is based on a recurrent neural network (RNN) layer to which the energy-loss vector is passed and a subsequent fully connected network layer that receives a combination of the RNN output, the energy proxy S_{125} , and the reconstructed zenith angle from the standard reconstruction [200]. Finally, the primary energy and the number of muons above 500 GeV on the surface are predicted. In contrast to the reconstruction of the muon density at large distances, this procedure works on an event-by-event basis. This is of particular importance for tests of hadronic interaction models, for which studies of the correlations of low- and high-energy muons for the same showers can be used to derive tight model constraints as they relate to the muon-energy spectrum. This is one main motivation for the reconstruction of the muon content using the two-component LDF developed within this thesis, as it provides an event-by-event based estimate of the low-energy muons, and therefore enables such correlation studies with IceCube.

The neural network output is used to reconstruct the average high-energy muon number as a function of primary energy. Similar to the muon density analysis, systematic reconstruction biases of this method are taken into account by means of a correction factor. However, a more advanced treatment of the correction based on an iterative procedure is applied. This procedure utilizes the linear dependence of the reconstruction bias on the logarithm of the mass number $\ln A$ and works without the need to assume a specific mass composition (see [41, 201] for a detailed overview). The average reconstructed muon number as a function of primary energy is shown in Fig. 4.19 for Sibyll 2.1, EPOS-LHC,

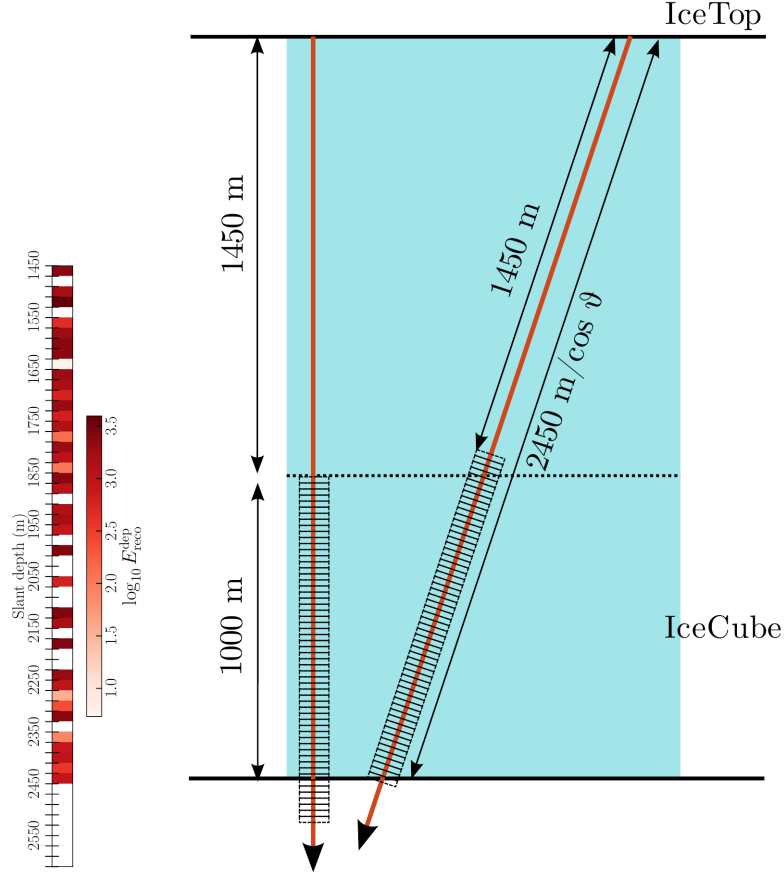


Figure 4.18.: Schematic view of the construction of an energy-loss vector that is passed to the neural network for the reconstruction of the high-energy muon multiplicity. The energy deposit is obtained in 20 m segments [202] along the reconstructed track. The length of the input vector is constant and defined by the maximum zenith angle included in the analysis. Therefore, the vector is padded with zero entries at the top or the bottom depending on the inclination of an event. Figure taken from [41].

and QGSJet-II-04. Similar to the muon density analysis, the results are shown also as z -values and compared to the flux models H4a, GST, and GSF. Systematic uncertainties include detector systematics (dominated by the uncertainties in the ice model used in the simulations and the DOM efficiency [200]) and a systematic uncertainty introduced through the correction procedure. In contrast to the measurement of the low-energy muon density at large distances, agreement is found between the average high-energy muon number and the modern flux models within the systematic uncertainties for all tested hadronic interaction models. Therefore, a tension is observed between the measurement of low- and high-energy muons for EPOS-LHC and QGSJet-II-04, indicating an insufficient description of the shower development by the two post-LHC models. However, it is discussed in section 8.3, that Sibyll 2.1 also does not produce a consistent description of all observables. Consequently, stronger model tests are needed in order to improve the

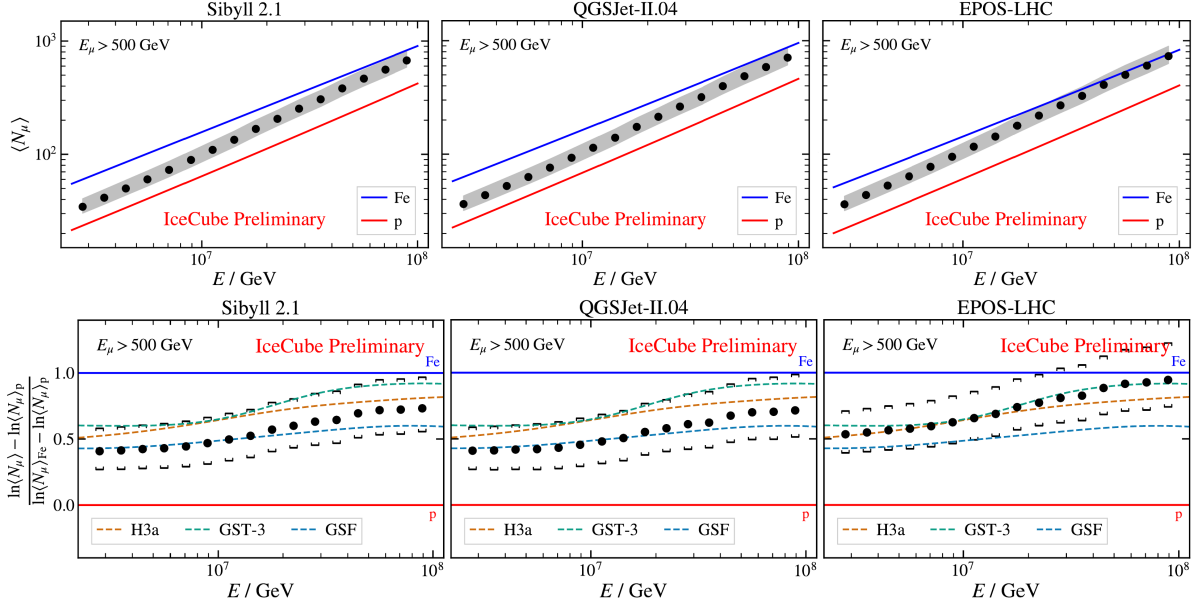


Figure 4.19.: Average reconstructed muon number above 500 GeV as a function of primary energy for near-vertical showers for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 compared to the MC expectations for a pure proton and iron composition (upper row). Systematic uncertainties are illustrated as gray shaded band. The average reconstructed muon number shown in the upper row expressed as z-values and compared to the flux models H4a, GST, and GSF, is shown in the lower row. Systematic uncertainties are shown as brackets. Figures taken from [200].

understanding of the measured data and reduce the systematic uncertainties introduced by hadronic interaction models. The results of the high-energy muon multiplicity analysis are further discussed in section 9.6.

4.4. Simulation set

The interpretation of measured air-shower data is based on MC simulations. As large differences in the expectations of shower observables are present between different high-energy hadronic interaction models (see section 3.6), the data needs to be interpreted using simulation sets produced with different models to take into account the resulting systematic uncertainties. For this reason, the analyses introduced in this section as well as the analysis presented in this work employs simulation sets produced with Sibyll 2.1, EPOS-LHC, and QGSJet-II-04. A further complication arises specifically for simulations used for the interpretation of IceTop data, since the snow accumulation on top of the IceTop tank increases over the years, leading to the necessity of the production of new simulation sets for each year with updated snow levels. For the purpose of this work, how-

ever, only the simulation set produced for the full 86 string detector configuration for the year 2012 (IC86.2012) is used. The snow accumulation used in the IC86.2012 simulations is chosen according to in-situ measurements in October 2012 (shown in Fig. 4.5 (right)), which roughly corresponds to the average accumulation observed in the corresponding data-taking period [42]. Accordingly, the measured data studied in this work includes the data-taking period from 15th of May of the year 2012 to the 2nd of May of 2013¹⁸.

In the following, the details of the production of the standard simulation set for 2012 used for this work are introduced. In section 4.4.1, the details of the production of the CORSIKA simulations are introduced. Then, in section 4.4.2, the specifics of the subsequent detector response simulations are discussed.

4.4.1. CORSIKA

For the production of EAS simulations for the standard IceTop simulation set, the version 7.3700 of CORSIKA is used. Hadronic interactions at low energies below 80 GeV are modeled with FLUKA2011.2b. As mentioned, high-energy hadronic interactions are described using the pre-LHC model Sibyll 2.1, and the post-LHC models EPOS-LHC and QGSJet-II-04. For all three models, individual simulation sets are produced. While for Sibyll 2.1 a total of 20000 individual EAS are simulated for four different primaries, proton, helium, oxygen, and iron, for the primary energy range of 100 TeV to 100 PeV and the zenith range of $0^\circ - 65^\circ$, for the post-LHC models only proton and iron primaries with more limited statistics are available. An overview of the entire set of EAS simulations from IC86.2012 used in this work is shown in Tab. 4.1. It should be noted, that an additional high-energy simulation set is present for Sibyll 2.1 for primary energies of $16 \leq \log_{10}(E/\text{eV}) \leq 18.6$ in the IC86.2012 set. Due to the significantly increase in computation time as a function of the primary energy, the high-energy set uses thinned showers. However, for the purpose of this work, only non-thinned showers up to 100 PeV are used.

For each of the different simulation sets, a fixed number of showers is produced per $\log_{10} E$ bin with a bin width of 0.1. Therefore, the simulation sets are produced according to a E^{-1} spectrum. The primary zenith and azimuthal angles are generated according to an isotropic distribution.

To reduce the computation time and memory usage in the simulation of EASs, particles that fall below a certain cutoff energy are discarded as they are unlikely to be detected at the observation level. For the IC86.2012 simulation set, the cutoff energy for electrons/positrons and photons is set to 0.01 GeV and 0.002 GeV, respectively. Muons and hadrons are discarded for energies below 0.05 GeV.

¹⁸Note that this simulation and data set is also included in the analyzes presented in section 4.3.2, which allows a later comparison of the results.

Table 4.1.: Overview of the IC86.2012 simulation set used in this work.

Hadronic model	Primary	$\log_{10}(E/\text{eV})$	$\theta/^\circ$	$\#_{\text{Showers}}$	Thinned
Sibyll 2.1	H	14 – 17	$0^\circ - 65^\circ$	20000	No
Sibyll 2.1	He	14 – 17	$0^\circ - 65^\circ$	20000	No
Sibyll 2.1	O	14 – 17	$0^\circ - 65^\circ$	20000	No
Sibyll 2.1	Fe	14 – 17	$0^\circ - 65^\circ$	20000	No
EPOS-LHC	H	14 – 17	$0^\circ - 65^\circ$	6000	No
EPOS-LHC	Fe	14 – 17	$0^\circ - 65^\circ$	6000	No
EPOS-LHC	H	14 – 17	$0^\circ - 20^\circ$	6000	No
EPOS-LHC	Fe	14 – 17	$0^\circ - 20^\circ$	6000	No
QGSJet-II-04	H	14 – 17	$0^\circ - 65^\circ$	6000	No
QGSJet-II-04	Fe	14 – 17	$0^\circ - 65^\circ$	6000	No
QGSJet-II-04	H	14 – 17	$0^\circ - 20^\circ$	6000	No
QGSJet-II-04	Fe	14 – 17	$0^\circ - 20^\circ$	6000	No

As discussed in section 3.1 on the basis of an isothermal model, the atmosphere has a significant impact on the shower development. For the production of the IC86.2012 simulation set, a more realistic atmospheric model based on five years of measurements of the atmospheric temperature from 2007 to 2011 is chosen [42]. From studies of the average monthly atmospheric profiles, the atmospheric profile for the month of April has been chosen for the application in the CORSIKA production (see Fig. 3.1), since it approximately represents the average of the entire year. This is beneficial in the context of seasonal atmospheric variations, as they only smear the measured data with respect to the average atmosphere and do not result in systematic effects [42].

The development of the shower is simulated down to the observation level, which is set to 2837m above sea level. Due to increasing snow accumulation over the years, the observation level has to be adjusted accordingly to be above the maximum snow level.

4.4.2. Detector response

To increase the statistics given the limitations in the production of CORSIKA simulations due to the large computation time, the EASs produced for the IC86.2012 simulation set are resampled one hundred times for the production of detector response simulations. For this purpose, the core position of the EAS is chosen randomly within a circle around the center of IceTop with an energy-dependent radius. The radius extends beyond the

Table 4.2.: Overview of the energy-dependent re-sampling radius used in the production of detector response simulations.

$\log_{10}(E/\text{eV})$	Radius/m
14 – 15	800
15 – 16	1100
16 – 17	1700

IceTop area and is chosen to ensure a significant probability that a shower within a certain energy range will produce an IceTop trigger. Therefore, the simulation set contains a large fraction of events with core position outside of IceTop. Since the reconstruction quality for such events is significantly worse than for contained events, dedicated quality cuts are applied for standard analyses and for the analysis presented in this work to remove them (see section 6.3 for a detailed discussion). The energy-dependent resampling radius is summarized in Tab. 4.2.

After sampling of the simulated EASs, the particles present at the observation level are propagated through the snow (modeled with a density of 0.38 g/cm^2 [42]) and IceTop tanks via Geant4 [203]. Each particle that could intersect with an IceTop tank (including a safety margin of 30 cm around the tank) is passed to the detector simulation one by one, where the signal deposit is simulated (see section 3.6 for more details). The output of the detector response simulations is then fed to the standard processing discussed in this section.

4.5. The future of IceCube

The IceCube Neutrino Observatory is operating since 2011 with an up time of $> 99\%$ [204]. Its successful operation and physics results motivate the continuation and further upgrade and enhancement of the IceCube detector [205]. Therefore, the *IceCube upgrade* and *surface array enhancement* will be deployed. In addition, the planned next-generation experiment *IceCube-Gen2* is in development. The corresponding science cases are introduced in this section.

4.5.1. IceCube upgrade and surface array enhancement

The IceCube upgrade comprises an extension of IceCube with seven additional strings and its deployment is planned for the 2025/26 polar season [208]. The new strings feature

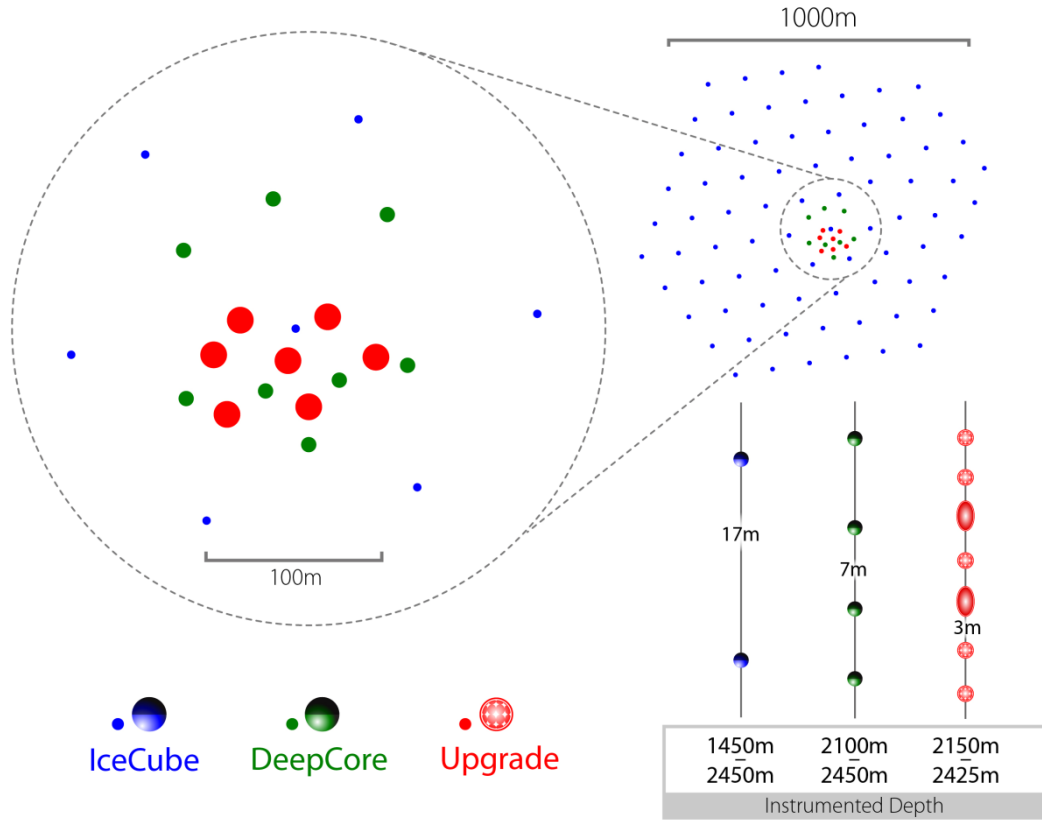


Figure 4.20.: Schematic view of the geometry of the IceCube upgrade (red). The configuration of the two different DOM types, the *mDOM* [206] and the *D-Egg* [207] of the upgrade are shown as red circles and ovals on the right string. Figure taken from [208].

a denser string and DOM spacing. Furthermore, new calibration devices on the upgrade strings will allow for more detailed studies of the optical properties of the ice, which will be beneficial for the entire IceCube detector. The upgrade will result in a lower threshold for the measurement of neutrinos ($\sim \text{GeV}$) and an improved angular and spatial resolution. This allows for revaluation and improved accuracy of the existing analysis in addition to new data. This will also be beneficial for the measurement of the muon bundle produced in EAS events. The IceCube upgrade is the first stage towards the development of IceCube-Gen2 as it tests the prototype instrumentation of the full-scale IceCube-Gen2 detector [208]. An overview of the geometry of the IceCube upgrade is shown in Fig. 4.20.

In addition to the IceCube upgrade, a complementary enhancement to the existing IceTop array is currently under construction. The surface array enhancement (SAE) comprises stations of elevated plastic scintillation detectors and radio antennas. The elevation is necessary due to the increasing snow accumulation over the years. In total, 32 stations

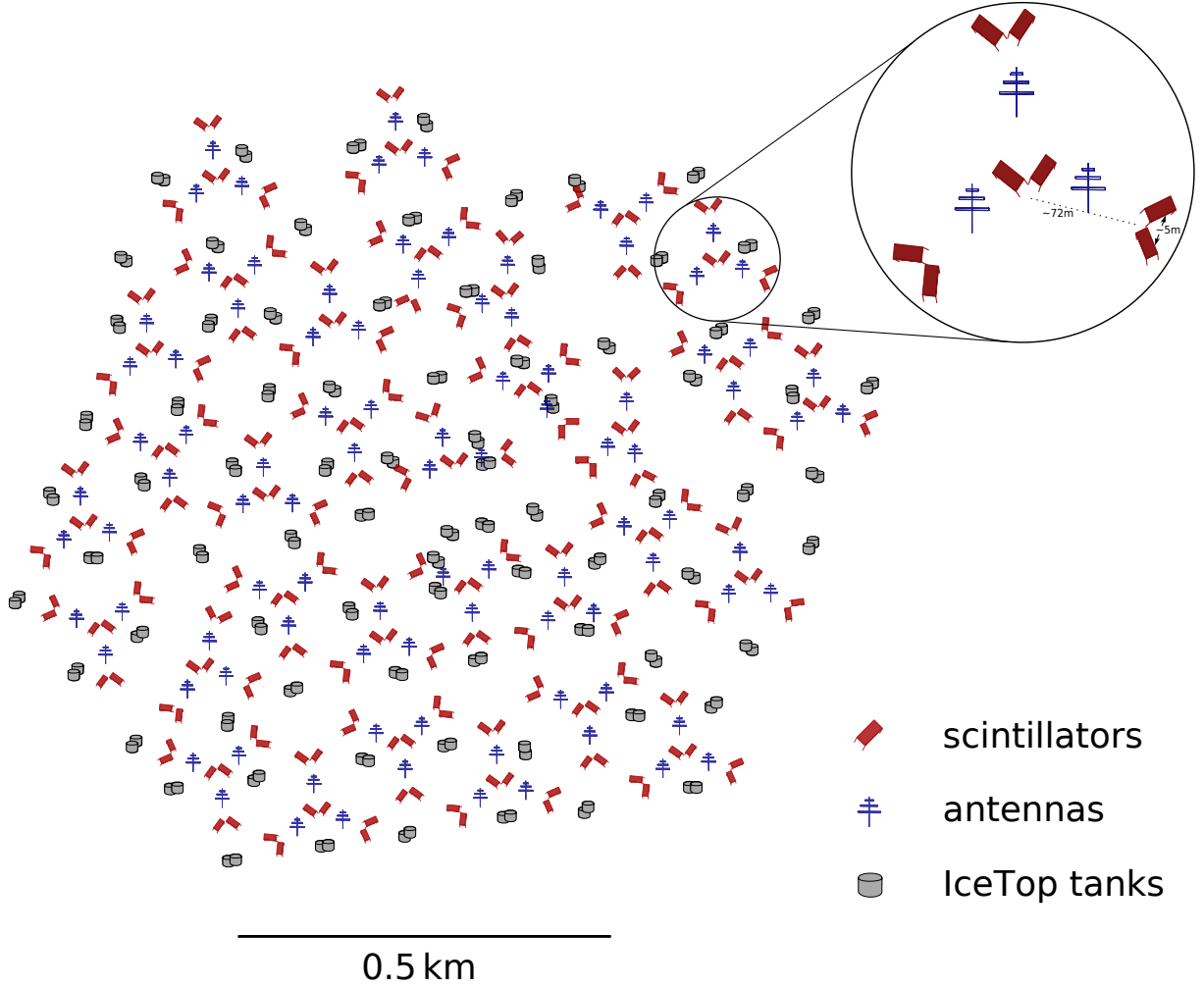


Figure 4.21.: Overview of the geometry of the surface array enhancement (top). Figure inspired by [194].

with 8 scintillation panels and 3 radio antennas will be arranged with a uniform spacing [209]. Each station has a triangular shape, where the scintillation panels are ordered as 4 pairs. An overview of the geometry of the SAE is shown in Fig. 4.21.

While the scintillation panels can be used for calibration purposes of the snow attenuation [194] and for the measurement of EAS particles, the radio antennas provide sensitivity to X_{max} . Scintillation detectors constitute a complementary detector type to the IceTop, as they are more sensitive to electrons. The signal differences between scintillation detectors and ice-Cherenkov tanks can therefore be used, e.g., for mass discrimination studies [194]. Due to the increased sensitive detection area and lower threshold, the scintillation detectors will provide a lower threshold for the detection of EASs [211], enabling the measurement of cosmic rays below the knee and increases the veto capabilities for studies of astrophysical neutrinos with IceCube [194].

Moreover, the hybrid array with its radio antennas will allow the measurement of the EM

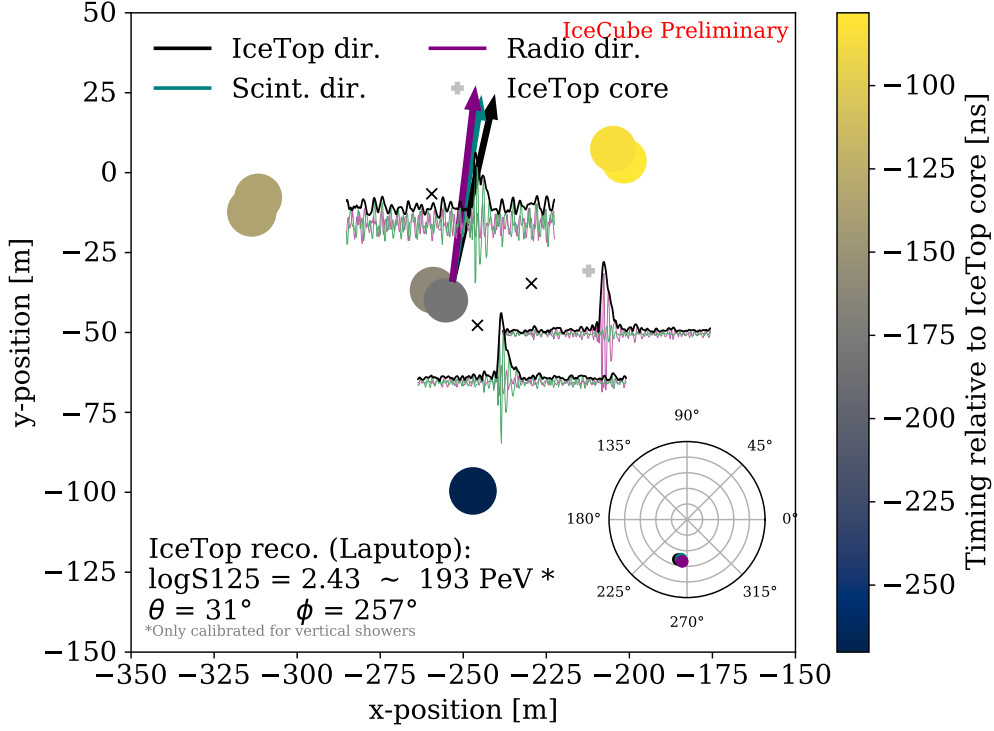


Figure 4.22.: Example EAS event observed with the prototype station. Charge and timing information of the scintillator hits are represented as size and color of the points, respectively. Radio antennas are shown as black crosses and include the measured waveforms. The reconstructed core position and directions are indicated as gray plus and arrows, respectively. Figure taken from [210].

shower energy and $X_{\max}$, which is of great interest for composition studies [212]. However, while the scintillators as effectively two-dimensional detectors are suitable for the measurement quasi-vertical showers, radio antennas are more sensitive to inclined showers and generally feature a higher energy threshold [213]. Therefore, the energy range between the knee and the second knee can be studied for a large range of zenith angles. In addition, the sensitivity to more inclined showers can further enhance the veto capabilities of the surface array. Since photon-induced air showers feature slightly stronger radio emission compared to primary hadrons, the radio array also allows searches for PeV photons [212]. A complete prototype station with the final IceTop enhancement design has been in operation since 2023 [108]. In the 2024/25 season, two new stations were deployed. Studies of EAS measurements with this small sub-array of the full SAE are ongoing at the time of writing. For hybrid detection of EASs with the SAE, the scintillation panels provide a trigger for the radio detectors. An example of a hybrid detection that includes a rudimentary reconstruction and is compared to IceTop is shown in Fig. 4.22.

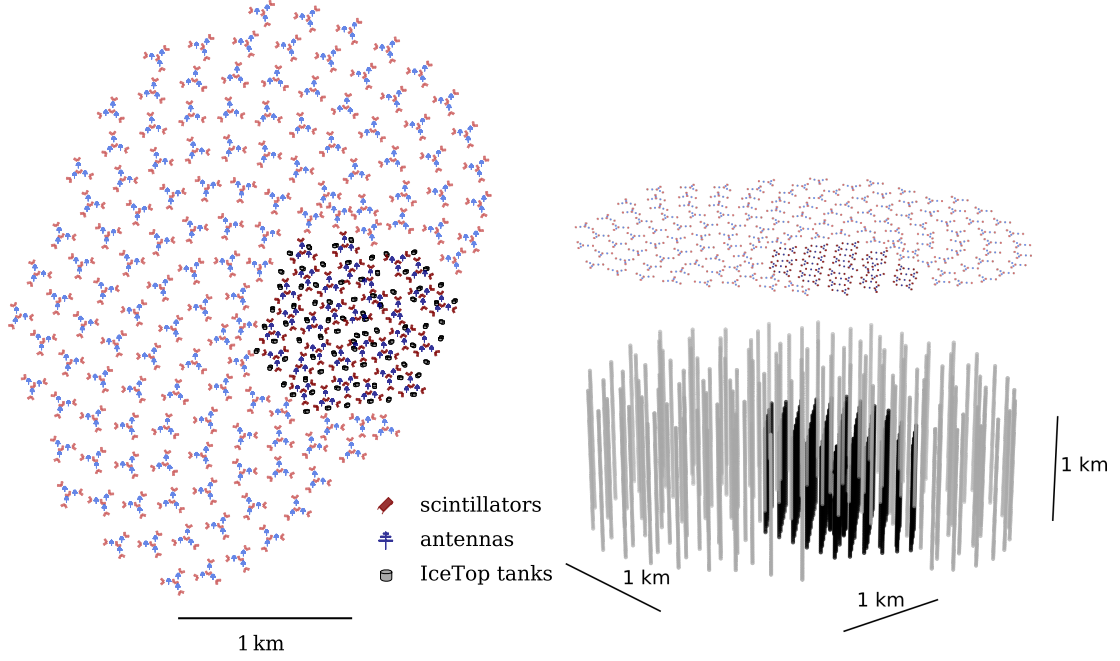


Figure 4.23.: Bird's eye view of the IceCube-Gen2 surface array (left) and the overview of the IceCube-Gen2 surface and in-ice optical array (right). Gray strings indicate Gen2 strings, while existing IceCube strings are shown in black. Right figure taken from [214].

4.5.2. IceCube-Gen2

The planned next-generation experiment, IceCube-Gen2, will extend the existing IceCube detector by three additional components. Namely, an in-ice radio and optical array that encompasses the existing in-ice array, and a surface array [198].

Increasing the detector volume by a factor of ~ 8 , the focus of the IceCube-Gen2 optical array is on high-energy neutrinos in the 10 TeV to 10 EeV range [215]. In total, the baseline design foresees the deployment of 120 new strings with 80 DOMs each and a spacing of 240 m. The planned DOM design for IceCube-Gen2 is expected to increase the light yield three times compared to IceCube DOMs [198]. The strings will be arranged in a sunflower geometry around IceCube as shown in Fig. 4.23.

The in-ice radio extension of IceCube-Gen2 (not shown in Fig. 4.23) will allow the measurement of the radio signal produced of in-ice showers produced by high-energy neutrinos. The radio array comprises 200 stations with shallow and sub-surface antennas and will be distributed over 500 km^2 [198]. This large effective volume features a detection threshold for neutrinos of $\gtrsim 30 \text{ PeV}$.

The IceCube-Gen2 surface array is planned to follow the footprint of the optical in-ice array. It employs surface stations that use the same design as for the SAE. It will act as both a veto for the in-ice array and as a standalone hybrid air shower observatory. Of particular interest for cosmic-ray analyses is the 30 times increase in aperture for coincident

events compared to IceCube [216]. The geometry of the IceCube-Gen2 surface array is illustrated in Fig. 4.23. The ~ 8 times increase in surface area, the IceCube-Gen2 surface array can measure EASs up to a few EeV, with an expectation of a few hundred events per year at ~ 1 EeV with coincident surface and in-ice information [198, 214]. Similar to the SAE, hybrid measurements can be of great benefit for composition analyses in the transition region [217].

Muon tank response

The reconstruction of air-showers is typically performed via the application of detailed likelihood methods. In the case of the IceTop standard reconstruction introduced in section 4.3.1, separate likelihood functions for the description of HLC signals, saturated and silent detectors, as well as for the shower front are employed and the combined negative log-likelihood is minimized to derive the characteristics of EASs. By construction, the standard reconstruction is dominated by the contribution of EM particles, as only HLC stations are included in the calculation of the likelihood, which occur mainly close to the shower axis. For the accurate description of individual shower components using the response of surface detectors, the corresponding underlying physical distributions have to be well understood. Due to the multiplicative character of the shower development, the fluctuations of the shower size are in first order proportional to the number of particles and are therefore log-normal distributed [8]. In addition to these shower-intrinsic fluctuations also detector-intrinsic fluctuations contribute to the measured signal spread. The latter are influenced by the energy spectrum of the arriving particles¹ contain fluctuations in the reflection and absorption of produced photons inside the tank as well as the possibility of the induction of small sub-showers. It is shown in [189], that the tank intrinsic fluctuations follow a Gaussian distribution in linear scale and are subdominant compared to the fluctuations of the shower size. Consequently, the total measured signal fluctuations are log-normal distributed. As discussed in more detail section 4.3.1, the expected signal distribution of EM particles is therefore also log-normal. This circumstance is therefore theoretically and experimentally motivated (see also section 7.3) and is crucial for the accurate description of the EM component of air showers measured with IceTop.

Since IceTop does not feature dedicated muon detectors, the EM and muon components need to be disentangled based on the corresponding detector response. In principal, the separation of the muon component becomes more straight forward at large distances from the shower axis where the relative contribution of EM particles decreases and, in the case of IceTop, the snow accumulation leads to an additional attenuation of the EM component. However, due to the stochastic nature of the shower development, a detailed

¹The bulk of the arriving particles are photons and electrons/positrons with energies $\lesssim 1$ GeV [189].

understanding of the underlying probability distributions is generally required for the separation of different shower components. Since this work aims to reconstruct the muon content in air showers measured with IceTop, the accurate modeling of the muon and EM signal probability distributions is crucial. As discussed, the case of the EM contribution, the signal probability distribution is well described by a log-normal distribution. However, due to their nature as minimum ionizing particles, muons exhibit a more complex signal response distribution. For this purpose, dedicated signal response simulations are produced to accurately model the underlying signal probability distributions of muons which can be used in a likelihood based reconstruction of the muon content described in chapter 6. Firstly, in section 5.1, the underlying physics of the IceTop tank response to muons is discussed. Successively, the techniques utilized for the production of tank response simulations to muons as well as the derivation of muon signal probability distributions are introduced in section 5.2. Further, the influence of the snow accumulation on top of the IceTop tanks on muons is studied in section 5.3. Lastly, various details of the average single muon response such as its dependence on the muon energy and inclination are characterized in section 5.4.

5.1. Probability density functions

In order to derive a likelihood function that can be used for the reconstruction of the muon component, dedicated IceTop tank response simulations are produced. For this purpose, muons with given multiplicity, inclination and energy are injected into IceTop tanks, followed by a simulation of the resulting energy deposit with Geant4 [218]. The choice of the energy and inclination of the injected muons is not entirely straightforward but can be optimized for a given analysis goal. Generally, either a fixed muon energy and inclination or an injection spectrum can be chosen. For all cases, muon response functions are derived and tested with respect to the observed reconstruction performance (see section 7.3). Fig. 5.1 (left) shows the muon energy spectrum at the observation level of the IceTop array for near-vertical showers ($\cos \theta_{\text{prim}} > 0.9$) with primary energies around 10 PeV for different hadronic interaction models. It is clearly visible, that all hadronic interaction models predict different shapes in the produced energy spectra due to the differences in the expected muon yields as a function of energy. The use of a particular muon energy spectrum for the production of tank response simulations therefore introduces a hadronic model dependence on the underlying signal model. In particular, for small muon energies, differences in the injection spectrum can have a significant impact on the resulting tank response model. This is due to muons that fall below the Cherenkov threshold before crossing the entire tank volume, which can be observed in the sub-GeV regime. These *stopping muons* contribute to the shape of the signal response, as their track length

inside the sensitive volume along which energy is deposited via Cherenkov radiation is correspondingly smaller. Depending on the muon energy and inclination, this results in an enhancement in low signal deposits. The second option is the injection of muons at a fixed energy. Since the muon spectra peak in the GeV range, an injection energy of 1 GeV has been chosen for the injection scenario with mono-energetic muons. Similarly to the energy distribution of muons produced in air-showers, both a zenith distribution as well as a fixed zenith angle can be considered. In the case of a fixed muon inclination, multiple options can be tested and evaluated in the context of the reconstruction performance. In a simplified model, the muon zenith angle can be approximated to the primary zenith angle, which is determined during the reconstruction algorithm. In reality, however, muons possess a finite spread around the primary axis, which can be described as

$$\sin \alpha = \frac{cp_t}{E_i} . \quad (5.1)$$

Here, α describes the muon angle with respect to the primary direction, p_t the transverse momentum and E_i the energy of the muon at the production point [61]. Thus, the magnitude of the muon angular spread depends on the muon energy. Fig. 5.1 (right) shows the angular spread distribution of atmospheric muons derived from CORSIKA simulations produced with Sibyll 2.1 as a function of muon energy at the observation level. For the injection scenario with mono-energetic (1 GeV) muons, a muon spread of around 10° is observed. For simplicity, only the muon response for fixed muon inclinations is produced and will be used as basis for the parametrization as a function of the muon zenith angle. Thus, the impact of the simplifying assumption of a negligible muon angular spread as compared to a parametrization of the muon spread can be tested at a later stage (see section 7.3).

For muon injection, the *topsimulator*² framework within the icetray software is utilized. It features both injection and detector response simulation services for different detector types. Relevant for the muon response parametrization use case is the single-particle injection into IceTop tanks using specific injection settings. A general overview of the injection parameters used for this work can be found in Tab. 5.1. In the case of the mono-energetic injection scenario, only 1 GeV muons are used. Furthermore, an additional margin of 2 m above the IceTop tank (injection height) is used for the injection. The injection height varies as a function of the snow height used in the simulation, ensuring a constant 2 m margin above the detector and snow volume. For the production of muon-energy spectrum-weighted response simulations, instead of a constant muon energy, muons are injected with a flat energy spectrum between 0.1 GeV and 100 GeV. In all scenarios, 10^5 muons are injected per zenith angle and per snow height to provide sufficient statistics for the response parametrization.

²<https://github.com/icecube/icetray/tree/main/topsimulator>

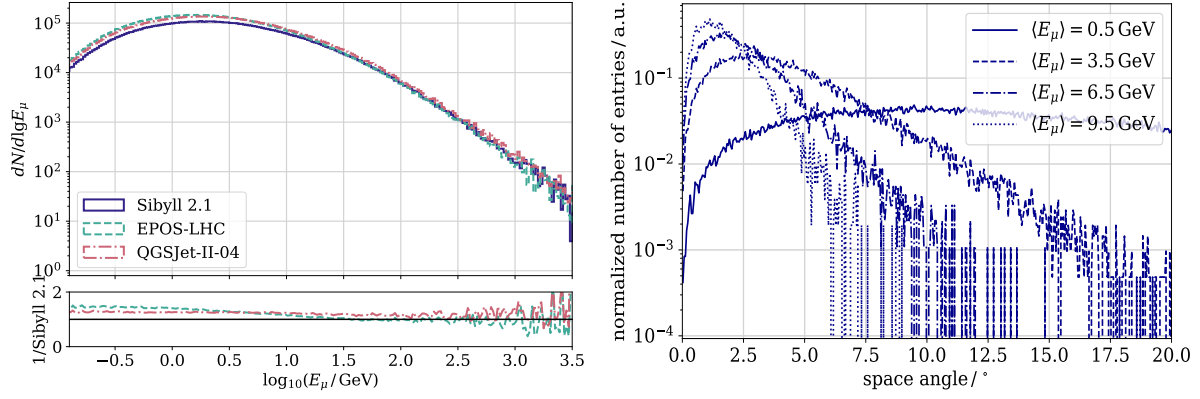


Figure 5.1.: Muon energy spectrum for different hadronic interaction models as derived from CORSIKA for proton- and iron-induced air showers around 10 PeV (left). The bottom panel shows the ratio of the energy spectra with respect to Sibyll2.1. Muon angle with respect to primary axis for different muon energies as indicated with the color scale (right).

Table 5.1.: Injection parameters for the muon spline production.

type	$E_{\mu,\text{inj}} / \text{GeV}$	n_{inj}	$h_{\text{inj}} / \text{m}$	$h_{\text{snow}} / \text{m}$	$\theta / ^\circ$	$\phi / ^\circ$
mono-energetic	1	10^5	$h_{\text{snow}} + 2$	[0,5]	[0,60]	[0,360]
muon spectrum	[0.1,100]	10^5	2	0	[0,60]	[0,360]

Fig. 5.2 illustrates the injection geometry used for all scenarios with the injection radius

$$r_{\text{inj}} = r_{\text{tank}} + (h_{\text{tank}} + h_{\text{inj}}) \tan(\theta). \quad (5.2)$$

For the purpose of this analysis, the injection algorithm is specifically adjusted to count only muons as hits for which the theoretical trajectory intersects the sensitive detector volume.

5.2. Spline fits

After the detector response simulation, the resulting probability density distributions for all different injection scenarios can be obtained from the calibrated tank pulse series. An example histogram for the injection of mono-energetic muons is shown in Fig. 5.3 (top left). It can be clearly observed that the muon signal response is in first order a function of the detector geometry. The position of the peak as a function of the muon inclination scales with $1/\cos\theta$, since the muon track length increases accordingly. Naturally, this is only true for a sufficiently high muon energy, which is necessary for the emission of

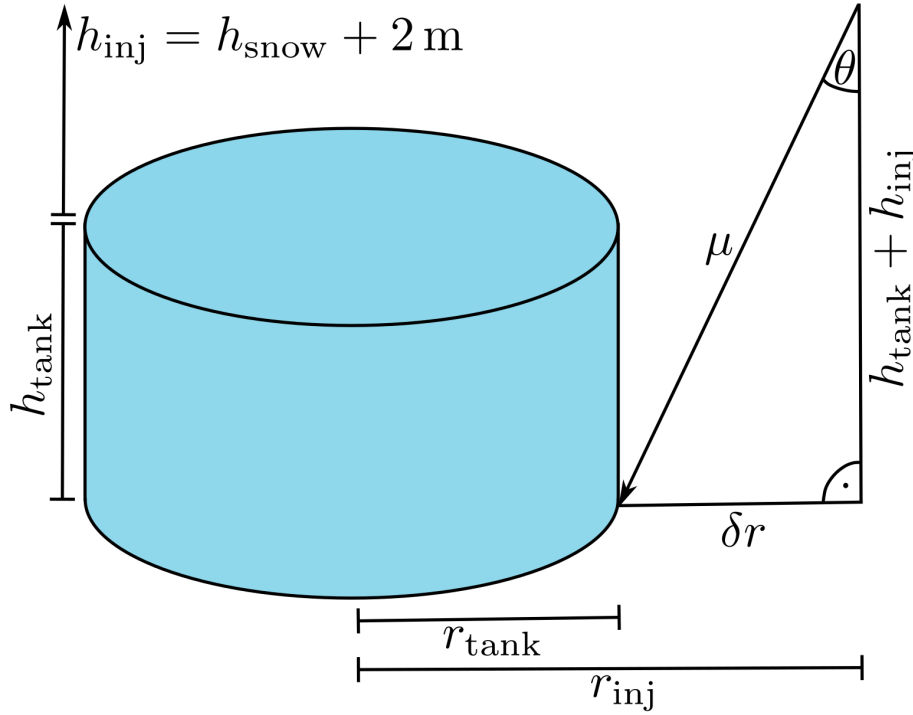


Figure 5.2.: Illustration of the injection geometry used for the muon response simulation.

Cherenkov radiation along the entire track. This can be easily observed in the mean signal deposit as a function of the muon energy in Fig. 5.6 (left). For a muon energy of 1 GeV, the tank response is, in good approximation, a function of the track length inside the tank even for realistic snow heights. However, even for sub-GeV muons of $E_\mu \gtrsim 200 \text{ MeV}$, a mean signal of 0.7 VEM is observed. The variation in snow levels from tens of centimeters to $\sim 2 \text{ m}$ for the year 2012 results in lower energy muons contributing to the observed muon peak in the measured data [199]. For muon energies sufficient to produce Cherenkov radiation across the entire sensitive volume, the Cherenkov yield increases with the muon energy. The contribution of muons passing through only the edge of the tanks increases with increasing muon inclination. These *corner clipping muons* result in small signal deposits due to their smaller track length inside the sensitive volume. Overall, this leads to a larger spread of the tank response distributions for inclined muons. This attribute is incorporated into the signal likelihood calculation by means of the muon signal uncertainty (see section 6.3). For a muon injection that follows an assumed energy spectrum, the resulting response distribution exhibits only minor differences compared to the mono-energetic scenario. This is due to the fact that, for the latter, a muon energy of 1 GeV is chosen. This energy regime around 1 GeV contains the peak of the energy regime which consequently has the largest impact on the resulting response distribution. Muons that are injected with energies above a few GeV to tens of GeV range lead to an increased contribution of larger signal deposits. Additionally, a slightly enhanced contribution at low signal deposits arises, caused by the influence of sub-GeV muons. The

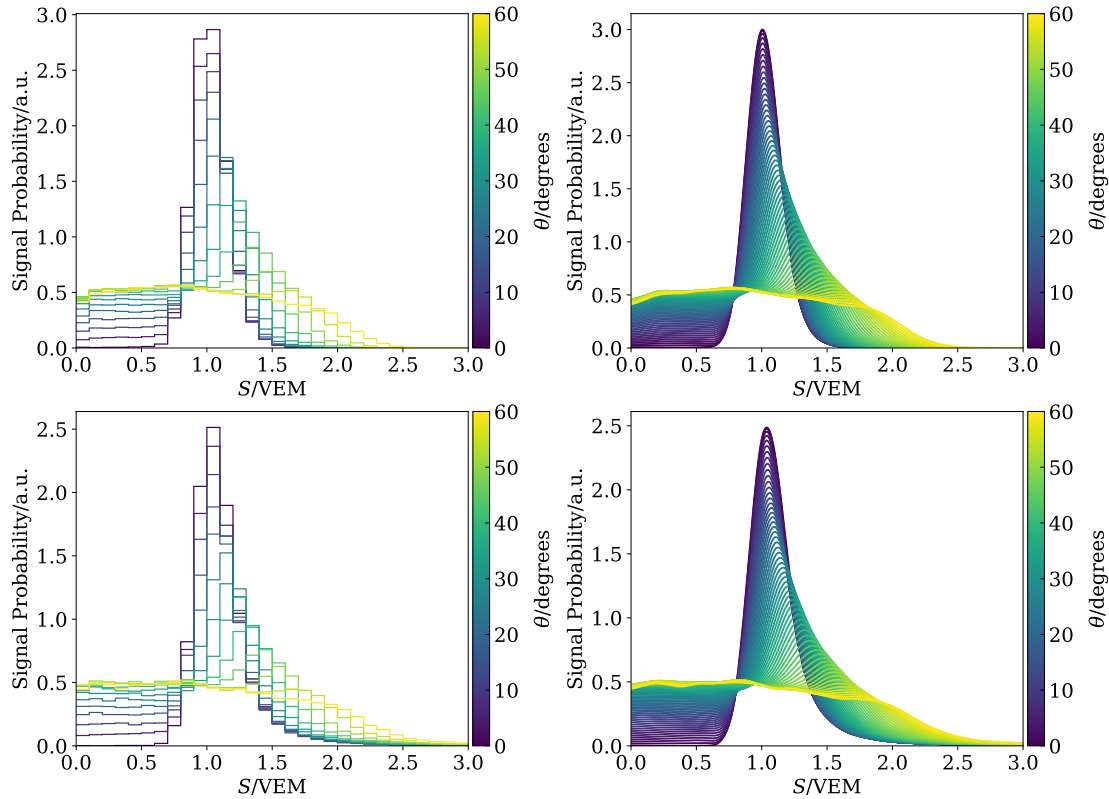


Figure 5.3.: Probability density distribution for tank response simulations for the injection of one 1 GeV muon (top left) and muons weighted an energy spectrum based on Sibyll 2.1 (bottom left) at different inclinations. The corresponding spline fits to the tank response distributions as a function of muon inclination are shown in the right column.

differences between the probability distributions for both scenarios is further discussed in section 5.4.

For each muon number, the probability distribution is then fitted using B -splines. The resulting spline fits for the mono-energetic scenario and the spectrum-weighted distribution for the injection of one muon as a function of inclination are shown in Fig. 5.3. The fitting itself is performed via *photospline*³, a specialized framework for the application of penalized spline fits (see [219] for details) using B -splines.

B-spline fitting

In general, B -splines can be applied as non-parametric descriptions [219] in a variety of use cases. B -splines (*basic splines*) are comprised of piecewise polynomials of degree p connected by a set of breaking points. These *knots* partition the polynomials, defining sections at which the polynomials join. A combination of piecewise polynomials of degree

³<https://github.com/icecube/photospline>

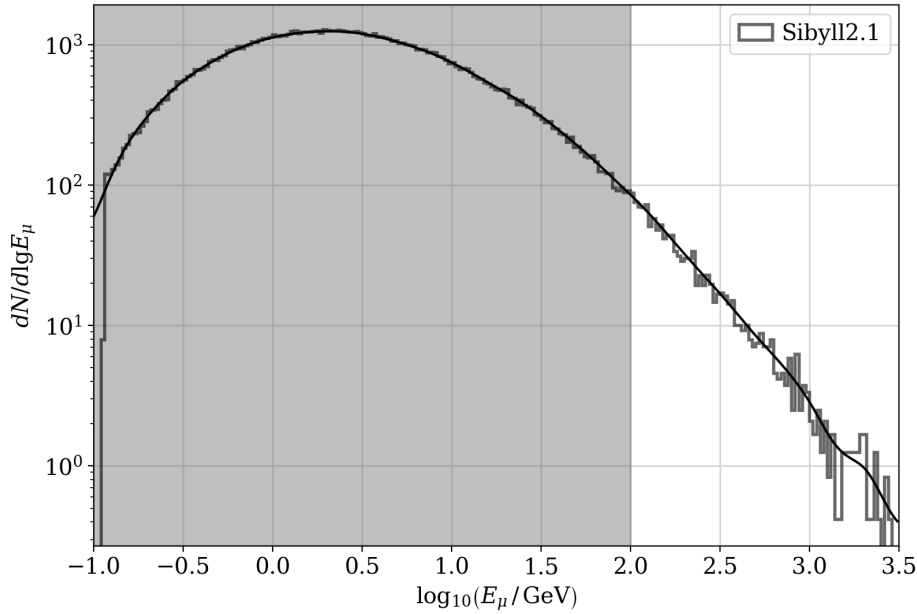


Figure 5.4.: Muon energy spectrum for Sibyll2.1 with corresponding spline fit (black line). The grey area indicates the muon energy sampling for the spectrum-weighted muon spline production.

p would thus define a B -spline of order $p - 1$ [220]. Since the choice of knots determines the position of a B -spline, a custom ensemble of knots is used for the application on the muon tank response. In combination with the specialized fitting penalty based on the differences of the coefficients of neighboring B -splines [219], this results in stable spline fits. The objective function for the spline fit can then be written as [219]:

$$S = \sum_{i=1}^m \left[y_i - \sum_{j=1}^n a_j B_j(x_i) \right]^2 + \lambda \sum_{j=k+1}^n (\Delta^k a_j)^2, \quad (5.3)$$

where (x_i, y_i) describe the set of m points which are to be fit by a set of n corresponding B -splines, B_j . The latter are constructed as linear combinations with the coefficients a_j . The first sum in Eq. (5.3) describes the least squares part of the objective function. The second sum is the corresponding penalty term utilizing the derivative of order k . The influence of the penalty term can be adjusted in a continuous manner by means of a smoothness parameter λ which, again, is tuned for the application to the tank response distributions. The spline fit settings for different muon multiplicities in the injection are presented in Tab. 5.2⁴. It should be noted, that different smoothness parameters are applied for each dimension depending on the muon multiplicity. As the shape of the muon signal PDFs become broader for higher multiplicities and with increasing zenith angles, this ensures sufficient accuracy of the spline fits while preventing overfitting. A

⁴The settings for the three-dimensional, snow dependent spline fits differ slightly and are shown in App. A.

Table 5.2.: Spline fit settings for the application on muon tank response distributions as a function of signal strength and zenith angle.

n	signal bin step size / VEM	number of knots		smoothing factor	
		signal	zenith	signal ($\cdot 10^{-5}$)	zenith ($\cdot 10^{-7}$)
1	0.1	218	21	1.0	100.0
2	0.15	218	21	1.0	50.0
3	0.2	226	21	10.0	50.0
4	0.15	233	21	10.0	50.0
5	0.3	234	21	10.0	50.0
6	0.35	241	21	100.0	50.0
7	0.4	240	21	100.0	50.0
8	0.45	246	21	100.0	10.0
9	0.5	250	21	100.0	10.0
10	0.55	256	21	100.0	5.0
11	0.6	260	21	100.0	5.0
12	0.65	266	21	100.0	5.0
13	0.7	270	21	100.0	5.0
14	0.75	276	21	100.0	5.0
15	0.8	280	21	100.0	5.0

more detailed overview of the custom knot placement can be found in App. A.

In case of the flat muon injection spectrum, the probability density is derived by applying weights to each muon as determined from the muon-energy spectrum shown in Fig. 5.4 to resemble a muon PDF based on a realistic spectrum. For the spline fits, additional weights are assigned to each probability density value according to their Poisson uncertainty. The resulting spline fit for one muon as a function of the muon inclination is shown in Fig. 5.3 (right). With the chosen smoothing, bin size, and knot settings, accurate and smooth spline fits are achieved for all simulated multiplicities and zenith angles (see Fig. A.1).

The B -splines defining the muon signal PDFs are saved using the *photospline* framework, which can be utilized within the reconstruction framework to retrieve the probability of observing a particular amount of muons, $p_{\mu,\text{sig}}(S|\theta, n)$, given a measured signal strength

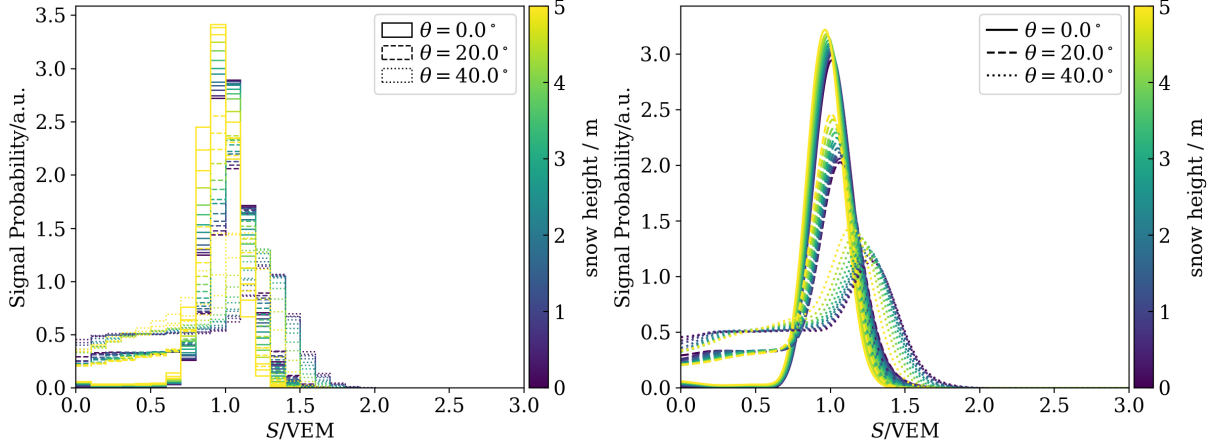


Figure 5.5.: Average signal deposit for vertical muons as a function of muon energy (left). The color code indicates different snow heights on top of the IceTop tank. Evolution of the muon spline fits for 1 GeV muons for two different inclinations as a function of snow height (right).

and zenith angle.

5.3. Snow attenuation

In Fig. 5.6 (left) it is shown, that the average signal deposit produced by vertically traversing muons is in good approximation constant for snow heights relevant for this work. However, for inclined muon tracks, the snow attenuation may prevent the muons from traversing through the entire tank volume. This can affect the average value as well as modify the muon signal PDF. To gauge the influence of different snow heights on the resulting muon signal PDFs, dedicated tank response simulations are produced in addition to the mono-energetic and spectrum-weighted scenarios. For computational reasons, the production of snow-dependent muon spline fits is limited to mono-energetic muons of 1 GeV. However, since this energy roughly corresponds to the peak of the muon energy spectrum, this simplification is sufficient to gauge the impact of the snow attenuation on the muon tank response. For the production of snow-dependent splines, the fits need to be performed with an additional snow height dimension. For this reason, the snow height for the tank response simulations is varied in steps of 0.5 m from no snow to 6 m of snow accumulation. The muon injection height is adjusted accordingly to keep a constant offset of 2 m above the snow level (see Tab. 5.1). Fig. 5.5 (left) shows the resulting probability distribution as a function of snow height for three different inclinations. The corresponding spline fits are shown in the right figure. A clear shift of the muon response distributions can be observed towards lower signal deposits caused by the attenuation of

muons through the snow. This effect is stronger for higher muon inclinations, as the track length through the snow increases. At the same time, the contribution of small signals decreases slightly as a function of snow height for muons with inclined tracks. In the relevant range for this work, i.e., for snow heights $\lesssim 2$ m, the form of the spline fits does not differ significantly compared to the case of no snow attenuation. The introduction of an additional snow dependence is therefore not expected to be of significant importance for the application of the muon signal PDFs as the basis of the advanced air-shower reconstruction introduced in chapter 6. It should be noted, however, that due to the increasing snow accumulation over the years, the validity of the assumption of a negligible muon attenuation through the snow decreases. For studies of more recent years, the importance of a snow-dependent muon signal model has increased. This is emphasized by the more rapid change of the response distributions for snow heights in the multiple-meter range. In particular the energy threshold required for muons to produce Cherenkov emission along their entire track is modified significantly by a large snow accumulation and should be tuned for each year. The influence of additional snow dependence on the underlying muon probability distributions will be studied further in section 7.3.

5.4. Average single muon response

A significant difference between the production of muon response distributions between the spectrum-weighted and the mono-energetic scenario is the presence of sub-GeV muons. For these muons, the energy can be too small for the production of Cherenkov radiation along their entire track inside the sensitive detector volume. With increasing snow accumulation on top the tanks, this threshold also shifts to larger muon energies. In order to produce Cherenkov radiation, the kinetic energy of a muon is required to be above the Cherenkov threshold. Thus, the particle velocity must exceed the phase velocity of light in the medium, $\beta > c/\eta$, classified by the refractive index η . The Cherenkov threshold for a muon can therefore be calculated via relativistic kinematics [221]

$$T_{\mu,\text{Ch}} = m_{\mu} \left(\frac{\eta}{\sqrt{\eta^2 - 1}} - 1 \right), \quad (5.4)$$

with the mass of the muon, $m_{\mu} \approx 106$ MeV. For modeling IceTop tanks, the ice is assumed to have a refractive index of 1.33 [222]. The Cherenkov threshold for muons observed with IceTop, therefore, computes to $T_{\mu,\text{Ch}} \approx 55$ MeV. To produce Cherenkov radiation along their entire track, the kinetic energy of muons is required to lie above this threshold until they eventually leave the sensitive detector volume. For this reason, ionization losses of the muons crossing the detector have to be considered to estimate a corresponding threshold. Assuming a typical ionization loss of 2 MeV/cm, the density of the ice inside

the tank of 0.92 g/cm^3 [171], and a height of the ice volume inside the tank of 90 cm, the total ionization loss of a vertically traversing muon is of the order

$$E_{\text{Ion},0^\circ} \approx 2 \text{ MeV} \frac{\text{cm}^2}{\text{g}} \cdot 0.92 \frac{\text{g}}{\text{cm}^3} \cdot 90 \text{ cm} \approx 166 \text{ MeV}. \quad (5.5)$$

The energy threshold required to produce Cherenkov photons along a vertical track therefore is

$$E_{\mu,\text{min},0^\circ} = T_{\mu,\text{Ch}} + E_{\text{Ion},0^\circ} \approx 221 \text{ MeV}. \quad (5.6)$$

For muons traversing the tank on an inclined track, this energy threshold can be simply modified by the increasing ionization loss

$$E_{\text{Ion},\theta} \approx 2 \text{ MeV} \frac{\text{cm}^2}{\text{g}} \cdot 0.92 \frac{\text{g}}{\text{cm}^3} \cdot 90 \text{ cm} / \cos \theta. \quad (5.7)$$

Considering additionally the snow accumulation on top of the IceTop tanks, the energy threshold is further shifted toward higher energies due to the additional ionization loss muons undergo when passing through the snow. The additional energy loss is calculated using the density of the South Pole snow, which is estimated at 0.38 g/cm^3 [171]. The resulting energy threshold for muons to produce Cherenkov radiation along their entire path through the sensitive detector volume as a function of their inclination and the snow accumulation is shown in Fig. 5.6 (right). Clearly, the threshold energy is sensitive to the muon inclination as the muon track length inside the sensitive volume increases. This is even more important for large snow accumulations. Among others for this reason, this work focuses on near-vertical air showers and only uses MC simulations and measured data from 2012, where maximum snow heights of $\sim 2 \text{ m}$ are observed. In future analyses including data from more recent years, the snow attenuation of muons and the resulting increase of the threshold energy has to be considered in more detail. The average signal deposit of vertical muons obtained from the tank response simulations is shown in Fig. 5.6 (left) as a function of the muon energy and snow accumulation. For the purpose of this study, a different set on tank response simulations with a lower statistic of 1000 injected muons per muon energy is produced. Muon energies are sampled from 0.1 GeV to 2 GeV in steps of 100 MeV for snow heights up to 5 m . The error bars of the resulting average signal deposits illustrate the corresponding standard deviation. For muons in the sub-GeV range, the impact of the muon threshold energy is clearly visible and shifts toward higher energies with increasing snow height. However, as motivated in [199] and validated by Fig. 5.6 (left), already above $\sim 210 \text{ MeV}$, muons have a significant impact on the muon peak observed for near-vertical air showers for negligible snow heights. For snow heights around 2 m , the muon energy required to contribute to the muon peak increases to $\sim 420 \text{ MeV}$. In fact, for muons above these energies and snow heights below 2 m , the average signal response roughly levels around 1 VEM . Therefore, the tank response for such muons can be approximated as a function of the tank geometry. With increasing

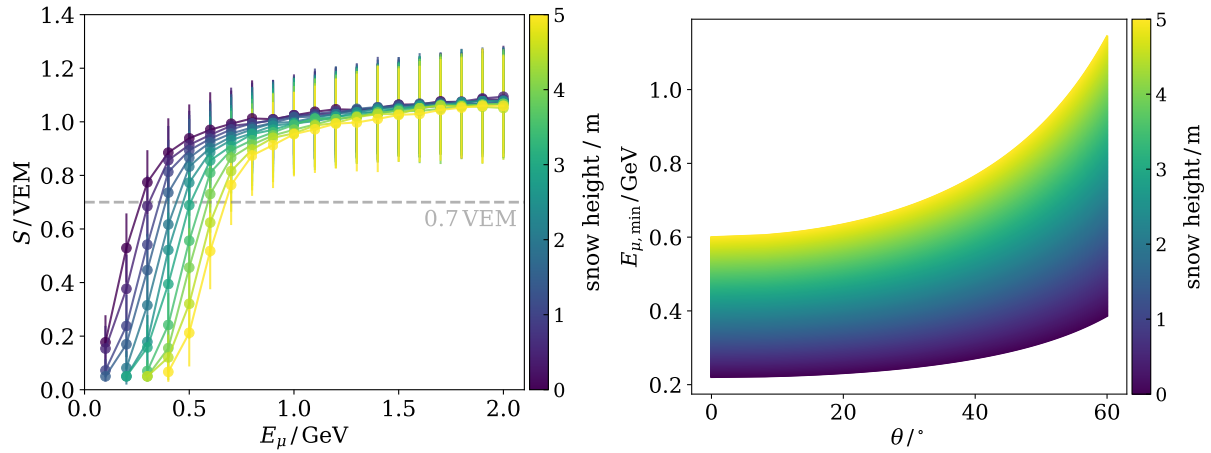


Figure 5.6.: Average signal deposit for vertical muons as a function of muon energy (left). The color code indicates different snow heights on top of the IceTop tank. Muon energy threshold for the production of Cherenkov radiation along the entire track through the sensitive volume as a function of the muon inclination and the snow accumulation on top of the detector (right).

muon energies, the muon energy loss increases as well, leading to a slight increase in the number of Cherenkov photons produced [223].

5.4.1. Average track length

Based on Fig. 5.6, the signal response to muons exceeding the energy threshold is assumed to be a function of their track length. To test this assumption, the average muon track length can be derived based on analytical calculations and compared to the signal response obtained from simulations. This is of particular importance for the derivation of the muon signal uncertainty, for which the variation of the muon track lengths contribute significantly to the measured signal fluctuations. A detailed derivation of the average track-length distribution along with their fluctuations as discussed in the following can be found in [224]. In this simplified response model, it is assumed that the muon response is purely a function of the tank geometry. For this purpose, the geometry of a Cherenkov tank can be decomposed in three components describing different case scenarios for muon trajectories through the tank. Fig. 5.7 (left) illustrates the three components, the *lid-base* (lb), the *lid-lateral* (li), and the *lateral-lateral* (la) components. These components refer to the cases of muons traversing the tank from the lid to the base, from the lid to the side

of the tank (lateral), and from side to side, respectively. Using the unit-less variables⁵

$$\begin{aligned} l &= \frac{l_{\text{track}}}{2r_{\text{tank}}}, \\ h &= \frac{h_{\text{fill}}}{2r_{\text{tank}}}, \end{aligned} \quad (5.8)$$

the track-length distribution can be expressed as the sum of all three components:

$$p(l, \theta) = p_{\text{lb}}(l, \theta)P(\text{lb}, \theta) + p_{\text{li}}(l, \theta)P(\text{li}, \theta) + p_{\text{la}}(l, \theta)P(\text{la}, \theta). \quad (5.9)$$

Here, $p_i(l, \theta)$ represent the probability distribution functions for the different components, and $P(i, \theta)$ are the corresponding case probabilities. The latter can be derived as

$$\begin{aligned} P(\text{lb}, \theta) &= \frac{a_{\text{lb}}(\theta)}{a(\theta)}, \\ P(\text{li}, \theta) &= \frac{a_{\text{li}}(\theta)}{a(\theta)}, \\ P(\text{la}, \theta) &= \frac{a_{\text{la}}(\theta)}{a(\theta)}, \end{aligned} \quad (5.10)$$

with the partial areas, $a_i(\theta)$, of the three components as a function of zenith angle and in relative units analogously to the Eq. (5.8) (see [224] for details). The normalization, $a(\theta)$, is defined in units of the tank area for vertical incidence ($A_{\text{tank}} = \pi r_{\text{tank}}^2$):

$$a(\theta) = \frac{A_{\text{tank,eff}}}{A_{\text{tank}}}, \quad (5.11)$$

with the effective tank area, $A_{\text{tank,eff}}$, that is, the tank area projected along the incident direction:

$$A_{\text{tank,eff}} = \pi r_{\text{tank}}^2 \cos \theta + 2r_{\text{tank}} h_{\text{tank}} \sin \theta. \quad (5.12)$$

The probability distribution functions for the different components are given by [224]

$$\begin{aligned} p_{\text{lb}}(l, \theta) &= \delta(l - l_{\text{max}}), \\ l_{\text{max}} &= \begin{cases} h / \cos \theta & , \tan \theta \leq 1/h \\ 1 / \sin \theta & , \text{else,} \end{cases} \\ p_{\text{li}}(l, \theta) &= \frac{1}{a_{\text{lb}}(\theta)} \begin{cases} 4/\pi \sin(2\theta) \sqrt{1 - (l \sin \theta)^2} & , 0 \leq l \leq l_{\text{max}} \\ 0 & , \text{else,} \end{cases} \\ p_{\text{la}}(l, \theta) &= \frac{1}{a_{\text{la}}(\theta)} \begin{cases} \frac{4[l \sin^3 \theta (h - l \cos \theta)]}{\pi \sqrt{1 - (l \sin \theta)^2}} & , 0 \leq l \leq l_{\text{max}} \\ 0 & , \text{else.} \end{cases} \end{aligned} \quad (5.13)$$

⁵The original track-length distribution as a function of l_{track} can be recovered via $p(l_{\text{track}}, \theta) = (2r_{\text{tank}})^{-1} p(l, \theta)$ [224].

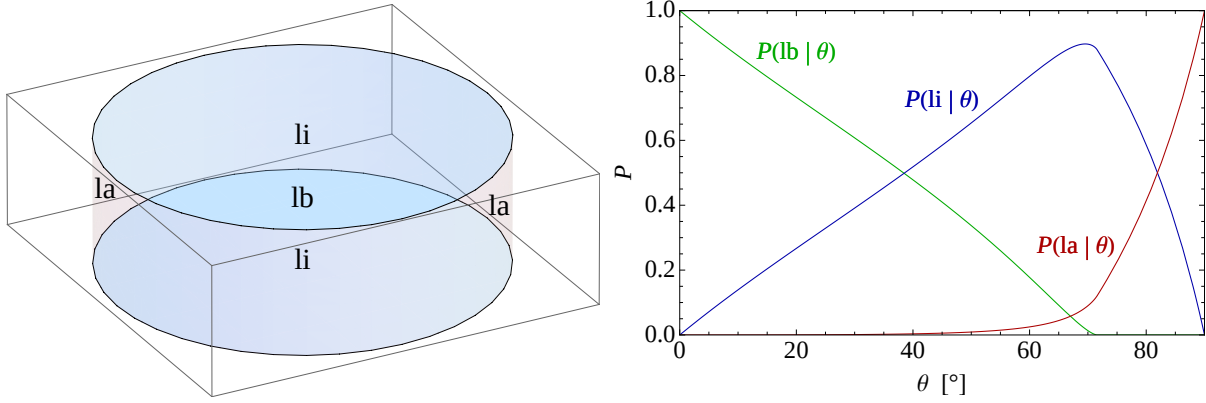


Figure 5.7.: Projection of the tank along the muon direction ($\theta = 50^\circ$) with a distinction of the three different components to the track-length distribution (left). Corresponding case probabilities for the three components as a function of muon inclination (right). Figures taken from [224].

In the case of muons traversing the tank from the lid to the bottom, the probability density distribution is a simple delta function determined by the maximum muon track length, $l_{\max}$. Fig. 5.7 (right) shows the case probabilities as a function of zenith angle. For vertical muons, only the lid-base trajectory contributes to the track-length distribution. For more inclined muons, the lid-lateral term becomes increasingly important and eventually has a higher contribution than the lid-base term for $\theta \gtrsim 40^\circ$. This leads to a constant increase in the width of the muon signal PDFs derived from tank response simulations as shown in Fig. 5.3. Muons crossing the tank from side to side only significantly contribute to the track-length distribution for zenith angles above $\sim 60^\circ$ and are therefore not relevant for the analysis presented in this work. The average track length can be derived simply by dividing the tank volume, $V_{\text{tank}} = h_{\text{tank}} \pi r_{\text{tank}}^2$, by the effective tank area [224]:

$$\langle l_{\text{track}} \rangle(\theta) = \frac{V_{\text{tank}}}{A_{\text{tank,eff}}} = \frac{h_{\text{tank}}}{\cos \theta + 2h_{\text{tank}} \sin \theta / (\pi r_{\text{tank}})}. \quad (5.14)$$

Therefore, in the approximation that all muons cross the entire tank along their trajectory, the volume of the tank is given by the multiplication of the average track length with the projected area of the tank. This is because the tracks of muons that arrive as a particle disc that covers the entire detector can be viewed as small volume elements ($dV = l_{\text{track}} dA$) that add up to the entire volume of the tank [224].

5.4.2. Muon energy dependence

To derive the average signal response for single muons as a function of zenith angle, the muon signal response shown in Fig. 5.3 is used to obtain the weighted average and

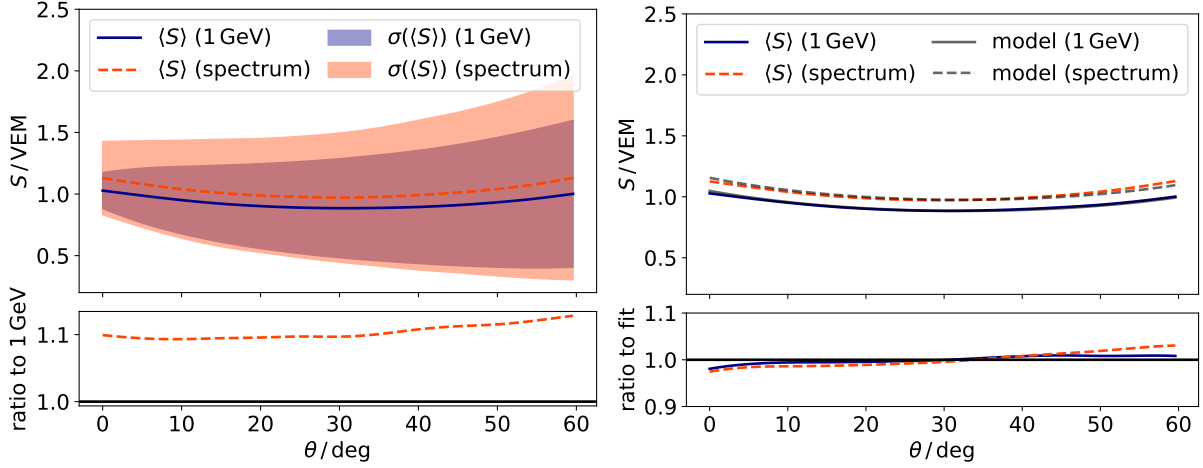


Figure 5.8.: Average single muon response and standard deviation for IceTop tank response simulations for injected 1 GeV muons and a realistic muon energy spectrum as a function of zenith angle (left). The lower panel shows the ratio between the corresponding average values. Small fluctuations in the ratio are caused by imperfections in the spline fits. Average signal responses fit with the idealized model Eq. (5.16) based purely on the tank geometry (left). The ratio to the model is shown in the lower panel.

standard deviation

$$\begin{aligned} \langle S \rangle &= \frac{\sum_{k=1}^N w_k s_k}{\sum_{k=1}^N w_k}, \\ \sigma(\langle S \rangle) &= \sqrt{\frac{\sum_{k=1}^N w_k (s_k - \langle S \rangle)^2}{\sum_{k=1}^N w_k}}, \end{aligned} \quad (5.15)$$

where the weights, w_k , are the values of the muon signal PDFs in each signal bin s_k . Both quantities can be described by spline fits in one dimension using the setup described for the muon signal PDFs. The settings used for the spline fits is listed in Tab. 5.3

The average single muon response and standard deviation are shown in Fig. 5.8 (left) for the mono-energy and muon-spectrum weighted scenario. As the zenith angle increases, the average signal for the mono-energy scenario first decreases from ~ 1 VEM to ~ 0.9 VEM around 30° and then starts to increase again. For the spectrum-weighted tank response, the same zenith dependence is observed, however, with a signal offset of ~ 0.1 VEM. This offset is caused by influence of muons in the multiple GeV energy regime and above, which lead to an increased number of observed Cherenkov photons. Under the assumption that the muons cross the entire tank and produce Cherenkov radiation along their full trajectory, the average muon signal response can be described by [225]

$$\langle S \rangle(\theta) = p_S \cdot \langle l_{\text{track}} \rangle(\theta), \quad (5.16)$$

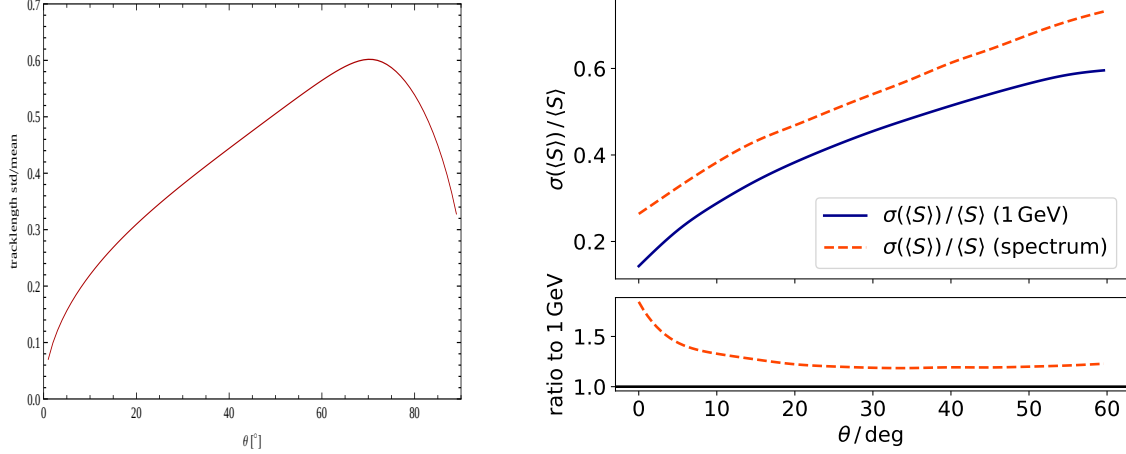


Figure 5.9.: Relative standard deviation, $\sigma(p(l_{\text{track}}, \theta))/\langle l_{\text{track}} \rangle(\theta)$, obtained for the analytical track-length model as a function of zenith angle (left). Figure taken from [224]. Relative standard deviation obtained for the tank response simulations for injected 1 GeV muons and a realistic muon energy spectrum as a function of zenith angle (right). The ratio between them is shown in the lower panel.

with the average track length given by Eq. (5.14) and an arbitrary offset parameter, p_S [VEM/m], that accounts for the signal scaling. Fig. 5.8 (right) shows the average signal response for the mono-energy and spectrum-weighted scenarios compared to corresponding fits with Eq. (5.16). For the mono-energy, the muon signal response is well described by the analytical model over the entire zenith range and is therefore in agreement with the expectation of a purely geometry-based muon response. However, for the spectrum-weighted scenario small deviations from the idealized signal model are visible. This is due to the presence of sub-GeV muons and muons in the multiple GeV range and above. For the former, muons can fall below the Cherenkov threshold before crossing the entire sensitive detector volume and they produce a smaller amount of Cherenkov photons compared to muons in the GeV range. For the latter, the combination of a larger amount of produced Cherenkov radiation and an increased track length leads to a slightly larger average signal compared to the idealized model. Therefore, in this scenario, the underlying assumptions of Eq. (5.16) are not strictly valid. Nevertheless, in first order, the muon signal response can be approximated as a function of the tank geometry for both scenarios.

A relevant quantity for the utilization of the muon tank response simulations is the relative standard deviation, as it describes the relative uncertainty for a given average muon signal. The signal uncertainty is incorporated into the likelihood function used in the reconstruction procedure (see section 6.3) and therefore effectively influences the relative weighting of a given expected muon signal. The relative standard deviation obtained from the idealized track-length based response model is illustrated in Fig. 5.9 (left) as a

Table 5.3.: Spline fit settings for the application on the average signal response and its standard deviation as a function zenith angle.

zenith bin (min,max,step) / $^{\circ}$	number of knots	knot settings (min,max,step) / $^{\circ}$	zenith smoothing factor
(0,1.047,0.087)	21	(-0.349,1.396,0.087)	10^{-12}

function of the zenith angle. For the zenith angle range relevant for this work, the relative standard deviation increases smoothly as a function of inclination. Only above $\theta \gtrsim 70^{\circ}$, the probability of muons crossing the tank from side to side increases rapidly, which leads to a decrease in the relative fluctuations of the track length. A similar behavior is visible in the relative standard deviation obtained from the muon tank response simulations (see Fig. 5.9 (right)). However, the magnitude of the relative standard deviation is overall larger compared to the idealized model, since the detector response includes the simulation of optical properties of the tank, such as the DOM efficiency and the reflectivities of the inner tank surfaces [171]. In the case of the spectrum-weighted scenario, the relative standard deviation is significantly larger for near-vertical muons. This is because, due to the energy dependence in the yield of Cherenkov photons, sub-GeV muons have a larger relative impact at small inclinations. The influence of the increase in the relative uncertainty relative to the mono-energy scenario is studied further in section 7.3.

Additionally, taking into account snow accumulation on top of the IceTop tank further influences the average muon signal response. Fig. 5.10 (left) shows the average muon signal and its standard deviation as a function of zenith angle and snow height as obtained from the tank response simulations with additional snow height dependence. Due to attenuation, the average muon signal decreases with increasing snow accumulation. As a consequence, the phase space for the signal fluctuations also decreases. Because of the interplay between snow attenuation and the muon-energy dependent yield of Cherenkov photons, the exact evolution of the average muon response and its standard deviation is not trivial. Although the signal spread decreases smoothly as a function of snow height, the difference in the average muon signal reaches its minimum between $20^{\circ} - 30^{\circ}$, depending on the snow height. This is likely caused by the decrease in the average track length up to $\theta \sim 30^{\circ}$ in combination with the energy dependent signal response. As the average track length decreases, the differences in the average signal decrease as well (see Fig. 5.8 (left)). The relative standard deviation as a function of zenith angle and snow height is shown in Fig. 5.10 (right). Except for the region below $\sim 3^{\circ}$, the relative standard deviation decreases with increasing snow heights. For inclinations $\lesssim 3^{\circ}$, the

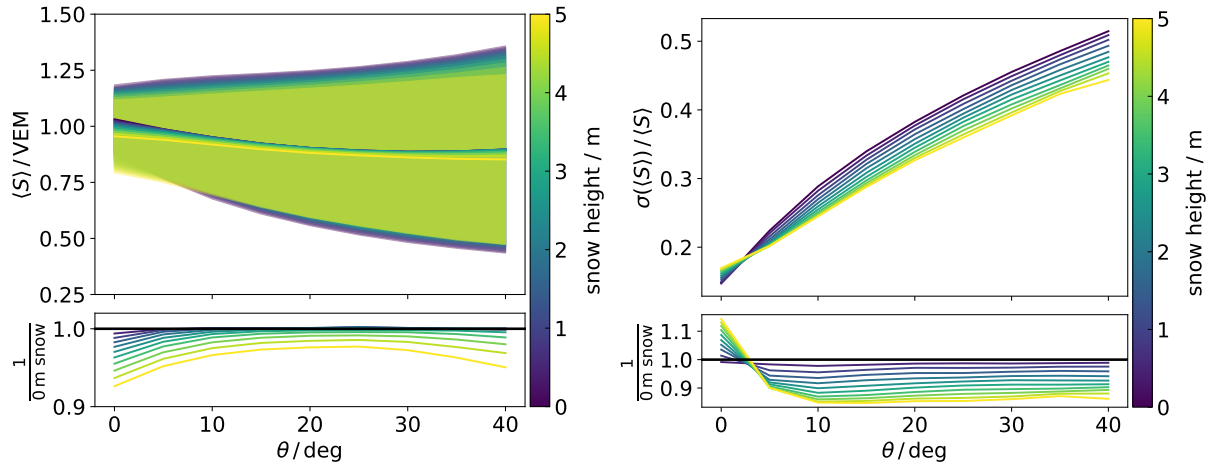


Figure 5.10.: Average single muon response (lines) and standard deviation (shaded areas) for IceTop tank response simulations for injected 1 GeV muons as a function of zenith angle and snow height (left). The lower panel shows the ratio of the average signals to one obtained without snow. Corresponding relative standard deviation as a function of zenith angle and snow height. The ratio to the no-snow scenario is shown in the lower panel (right).

average signal is likely influenced by scattered muons that only traverse the edge of the detector and deposit a very small signal⁶. For zenith angles above $\sim 10^\circ$, the relative fluctuations decrease roughly constantly with increasing snow height. However, for snow heights relevant for this work, the difference to the no-snow scenario is only on the order of a few percent. For analyses using data of more recent years and, in particular, for IceCube-Gen2, the effect of muon attenuation can not be neglected and has to be studied in more detail.

The effects of different assumptions compared the mono-energetic scenario and the simplified muon inclination model are re-visited in section 7.3.

⁶The tank response simulation only requires the initial path of the injected muons to hit the sensitive volume of the detector. For inclined muons, the effect of muons that do not hit the detector is small compared to corner clipping muons.

Two-component LDF

In the previous chapter, the underlying probability distributions of the signal response to EM particles and muons is introduced. The obtained signal PDFs are required for reconstruction of the corresponding shower components using a likelihood-based approach. As discussed in sections 3.5 and 4.3.1, these reconstruction methods are usually based on the description of the signal and time lateral distributions with dedicated model functions. The event-by-event reconstruction of the muon content requires the separation of the EM and muon signal distributions¹ for single events. For this purpose, two separate LDFs are employed for the two shower components which are fit simultaneously using a combined likelihood function. A first version of this approach was introduced in [193, 226, 227, 228]. In this chapter, the technical details of this *two-component* approach are discussed. Since the two-component approach requires separate model functions for the description of the EM and muon components, corresponding candidate functions are introduced in section 6.1 tested for their ability to describe the expected lateral distributions through parameter optimizations in section 6.2. Finally, a detailed overview of the implementation of the two-component likelihood approach is given in section 5.3.

6.1. Lateral distribution function

Typically, to model the particle density distribution generated by air-shower events and observed as deposited charge in particle detectors (expressed in units of VEM in the case of IceTop), a lateral distribution function (LDF) is used. Generally, an LDF describes the particle density as a function of lateral distance at a given observation level. A proper model function for the lateral charge distribution is crucial for the reconstruction of the properties of an EAS. Parameters of interest are the air-shower geometry, i.e., the core position and the incident direction, as well as the energy and mass of the primary particle.

¹Note, that a separate treatment of the arrival time for the EM and muon component can also be beneficial for the reconstruction of air-shower characteristics. However, for the purpose of this work, the derivation of the shower direction based on the standard reconstruction has sufficient accuracy.

The latter can be related to the slope of the LDF, which is a measure of the electron-to-muon ratio and of the shower age [229]. The primary energy is related to the shower size, which is modeled via the LDF normalization.

The lateral distribution at the observation level is influenced by multiple factors in the shower development. The height of the first interaction, X_0 is strongly correlated with the shower age, leading to younger/older showers with decreasing/increasing X_0 for the same primary energy. EASs which are measured at an earlier stage of development tend to have a steeper lateral distribution [42] due to the smaller lateral spread of shower particles earlier in the development. Since, on average, proton and iron primaries of the same energy interact later/earlier in the atmosphere, respectively, the lateral distribution measured at ground is steeper/flatter. The slope of the LDF therefore contains information about the primary mass. The lateral spread of the charge distribution is produced by the transverse momentum of the particles produced during the shower propagation and scattering processes. The transverse momentum, p_T , is of high importance to the lateral spread for hadrons and the particles produced in their decay [86]. This is in particular important for the production of laterally separated muons (see [68] for details) as the p_T distribution for the interaction of nuclei depends on the corresponding energy per nucleon and is therefore sensitive to the primary mass. However, for the measurement of the lateral distribution with IceTop, only the EM component and low-energy muons play a role. For such low-energy muons which constitute the majority of the muon content in air showers, the muon transverse momentum distributions at the production level exhibit a universality for different primary masses. This is due to the fact that the bulk of muons are produced in later stages of the shower development with energies of the parent mesons around the critical energy. The main part of their transverse momentum is determined by the p_T the parent meson obtained in its last interaction [230]. In the EM component, multiple Coulomb scattering is the main source of the lateral spread. This also effects low-energy muons, which, in combination with the transverse momentum and the smaller attenuation compared to EM particles, can lead to a domination of the muon component over the EM component at larger lateral distances [86]. Additionally, the opening angles in Bremsstrahlung and pair production processes influence the lateral spread of EM shower particles [42], however, these effects are typically not significant compared to multiple Coulomb scattering [86]. Of course, the Earth's magnetic field additionally leads to a deflection of charged particles, causing curved particle trajectories and lateral separation [86]. The lateral spread caused by Coulomb scattering and magnetic deflection can be approximated with the radiation length, χ_0 , as

$$\begin{aligned} d_{\text{CS}} &= \frac{E_{\text{CS}} \chi_0}{E}, \\ d_{\text{Mag}} &= \frac{300 B \sin \psi \chi_0^2}{E}, \end{aligned} \tag{6.1}$$

respectively [86]. Here, E is the particle energy, B is the geomagnetic field strength, and ψ is the angle between the particle momentum and the direction of the magnetic field. For the radiation length for electrons, and the scattering energy², $E_{\text{CS}} \sim 21 \text{ MeV}$, the lateral separation caused by the Coulomb scattering is roughly 10 times larger compared to the magnetic deflection [86]. In the case of muons, both effects can be of the same order, which can produce azimuthal asymmetries of the lateral distribution. This effect becomes more relevant for highly inclined showers. The shower inclination itself has a significant influence on the slope of the lateral distribution measured at the ground. With increasing inclination, the effective path length particles have to traverse until they reach the observation level increases. Typically, this leads to flatter lateral distributions observed at the ground. In theory, however, a difference in the shower age depending on the lateral distance and azimuthal orientation is observed [86].

In practice, the choice of an appropriate LDF varies between different experiments. This is because the measured charge distributions depend on the specifics of the detector response, which is different for each experiment. In particular, different detectors such as Cherenkov tanks or scintillators have a significantly different response depending on the species of the measured air-shower particles and due to the different detector geometry. I.e., the functional form of an optimal LDF depends on the sensitivity of a detector array to the different shower components. In case of IceTop, where low-energy muons have a significant impact on the slope of the lateral distribution, a function that is able to model the flat muon distribution is preferred. Additionally, analytical derivations of LDFs are based on particle density calculations, which may not resemble the measured charge deposit. E.g., the most prominent example, the NKG function [232, 233], derived by Nishimura, Kamata and Greisen from an analytical approach to describe the lateral density distribution of the EM contribution, does not properly fit the lateral distributions measured with IceTop. This is caused by the fact that the measured charge deposit in IceTop is not purely a measure of the particle density, but is influenced by the energy distribution of the EM particles. Additionally, low-energy muons influence the lateral distribution, leading to a deviation from the NKG function. To derive suitable LDFs in the context of the two-component model, two different LDFs are investigated for the description of the EM contribution.

DLP function

The double logarithmic parabola (DLP) was empirically derived on the basis of simulations to describe the charge distribution measured with IceTop [42]. The charge distribution

²Characteristic energy defined as $E_{\text{CS}} = m_e c^2 \sqrt{4\pi/\alpha}$, with the fine-structure constant $\alpha = 1/137$ [231].

utilized in the standard IceTop reconstruction is dominated by EM contribution. However, at larger distances also low-energy muons have a significant impact, which reflects in a flatter LDF slope. The DLP function is defined as

$$S_{\text{DLP}} = S_{\text{ref}} \left(\frac{r}{R_{\text{ref}}} \right)^{-\beta - \kappa \log_{10} \left(\frac{r}{R_{\text{ref}}} \right)}, \quad (6.2)$$

which is a parabola in double logarithmic space. This form was found to well describe the IceTop distributions up to 1 km in lateral distance [234]. The parameter β is the slope of the LDF at the reference radius, R_{ref} . The shower size parameter (reference signal), S_{ref} , can be understood as the signal strength at R_{ref} and is measured in units of VEM. κ describes the curvature of the parabola and was found to be roughly constant for all hadronic showers and is fixed to $\kappa \approx 0.303$ for the standard IceTop reconstruction based on fits to lateral distributions using measured data [235]. The DLP function was shown to provide high stability in the reconstruction of EASs, likely caused by its comparably simple functional form. Even though it was derived based on hadronic showers, it was shown that κ tends to favor higher values for EASs induced by photons [189]. Since photon initiated showers are, in first order, purely EM showers, this suggests that the DLP function can be optimized to describe the EM component by means of a re-parametrization of κ . In fact, the DLP function was found to provide a suitable model function for the application on EASs measured with the scintillator arrays of the IceTop enhancement [194] and the IceCube-Gen2 surface array [101]. The scintillation detectors are most sensitive to electrons, which further proves a certain universality in the application of the DLP function for EAS reconstruction for different LDF shapes. Therefore, the DLP function is used and optimized for the description of the EM component in the context of the two-component LDF in section 6.2. After the optimization, the shower size parameter S_{ref} can be interpreted as the shower size of the EM component, $S_{\text{em,ref}}$. Although the DLP function has no intrinsic mathematical constraints, from a physical perspective, monotonically decreasing behavior is required. This requirement constraints the parameter space for β and κ accordingly³.

Modified NKG function

The muon lateral distribution measured with IceTop is shown to be well described by a modified version of the Nishimura-Kamata-Greisen (NKG) function of form

$$S_{\text{mod. NKG}} = S_{\mu} \left(\frac{r}{R_{\mu}} \right)^{-\beta_{\mu}} \left(\frac{r + 320 \text{ m}}{R_{\mu} + 320 \text{ m}} \right)^{-\gamma}, \quad (6.3)$$

³A kink like feature can be observed at small lateral distances for certain combinations of β and κ , which is unphysical and should therefore be prevented.

when $\beta_\mu = 3/4$ and γ is a free parameter [236]. This function was originally proposed by Greisen [237], where $\beta_\mu = 3/4$ and $\gamma = 2.5$ are found to well describe the muon LDF at sea level. Eq. (6.3) will be referred to as Greisen LDF in the following. Here, 320 m is the Greisen radius, which represents the lateral distance at which 50% of the shower muons are contained at sea level [237]. This approximately holds also for the observation level of IceTop [238]. The two slope parameters of the Greisen LDF are inherently correlated. However, β_μ has the largest impact on the slope close to the shower axis, while γ mostly controls the LDF tail. Due to the correlation between both parameters, in practice, it is sensible to only use one as a free parameter of an LDF fit. Similarly to the DLP function, R_μ is the muon reference distance and S_μ the reference signal at R_μ . S_μ is used as muon shower size parameter, i.e., describes the normalization of the Greisen LDF.

6.2. EM and muon average lateral distributions

The general applicability of the proposed LDFs can be tested by fitting them to average lateral distributions. Since the two-component LDF model aims to disentangle the EM from the muon air-shower component, access to the corresponding lateral distributions is required. For this purpose, simulated air-shower events have to be utilized instead of measured data. As a first test of the suitability of the proposed LDFs, the ability to describe the shape of the lateral distributions is tested in two different scenarios.

Particle density distributions

Firstly, the LDFs are fit to average particle density distributions derived from CORSIKA simulations. The simulation set used for the construction of average lateral distributions can be found in (section 4.4). Fig. 6.1 shows the particle density for electrons/positrons, photons, and muons at the observation level as a function of primary energy and zenith angle for EASs simulated with Sibyll 2.1. It is clearly visible, that photons have the highest contribution to the overall particle density distribution across all lateral distances studied. While the shape of the EM distribution falls off quickly at large distances, the muon contribution becomes more significant at distances beyond a few hundred meters due its comparably flat distribution. The slope of the lateral distributions increases slightly with energy since $X_{\max}$ shifts to larger values and therefore the measured shower age decreases. With increasing zenith angle, the amount of matter the shower needs to traverse to reach the ground increases. Hence, for a given energy, the measured shower age increases accordingly, leading to a more flat lateral distribution for more inclined EASs. In order to test the ability of the LDFs to describe the lateral shape of the particle

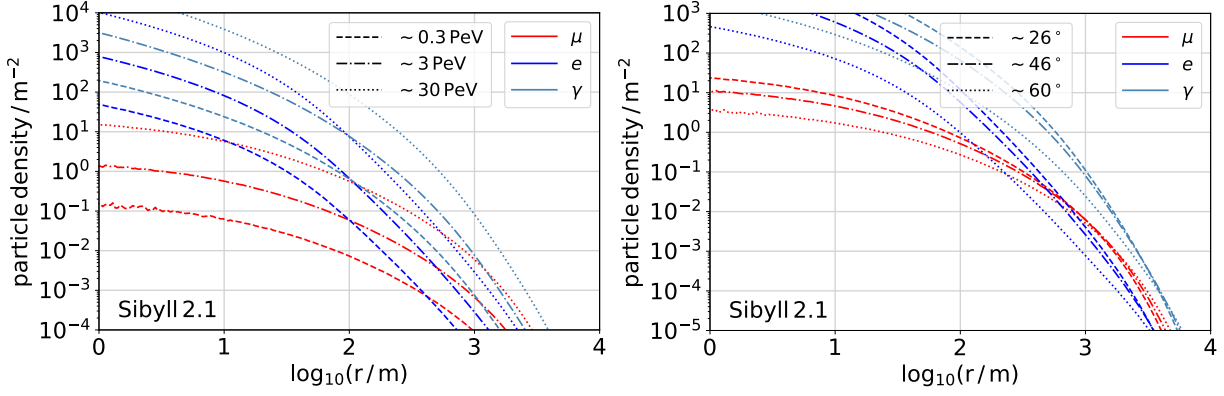


Figure 6.1.: Particle density distributions for electrons/positrons, photons and muons as derived from pure CORSIKA as a function of the primary energy (left) and zenith angle (right) for proton- and iron-induced showers. The average primary energy and zenith angle are indicated with different line styles. The right figure includes primary energies between 10 – 100 PeV.

density distributions, the model functions are fit to the distributions using a simple χ^2 minimization. For the EM part, electrons, positrons and photons are combined to an EM particle density. Fig. 6.2 shows the resulting fits for multiple bins in primary energy using different configurations of free parameters. In the fits only lateral distances between 10 – 1000 m are included, mimicking the fit range used in the IceTop reconstruction. It becomes clear, that with a fixed value of $\kappa = 0.303$ the DLP function does not describe the EM particle density sufficiently well for larger lateral distances for all energy bins. However, as discussed in section 6.1, a variation of κ allows for a significant increase in flexibility. With two free slope parameters, the DLP function describes the EM distribution well up to a few hundred meters. With two free slope parameters in the fit, the modified NKG function, allows an accurate description for distances up to 1 km, which is the maximum distance observed for EASs with core position contained within the IceTop array. This is not surprising, as the NKG function itself is derived specifically for the description of the EM particle density. In the case of the muon lateral particle density, the modified NKG function describes the shape of the distributions well for up to a few hundred meters in lateral distance for both one and two free slope parameters. Although two free parameters lead to a more accurate fit at small distances, a fixed value of γ seems to be preferred for the modeling of distances approaching 1 km. Since an accurate description of the muon slope far from the shower axis is of high importance for the two-component model, this hints that the application of two free slope parameters in the two-component LDF reconstruction is disfavored. This can be in particular beneficial for the fit stability, which increases for a decreased amount of degrees of freedom.

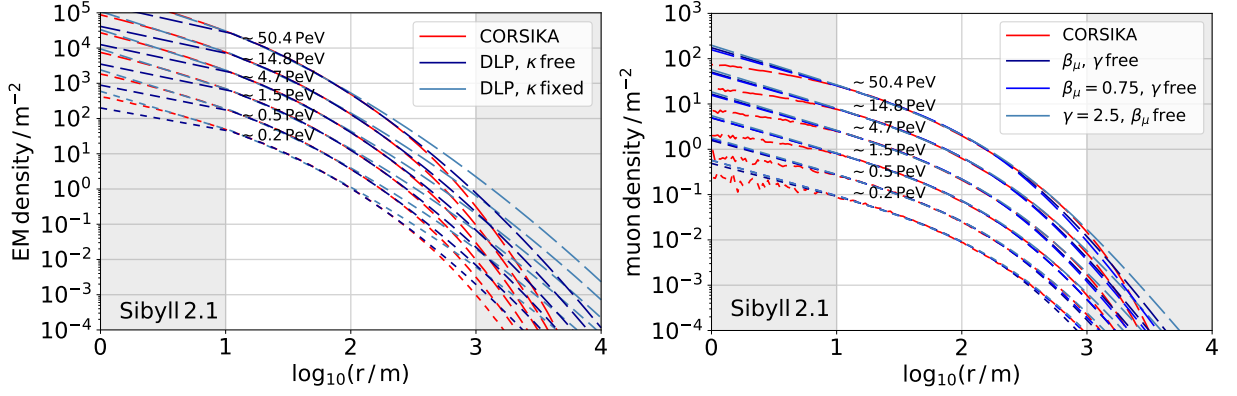


Figure 6.2.: Fits to the EM (left) and muon (right) particle density distributions obtained from pure CORSIKA simulations for different bins in primary energy and near-vertical proton and iron showers ($\cos \theta > 0.9$). The EM lateral distributions are fit with the DLP function with either one or two free slope parameters. The lower panels show the ratio of the corresponding fits to the true particle distributions. The gray shaded areas illustrate the lateral distance regions not included in the fits.

IceTop response

The charge distribution observed in the measurement does not necessarily represent the particle density distributions. In particular, for the EM component, the measured tank charges depend on the energy distribution of the particles and on the conversion rate of EAS photons inside the tank. Additionally, the snow coverage on top of the tanks leads to attenuation effects. Although muons are significantly less effected by the attenuation, low-energy muons can loose enough energy to fall below the Cherenkov threshold before they cross the entire tank. This leads to a shorter effective track length, reducing the observed signal deposit. However, for the bulk of muons which are above the GeV range, the snow attenuation can be approximately neglected. The muon density distribution should therefore be roughly proportional to the measured charge distribution. In contrast to that, the measured lateral distributions for EM particles can be significantly modified compared to the particle density. Thus, the LDFs need to be tested on average observed charge distributions. For each tank signal detected in a simulated event, the number of photoelectrons produced by a particular particle species is saved on the basis of CORSIKA information. The EM and muon contributions to each measured signal can then be distinguished. Additionally, the extracted pulses are calibrated to units of VEM using the proper calibration factors that are unique to each DOM. However, since information about different particle contributions to observed signals is saved before any pulse cleaning algorithms are applied, only detector signals that are present at Level3 of the data processing and are part of a chosen cleaned pulse series can be used for the extraction. For this purpose, pulses surviving a cleaning based on a $1 \mu\text{s}$ time window

with respect to a reconstructed shower plane (see section 4.3.1) are used. Since this procedure requires a preceding successfully performed standard reconstruction, providing an estimate of the air-shower geometry, this choice implies the application of quality cuts for this study given by

- **HLC multiplicity:** At least 5 triggered HLC stations, i.e., 10 tank triggers, are required to provide enough degrees of freedom for the standard IceTop reconstruction.
- **Thresholds for hottest HLC:** The largest measured charge deposit is required to be at least 6 VEM after snow correction using the simple snow model. At the same time, the neighboring tank in the same station has to measure a minimum of 4 VEM.
- **Containment of hottest station:** The HLC trigger with the highest charge deposit is not allowed to be on the edge of IceTop.
- **Fraction of HLCs within COG:** The fraction of triggered HLCs within a circle around the center of gravity of the measured charges is required to be at least 0.2. The outer radius of the circle is defined by the furthest triggered HLC.
- **Convergence:** The minimization procedure of the standard reconstruction has to converge.
- **Containment:** The reconstructed core position is required to be contained within a scaled factor of 0.96 of the IceTop surface area,

which follow analysis presented in [187]⁴. The quality cuts implicitly ensure sufficient quality of the simulated air-shower events included for the average charge distributions. This is beneficial for parameter optimizations based on average LDF fits, to mitigate any deterioration due to badly reconstructed or untypical events.

The resulting average lateral distributions for the EM and muon contribution are illustrated in Fig. 6.3 for near-vertical air showers ($\cos \theta_{\text{reco}} > 0.9$) in two example bins in the energy proxy S_{125} derived from the standard reconstruction. While the DLP function Eq. (6.2) is tested for the description of the average EM shower component, the Greisen function Eq. (6.3) is fit to the muon component. In both cases, the fit is performed via a simple χ^2 minimization procedure. It should be noted that, due to the increasing snow accumulation, the optimization of a chosen model function for the lateral distribution has to be optimized individually for each year. In particular, the attenuation of the EM shower component increases significantly with the snow level. Since in the later reconstruction procedure the LDF fit aims to describe the unattenuated signal distribution in order to estimate the air-shower parameters of interest, the EM signal component used in this study is corrected to account for the snow attenuation by means of the simple snow model

⁴A more detailed discussion of the quality cuts is given in section 6.3

described in section 4.3.1. Moreover, to resemble a density distribution, tanks without a signal ('silent' tanks) are included in the calculation of the average signal distribution as 0 VEM entries. To resemble a realistic flux, the contribution of each air-shower event to the average is weighted with the H4a flux model.

An interesting feature visible in the average LDF fits is the intersection of the EM and muon LDFs. The point of intersection is expected to be a function of the primary energy and zenith. Furthermore, due to the difference in the relative contribution of muons for different primary types, this characteristic can be studied in the context of mass composition studies. For all tested LDFs, the normalization parameters as well as both slope parameters are treated as free parameters in a least squares minimization to maximize flexibility. Firstly, in case of the average EM distributions, the DLP function allows for a sufficient description of both the large signal deposits and the shower tail. The main purpose of the LDF fit to the EM part of the shower is the reconstruction of the shower geometry and primary energy. In this context, proper modeling of the region close to the shower axis is crucial. However, for the application of the two-component LDF, i.e., for the convolution of the EM and muon contribution, a sufficient approximation of the shape of the expected EM tail is of high importance. The latter can be understood as a potential background for reconstruction of the muon content.

In case of the muon lateral distribution, the chosen LDF shape provides a good description of the observed distribution throughout all primary energies and the entire lateral distance range studied. For an overview of the average LDF fits for all S_{125} bins and for all hadronic interaction models, Sibyll2.1, EPOS-LHC and QGSJet-II-04, see App. B. The tested model functions provide a good description of the observed lateral distributions, therefore the chosen LDFs are suitable candidates for the application within the two-component LDF reconstruction. It should be noted, that this conclusion is purely based on the fit performance in the context of average lateral distributions. However, a main part of the uncertainty in the reconstruction of the characteristics of the primary particles initiating the EASs comes from shower-to-shower fluctuations which are effectively mitigated in the calculation of average distributions. Thus, the reconstruction performance based on single air-shower events is crucial for the choice of the LDF. Additionally, the simple χ^2 minimization applied for the average LDF fits does not necessarily lead to the same conclusions compared to the likelihood procedure implemented for the single event reconstruction. For this purpose, fits to single events using a sophisticated likelihood description of all signal models included in IceTop events are studied in sections 7.1 and 7.2.

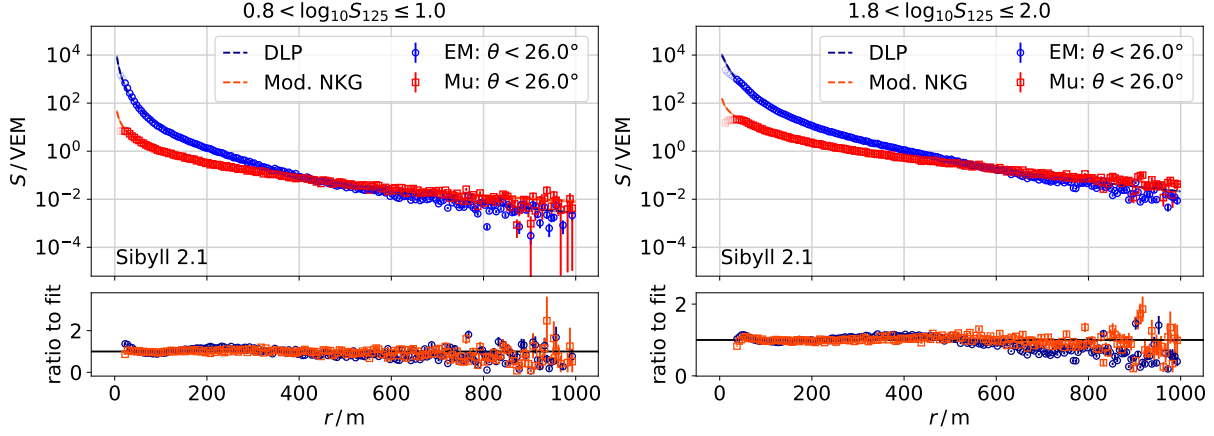


Figure 6.3.: Average lateral distributions from EM particles and muons obtained for proton and iron induced near-vertical air-showers (weighted to the H4a flux assumption) produced with Sibyll 2.1 for two different bins in the energy proxy S_{125} of the standard reconstruction (upper panels). Fits for two different LDFs are shown as dashed lines. Residuals for the LDF fits to the average EM and muon lateral distributions, respectively, are shown in the lower panels.

LDF parametrization

For the application of both LDFs within the two-component model, the LDFs are parametrized based on the fits to average distributions. Since the two-component reconstruction aims for a single-event-based reconstruction in which shower-to-shower fluctuations play an important role, too many free parameters can lead to an unstable reconstruction procedure. Additionally, the two slope parameters in each LDF are strongly correlated. For this reason, one slope parameter of each LDF is parametrized as a function of $\log_{10} S_{125}$, the energy proxy obtained from the standard reconstruction (see section 4.3.1). The fit results for the slope parameters β_{em} and κ of the EM LDF (Eq. (6.2)) and β_{μ} and γ of the muon LDF (Eq. (6.3)) in bins of $\log_{10} S_{125}$ and for the three hadronic interaction models are shown in Fig. 6.4. Interestingly, the energy evolution of the EM and muon lateral distributions are modeled most accurately with a combination of one decreasing ($\beta_{\text{em}}, \beta_{\mu}$) and one increasing (κ, γ) slope parameter. Both, κ and γ mostly influence the region far from the shower axis. While the overall lateral distribution becomes steeper with increasing energy due to the increase in X_{max} , for IceTop, in particular the tails of the EM distributions are strongly suppressed. This was also reported for lateral distribution function observed with the Pierre Auger Observatory [239] and is likely connected to attenuation effects. Therefore, the shape of the tail for a particular shower energy and primary depends on the atmospheric depth of a given air-shower array. For IceTop, however, the snow accumulation on top of the IceTop tanks further enhances the suppression of the shower tail. It was shown for the Pierre Auger Observatory, that an LDF modified

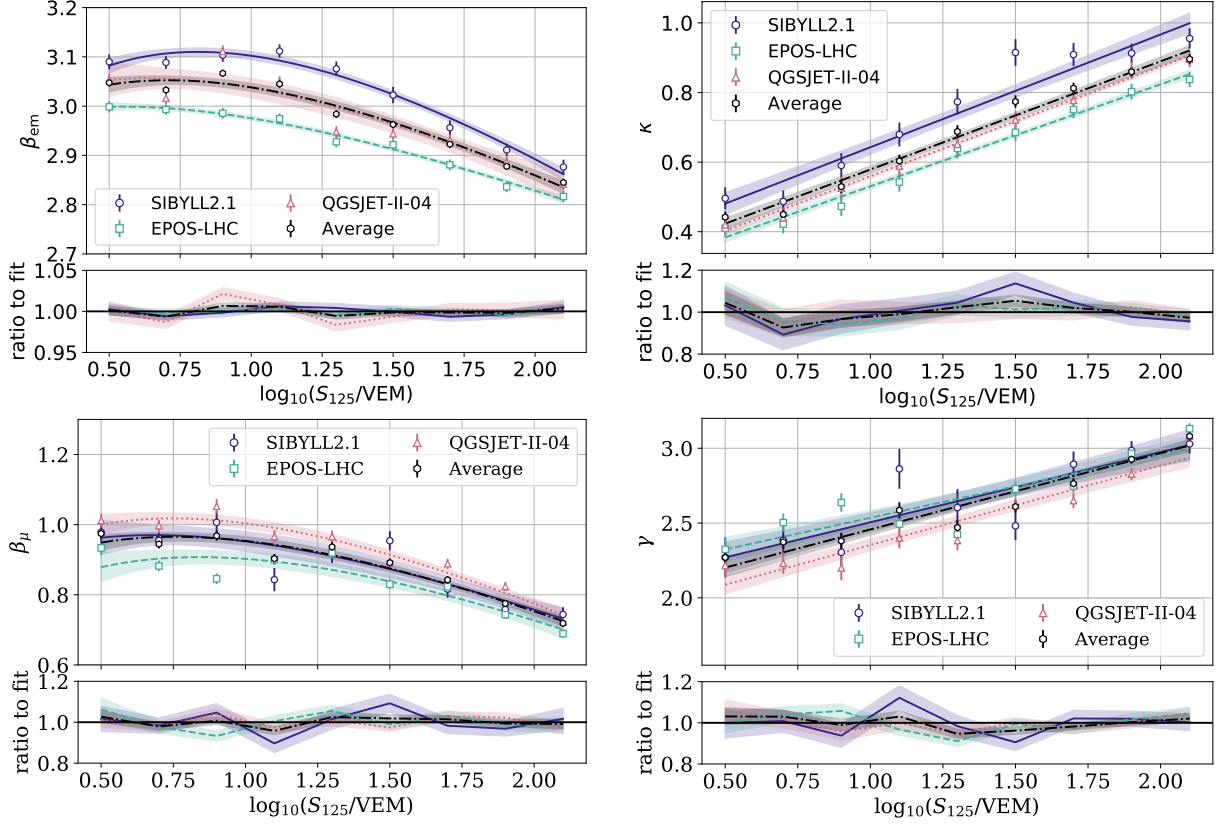


Figure 6.4.: Fit results and parametrization as a function of S_{125} for the slope parameters β_{em} (top left) and κ (top right) of the DLP function (upper row) and for the slope parameters β_{μ} (bottom left) and γ (bottom right) of the modified NKG function based on the average tank response to EM particles and muons, respectively.

by additional exponential suppression factor can be applied to describe the tail more accurately [239]. For the purpose of this work, in which simulations and measured data from the year 2012 are analyzed, the DLP function describes the observed EM distributions sufficiently well. However, for future studies including datasets from more recent years with higher snow accumulation, a similar approach could be studied for the application on the EM LDF used for the two-component model.

Another interesting observation is that the EM distributions are steepest for Sibyll 2.1. In principle, the post-LHC models EPOS-LHC and QGSJet-II-04, on average, lead to a deeper X_{max} compared to Sibyll 2.1 for the same primary energy. Thus, the shower age and consequently the flatness of the lateral distribution should be larger for Sibyll 2.1. However, the particle content for a given hadronic interaction model strongly depends on the atmospheric depth relative to X_{max} at which a shower is observed. The fact that Sibyll 2.1 leads to a steeper EM lateral distribution could therefore be a nontrivial effect caused by IceTop being situated at an atmospheric depth of 690 g/cm^2 , which is very close to X_{max} for the observed primary energies [240]. It should be noted, that this observation

Table 6.1.: Fit values for the parametrization of the LDF slope parameters obtained for the average of Sibyll 2.1, EPOS-LHC and QGSJet-II-04.

fit parameter	β_{em}	κ	β_{μ}	γ
p1	3.763	0.311	1.836	0.510
p2	-0.345	0.268	-0.408	1.947
p3	-3.422	-	-4.268	-

is in line with previous analyses of the lateral distribution in IceTop [42, 241, 242].

While β_{em} only varies within a few percent across the hadronic interaction models, the curvature of the DLP function, κ , shows variations on the few $\sim 10\%$ level. In case of the muon distributions, both slope parameters show maximum variations of $\sim 10\%$ between the different models. Since β_{em} and β_{μ} mostly describe the region close to the shower axis, they are more strongly constraint during the fit. This reflects in the smaller statistical uncertainties of the respective parameter values compared to κ and γ . Due to the increased number of low-energy muons in the post-LHC models, the overall muon LDF described by both β_{μ} and γ is slightly steeper for Sibyll 2.1. While the evolution as a function of $\log_{10} S_{125}$ of κ and γ can be well described by a linear fit ($f(\log_{10} S_{125}) = p_1 + p_2 \log_{10} S_{125}$), β_{em} and β_{μ} are modeled via

$$g(\log_{10} S_{125}) = p_1 + p_2 \log_{10} S_{125} + p_3(2 + \log_{10} S_{125})^{-2}. \quad (6.4)$$

The parametrizations relevant for the two-component model are derived for the average of the three hadronic interaction models. The resulting parameter values are listed in Tab. 6.1. The parametrizations for κ and γ are used to describe the energy evolution of the corresponding LDFs in the two-component reconstruction. For β_{em} and β_{μ} , they are used as first guess values for the LDF shapes as discussed in more detail in the next section.

6.3. Reconstruction algorithm

The implementation of the two-component LDF reconstruction is significantly more complex than the standard IceTop reconstruction introduced in section 4.3.1. In this model, the signal distributions measured with IceTop are reconstructed based on two lateral distribution functions. The measured time distributions are reconstructed analogously to the standard reconstruction. The goal of this procedure is the disentanglement of the EM and muon contributions to an observed lateral distribution on a single-event basis.

The primary reconstruction parameters of interest therefore are the shower size as proxy for the primary energy, the muon content, and the shower geometry (core position and primary direction). Additionally, the slope parameters of both LDFs as well as the ratio of EM and muon contribution to the measured signals as a function of lateral distance can be of interest for high-energy hadronic model tests as well as mass composition studies. Similarly to the standard reconstruction, the two-component reconstruction is realized as an iterative log-likelihood minimization procedure. Thus, the reconstruction parameters are correlated. In order to incorporate two different LDF functions simultaneously, the likelihood functions are based on convolved PDFs. In contrast to the starting point in the standard reconstruction, no dedicated algorithm is applied to derive seed values for the reconstruction parameters. Instead, for each air-shower event, the results of a standard reconstruction can be used as a high-quality seed for the two-component LDF reconstruction. This is only applicable for reconstruction parameters that are part of the standard reconstruction. This includes all parameters of the shower geometry and the energy proxy parameter, S_{125} . The standard reconstruction does not distinguish between different air-shower components. However, since only HLC tanks are included, which are dominated by the EM component, S_{125} can be used as an approximation of the EM shower size $S_{\text{em},125}$. In a similar fashion, the parametrization of the signal spread derived for the standard reconstruction [171] can be applied in the likelihood calculation of the EM contribution within the two-component LDF. In order to derive initial values for the slope parameters of the EM and muons LDF, the parametrizations as a function of S_{125} listed in Tab. 6.1 are used.

Numeric integration

The numeric integration of the signal PDFs is based on the trapezoid rule, which approximates an integral as a discrete sum of trapezoid areas

$$\int_0^{s_{\text{max}}} f(s') ds' \approx \sum_{k=1}^N \frac{f(s'_{k-1}) + f(s'_k)}{2} \Delta s'_k, \quad \Delta s'_k = s'_k - s'_{k-1}, \quad (6.5)$$

with the sampling size N that divides the integration interval into uniform steps of size $\Delta s'_k$. Since the accuracy of the numerical approximation is directly related to the chosen step size, in practice the accuracy and computational intensity have to be balanced. In the context of the two-component LDF, achieving this balance is not trivial since two PDFs with different functional forms are numerically integrated simultaneously by means of a convolution. Since in the implementation a numeric integration in linear space is chosen, the EM signal PDF is the bottleneck for the resulting numeric accuracy. This is in particular true for small signal expectation values, $\langle S_{\text{em}} \rangle$, due to the steep functional form of the log-normal distribution with the given parametrization. Fig. 6.5 (left) illustrates

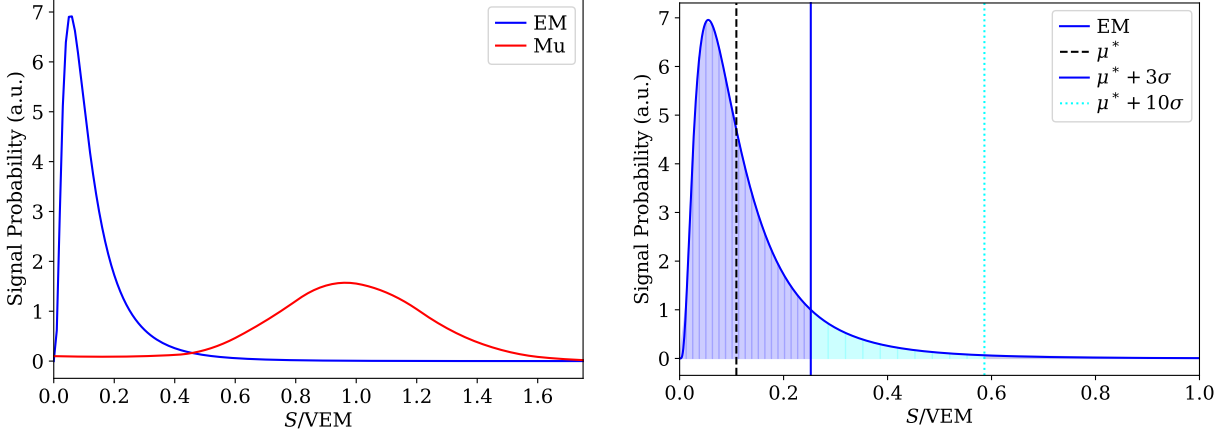


Figure 6.5.: Comparison of the PDFs for the EM and muon contribution, respectively, for the case of one vertical muon and an EM signal expectation value $\langle S_{\text{em}} \rangle = 0.1 \text{ VEM}$ (left). Illustration of the numeric integration regions as defined for the EM signal PDF (right).

this circumstance for an example configuration which occurs regularly during the negative log-likelihood minimization within the two-component reconstruction. In this case, an EM signal expectation value of $\langle S_{\text{em}} \rangle = 0.1 \text{ VEM}$ was chosen for the EM PDF. The muon PDF represents a probability distribution for one vertical muon. The narrow functional form of the EM PDF compared to the muon PDF is clearly visible and becomes more distinct for even lower $\langle S_{\text{em}} \rangle$. However, in particular an accurate description of the region in which small $\langle S_{\text{em}} \rangle$ are expected, i.e., at large lateral distances, is crucial for the reconstruction of the muon component. Thus, a flexible and nonuniform treatment of the step size $\Delta s'_k$ is chosen for the calculation of convolution integrals within the reconstruction:

$$\Delta s'_k = \begin{cases} \min(\Delta s'_{\text{max}}, \Delta s'_{\text{max}}/(\sigma_{\mu, \text{exp}}/(2\sigma_{\text{em}}))), & s' \leq \mu^* + 3\sigma_{\text{em}} \\ \min(\Delta s'_{\text{max}}, \Delta s'_{\text{max}}/(\sigma_{\mu, \text{exp}}/(5\sigma_{\text{em}}))), & \mu^* + 3\sigma_{\text{em}} < s' \leq \mu^* + 10\sigma_{\text{em}} \\ \Delta s'_{\text{max}}, & \text{else,} \end{cases} \quad (6.6)$$

where $\sigma_{\mu, \text{exp}}$ is defined via the expected average number of muons $\langle N_{\mu} \rangle$:

$$\sigma_{\mu, \text{exp}} = \sqrt{(\langle N_{\mu} \rangle \cdot \sigma_{\mu, 1}(\theta))^2 + \langle N_{\mu} \rangle}, \quad (6.7)$$

and μ^* and σ_{em} are the median and square root of the variance derived from the log-normal EM PDF. s' represents the signal value within the numeric integration, and s_{max} the upper integration bound. The median and square root of the EM PDF are given as [189]

$$\begin{aligned} \mu^* &= 10^{\log_{10} \langle S_{\text{em}} \rangle + \log(10) \sigma_{\log_{10} \langle S_{\text{em}} \rangle}^2 / 2}, \\ \sigma_{\text{em}} &= \sqrt{(10^{\log(10) \sigma_{\log_{10} \langle S_{\text{em}} \rangle}^2} - 1) \cdot 10^{2 \log_{10} \langle S_{\text{em}} \rangle + \log(10) \sigma_{\log_{10} \langle S_{\text{em}} \rangle}^2}}, \end{aligned} \quad (6.8)$$

with the signal uncertainty of the logarithm of the EM signal expectation, $\sigma_{\log_{10}\langle S_{\text{em}} \rangle}$. In the reconstruction, the implementation of $\Delta s'_k$ is used in Eq. (6.5) to allow for a more efficient integration of the PDFs, while maintaining a sufficiently fine sampling of the most relevant portions of a given integration phase space. This is true not only for the single PDF integration, but also for the application on convolution integrals by means of a maximum step size defined as $\Delta s'_{\text{max}} = \sigma_{\max(\sigma_{\text{em}}, \sigma_{\mu, \text{exp}})}/10$.

Normalization of the numeric convolution integrals

The first important feature of the numeric implementation of integrations within the two-component LDF is given by a flexible choice of the numeric resolution, which accounts for the different functional forms involved in a given convolution. However, due to numerical constraints introduced by the chosen sampling (Eq. (6.6)), a given integral can only be computed with finite precision. In the asymptotic approximation $N \rightarrow \infty$, the error of the trapezoid rule can be estimated as ([243])

$$\text{err} = -\frac{s_{\text{max}}^2}{12N^2} (f'(s_{\text{max}}) - f'(0)) + \mathcal{O}(N^{-3}) . \quad (6.9)$$

Therefore, in first order, the uncertainty of the numeric integration is inverse proportional to the square of the sampling size. In order to account for the finite accuracy, the integration result is additionally normalized by means of the full phase space. I.e., in case of a convolution of the EM and muon PDFs, the normalized convolution integral can be written as

$$\frac{\int_0^s p_{\text{em}}(S'_{\text{em}}|\theta, \langle S_{\text{em}} \rangle c_{\text{snow}}) p_{\mu}(s - S'_{\text{em}}|\theta, \langle N_{\mu} \rangle) dS'_{\text{em}}}{\int_{S'_{\mu}}^{s_{\text{upper}}} \int_{S'_{\text{em}}}^{s_{\text{upper}} - S'_{\mu}} p_{\text{em}}(S'_{\text{em}}|\theta, \langle S_{\text{em}} \rangle c_{\text{snow}}) p_{\mu}(S'_{\mu}|\theta, \langle N_{\mu} \rangle) dS'_{\text{em}} dS'_{\mu}} , \quad (6.10)$$

with the signal expectation values of the EM and muon contributions, $\langle S_{\text{em}} \rangle$, and $\langle S_{\mu} \rangle$, respectively. $\langle N_{\mu} \rangle$ describes the average expected number of muons and θ is the primary zenith angle. The denominator can be understood as a convoluted cumulative distribution function over the entire phase space which is normalized to 1 for $N \rightarrow \infty$ and $s_{\text{upper}} \rightarrow \infty$. In practice, the integration cannot be performed until infinity. Instead, the upper integration bound is adapted to a given integration scenario to reduce the computation time. Based on the characteristics of the EM and muon PDFs, the upper integration bound, s_{upper} , can be defined as

$$s_{\text{upper}} = \begin{cases} \max(S_{\text{max}} + 3\sigma_{\text{max}}, s), & \mu^* + 10\sigma_{\text{em}} \leq \max(S_{\text{max}} + 3\sigma_{\text{max}}, s) \\ \max(S_{\text{max}} + 5\sigma_{\text{max}}, s), & \text{else,} \end{cases} \quad (6.11)$$

where in case of an extended tail of the EM PDF a larger integration bound is chosen. The maximum signal strength classified as relevant to cover the entire phase space, S_{max} ,

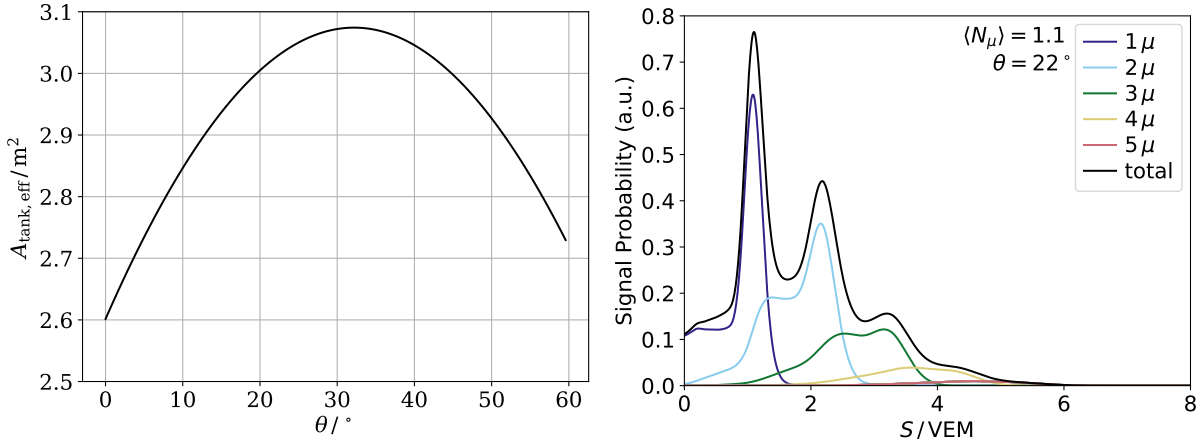


Figure 6.6.: Effective tank area as a function of the zenith angle (left). Poisson weighted muon signal PDFs for a contribution of 5 muons given an average expected number of muons of $\langle N_\mu \rangle = 1.1$ (right). Colored lines show the relative contributions of the different signal PDFs. The black envelope describes the corresponding muon PDF.

and the corresponding signal spread, $\sigma_{\max}$, are derived from both signal PDFs via

$$\begin{aligned}
 S_{\max} &= \max(\mu_{\mu,\max}, \mu_{\text{em}}), \\
 \sigma_{\max} &= \max(\sigma_{\mu,\max}, \sigma_{\text{em}}), \\
 \mu_{\mu,\max} &= N_{\mu,\max} \cdot \mu_{\mu,1}(\theta), \\
 \sigma_{\mu,\max} &= \sqrt{(N_{\mu,\max} \cdot \sigma_{\mu,1}(\theta))^2 + N_{\mu,\max}}.
 \end{aligned} \tag{6.12}$$

The mean and spread for a single muon, $\mu_{\mu,1}(\theta)$, and $\sigma_{\mu,1}(\theta)$, respectively, are determined by the spline fits introduced in chapter 5. The maximum expected spread from the muon contribution is then given by the signal spread for the maximum expected number of muons, $N_{\mu,\max}$, and the corresponding Poisson uncertainty, $\sqrt{N_{\mu,\max}}$, added in quadrature. $N_{\mu,\max}$ defines the maximum muon multiplicity included in the calculation of the convolution integral. The phase space of the muon multiplicity included in the likelihood calculation comprises the 3σ interval for the muon contribution, $n \in [N_{\mu,\min}, N_{\mu,\max}]$, with

$$\begin{aligned}
 N_{\mu,\max} &= \max\left(\langle N_\mu \rangle + 3\sqrt{\langle N_\mu \rangle}, 4\right), \\
 N_{\mu,\min} &= \min\left(\langle N_\mu \rangle - 3\sqrt{\langle N_\mu \rangle}, 0\right),
 \end{aligned} \tag{6.13}$$

where a minimum multiplicity interval of 0 – 4 muons is taken into account.

Likelihood construction

The implementation of two LDFs into a combined likelihood fit is a novel approach and is only possible within the modular *RockBottom* framework. As discussed in the context of the standard reconstruction, the likelihood for the EM contribution is based on the log-normal PDF

$$p_{\text{em}}(S|\theta, \langle S_{\text{em}} \rangle) = \frac{1}{\sqrt{2\pi} S \log(10) \sigma_{\text{em}, \log_{10} S}} \exp \left(-\frac{(\log_{10} S - \log_{10} \langle S_{\text{em}} \rangle)^2}{2\sigma_{\text{em}, \log_{10} S}^2} \right), \quad (6.14)$$

with the average expected EM signal $\langle S_{\text{em}} \rangle$. Here, the model for the uncertainty of the EM signal, $\sigma_{\text{em}, \log_{10} S}$, can be approximated with the standard parametrization (see section 4.3.1) derived using only HLC triggers. However, since even for HLCs low-energy muons can have a non-negligible impact on the signal distributions, a new parametrization based purely on the EM component is derived and compared to Eq. (4.13) in section 7.3. The underlying signal PDFs, $p_{\mu, \text{sig}}(S|\theta, n)$, utilized for the implementation of a likelihood function for the muon contribution are given by the spline fits derived in chapter 5. To obtain the muon PDFs, $p_{\mu}(S|\theta, \langle N_{\mu} \rangle)$, the muon signal PDFs are weighted with a Poisson factor accounting for the probability to observe a particular number of muons given an expectation value of the average number of muons

$$p_{\mu}(S|\theta, \langle N_{\mu} \rangle) = \sum_n \frac{\langle N_{\mu} \rangle^n}{n!} e^{-\langle N_{\mu} \rangle} p_{\mu, \text{sig}}(S|\theta, n). \quad (6.15)$$

The average expected number of muons, $\langle N_{\mu} \rangle$, can be determined by means of the effective IceTop tank area, $A_{\text{tank}, \text{eff}}$, via

$$\begin{aligned} \langle N_{\mu} \rangle &= \langle S_{\mu} \rangle A_{\text{tank}, \text{eff}}, \\ A_{\text{tank}, \text{eff}} &= \pi r_{\text{tank}}^2 \cos \theta + 2h_{\text{tank}} r_{\text{tank}} \sin \theta. \end{aligned} \quad (6.16)$$

The average expected muon signal for a given tank is proportional to the muon density independent of the muon inclination. This is because the muon signal deposit is proportional to its track length. The measured signal in VEM per tank can thus be converted to the average expected number of muons by multiplication of $A_{\text{tank}, \text{eff}}$. With increasing inclination, the projection of the tank area increases until $\sim 32^\circ$ and decreases as the contribution of the tank lid to the projected area decreases. The evolution of $A_{\text{tank}, \text{eff}}$ as a function of inclination is illustrated in Fig. 6.6 (left). An example for the resulting muon PDF (Eq. (6.15)) for a contribution of up to five muons given an average expected number of muons of $\langle N_{\mu} \rangle = 1.1$ and a zenith angle of $\theta = 22^\circ$ is shown in Fig. 6.6 (right). The muon spline fits are produced for muon multiplicities of up to $n = 15$. Already for $\gtrsim 10$ muons, the signal PDFs can be approximated by a Gaussian for all relevant zenith

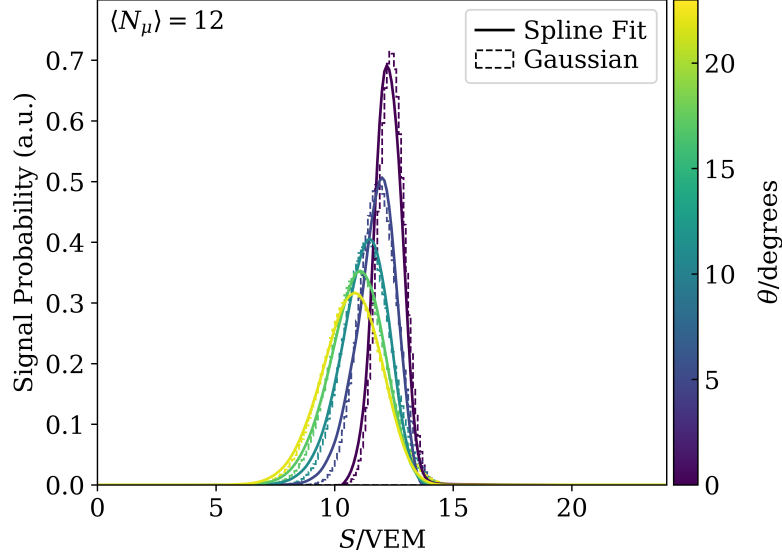


Figure 6.7.: Spline fit to the IceTop tank response for injected 1 GeV muons as a function of the muon inclination ($\theta \lesssim 26^\circ$) and for an injection multiplicity of $n = 12$. The histograms show a Gaussian approximation to each inclination.

angles. Fig. 6.7 shows a comparison of the Gaussian approximation based on the expected average signal deposit, $\mu_{\mu,1}(\theta)$, and signal uncertainty, $\sigma_{\mu,1}(\theta)$, derived from the single muon response and extrapolated to a given multiplicity and the spline fits for a muon multiplicity of $n = 12$. For all relevant zenith angles for the analysis presented in this work, the Gaussian approximation results in a satisfactory description of the distributions obtained from the full tank response simulations. For the reconstruction, a more conservative multiplicity threshold of $n = 15$ is chosen. In the case of larger muon multiplicities, the muon signal PDFs are approximated by a Gaussian function. Overall, the calculation of the muon PDF can be written as

$$p_\mu(S|\theta, \langle N_\mu \rangle) = \sum_{n=0}^{\infty} \frac{\langle N_\mu \rangle^n}{n!} e^{-\langle N_\mu \rangle} \begin{cases} p_{\text{sig}}(S|\theta, n), & n \leq 15 \\ \frac{1}{\sigma_{\mu,\text{res}}(\theta, n)\sqrt{2\pi}} \exp\left(-\frac{(S - \langle S_\mu \rangle)^2}{2\sigma_{\mu,\text{res}}^2(\theta, n)}\right), & \text{else,} \end{cases} \quad (6.17)$$

where the uncertainty of the muon response is defined as

$$\sigma_{\mu,\text{res}}(\theta, n) = \sigma_{\mu,1}(\theta)\sqrt{n}. \quad (6.18)$$

HLC signal model

Since HLC triggers tend to occur close to the shower axis, the observed HLC signal distribution is dominated by EM particles. In particular for large signal deposits at small

lateral distances, where large particle numbers are expected, the likelihood procedure has a limited ability to separate muon and EM contributions. Generally, the convolution of the likelihoods in the two-component model has the greatest potential to disentangle both components in the region where the underlying signal PDFs are most different from each other. This is the case when the signal distribution is expected to be produced mainly by the contribution of one or a few muons along with an EM contribution around the same order or smaller than that of the muon component. Therefore, the construction of the two-component likelihood benefits greatly from intrinsic constraints and simplifications based on knowledge about the shower physics.

Large signal regime

The domination of the EM contribution close to the shower axis can be implemented in the likelihood in different ways. Specifically, since the likelihood describes a lateral distribution, the description of the region close to the axis can be modeled by means of the lateral distance or the signal deposit itself. It should be mentioned, that a specific lateral distance or measured charge above which the EM signal can be defined as dominant depends on the characteristics of the shower. In particular, the shower size, the zenith angle and the primary mass influence the relative contribution of the shower components to the measured charge at a given lateral distance. Therefore, any MC-based implementation based on the lateral distance and charge deposit can potentially introduce a mass composition dependence and, thus, can depend on a chosen cosmic-ray flux model assumption. Additionally, different hadronic interaction models predict different numbers of EM particles and muons. In addition to a flux model dependence, therefore, also a hadronic model dependence can arise.

Since large signal deposits can be produced also at larger distances due to the hard EM component, an implementation based on the signal deposit is chosen for further analysis. In this context, the relative contribution of muons to the measured charge deposit is analyzed as a function of the cumulative charge in HLCs. For this purpose, information on the origin of a particular signal deposit as introduced in section 6.2 is utilized to obtain cumulative charge distributions weighted with the contribution of muons and EM particles, respectively. As such distributions depend on the shower size, this procedure is performed in bins of $\log_{10} S_{125}$. To ensure sufficient quality of the reconstructed air-shower events, a series of standard IceTop quality cuts similar to the cuts introduced previously which follow [187] is applied for this analysis. The resulting distributions are shown in Fig. 6.8 for near vertical air-showers ($\cos \theta > 0.9$) produced with Sibyll 2.1. Since the relative contribution of both components to an observed charge can be distorted if the tank is saturated, only HLCs with signals below their saturation thresholds are included. The weights, $w_{\mu,i}$ and $w_{\text{em},i}$, for a given HLC tank, i , contributing to a cumulative charge bin

are given as

$$\begin{aligned}
w_{\mu,i} &= w_{\text{flux}} \cdot f_{\mu,i}, \\
w_{\text{em},i} &= w_{\text{flux}} \cdot f_{\text{em},i}, \\
f_{\mu,i} &= \frac{S_{\mu,i}}{(S_{\mu,i} + S_{\text{em},i})}, \\
f_{\text{em},i} &= \frac{S_{\text{em},i}}{(S_{\mu,i} + S_{\text{em},i})},
\end{aligned} \tag{6.19}$$

where w_{flux} is the weight of a cosmic-ray flux model assigned on a signal event basis and f_{em} and f_{μ} are the EM and muon signal fractions defined on a single tank basis. The weighted histograms are then converted to a probability density. Each distribution then resembles the PDF for the contribution of EM particles and muons to the measured cumulative charge deposit. In other words, the integration of the PDF in one cumulative charge bin gives the probability of the contribution of the given particle species to the measured signal. The PDFs therefore describe the entire phase space for the EM and muon contribution to the HLC signal distributions measured with IceTop. Integrating the PDFs to a specific value in each $\log_{10} S_{125}$ bin is analogous to the inclusion of a specific portion of the corresponding phase space. In the PDF for the muon component, slightly above 1 VEM a peak is visible produced by single muon contribution. A second, less pronounced bump can be observed at 2 – 3 VEM, which comes mainly from the contribution of two muons to HLC signals. Both features are significantly smeared due to the binning in cumulative charge, which also prohibits the visibility of bumps at larger HLC signals produced by higher muon multiplicities. Another interesting point can be observed in the evolution of both bumps relative to each other as a function of the shower size. With increasing $\log_{10} S_{125}$, the size of the second bump increases relative to the first peak. This suggests an increasing contribution of muon multiplicities of $n > 1$ to the measured HLC signal distribution. The crucial characteristics of the interplay of EM and muon contribution to HLC signals becomes clear when comparing the evolution of the corresponding contribution PDFs. It can be clearly seen, that the PDF for the muon component has its largest contribution to the cumulative HLC charge and also relative to the EM contribution around 1 VEM and up to a few VEM. This corresponds to the contribution of one or a few muons to the measured HLC charges.

Since this is also the region in which the muon and EM PDFs differ the most, the signal range around a few VEM should always be included in the likelihood convolution within the two-component model. The PDFs for the EM contribution exhibit a much smoother distribution over the entire signal range. This is connected to the high regularity of the EM shower development. The phase space for EM contribution is significantly larger for large HLC signals above the tens of VEM region, this region will be referred to as *large signal regime*. This region is produced by signals that occur close to the shower axis. In addition to that, also the sub-VEM regime has a larger contribution produced by EM particles. This is an important point that will be discussed further in the next paragraph. For the large signal range, a threshold signal above which the EM contribution can be defined as dominant can be derived by integration of the PDFs for the muon contribution from small to large HLC signals. For the integration, the muon contribution PDFs are modeled via *B-splines* fits in each bin of $\log_{10} S_{125}$. The spline fits are then numerically integrated using the trapezoidal rule. In the spline fits, the relative uncertainty for each bin entry, j , is used as a weighting factor

$$\begin{aligned}
 w_{\text{spline},j} &= \left(\frac{\sigma_{p_\mu}}{p_\mu} \right)^{-1}, \\
 \sigma_{p_\mu,j} &= \frac{\sqrt{\sum_i w_{\mu,i}^2}}{\sum_{j,i} w_{\mu,j,i} \cdot 0.1}, \\
 p_{\mu,j} &= \frac{\sum_i w_{\mu,i}}{\sum_{j,i} w_{\mu,j,i} \cdot 0.1},
 \end{aligned} \tag{6.20}$$

where $p_{\mu,i}$ and $\sigma_{p_{\mu,i}}$ are the PDF value and its uncertainty, respectively. An additional factor of 0.1 comes from the bin width. To account for the propagated uncertainty in the resulting splines, the PDF values are re-sampled 100 times via bootstrapping using their corresponding uncertainties. The spline fits are then performed on each iteration. Fig. 6.8 shows the resulting 3σ bands around the spline fits, which is propagated as uncertainty in the PDF integration. Since the spline fits can slightly differ from the exact values of each histogram, an additional normalization in the numeric integration is performed, ensuring that the cumulative distribution function over the entire phase space equals one. Integrating the spline fits up to a particular value in each $\log_{10} S_{125}$ bin is then equivalent to including a particular fraction of phase space for the contribution of muons to the observed HLC signals. In Fig. 6.8, an integration up to a value of 0.7 is performed in each $\log_{10} S_{125}$ bin. The resulting cumulative signal regime that contains 70% of the phase space of the muon contribution is illustrated as red shaded region. The remaining 30% are contained in the blue shaded area, which can be classified as dominated by the EM contribution. Since the choice of a phase space threshold is somewhat arbitrary, it can be optimized in the context of the reconstruction performance and hadronic model

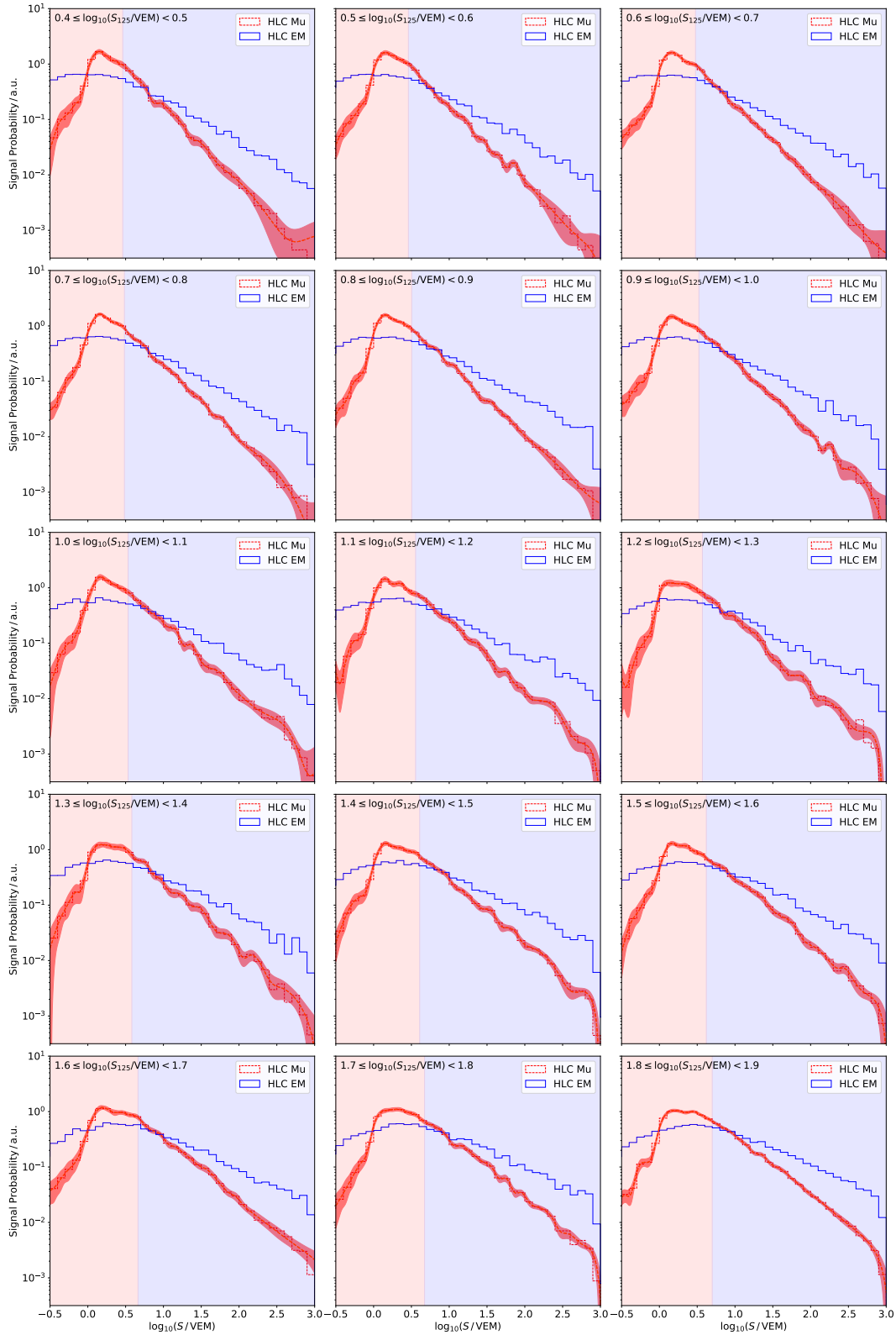


Figure 6.8.: Probability distributions for muons and EM particles in EASs produced with Sibyll 2.1 as a function of the cumulative signal measured in HLCs in bins of $\log_{10} S_{125}$. Muon distributions (red) and are modeled with spline fits. EM distributions (blue) are shown for reference, where the blue shaded area indicates the region above which the EM contribution is classified as dominant.

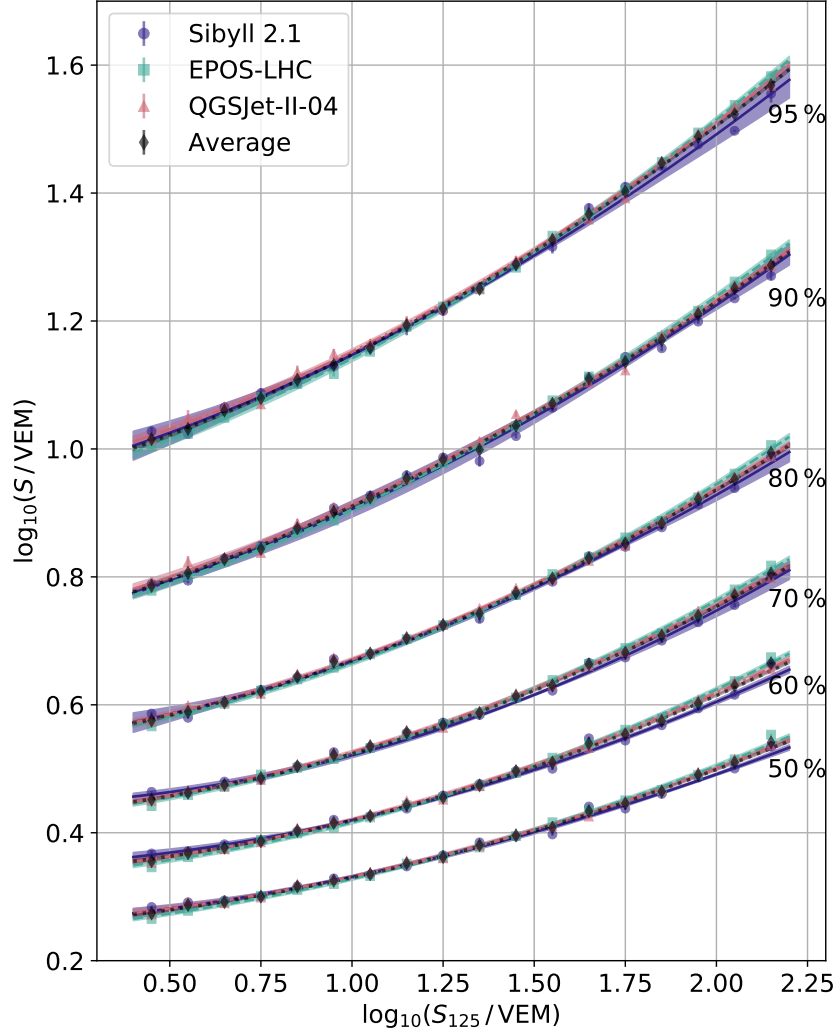


Figure 6.9.: Signal threshold for the inclusion of different amounts of the phase space for the muon contribution to the observed HLC signal distributions as a function of $\log_{10} S_{125}$. Shown are the parametrizations for the hadronic interaction models Sibyll 2.1, EPOS-LHC and QGSJet-II-04, as well as for the average of the three models.

dependence. Fig. 6.9 shows the HLC signal threshold obtained for the inclusion of different amounts of the muon contribution phase space as a function of $\log_{10} S_{125}$. Shown are the results for the hadronic interaction models Sibyll2.1, EPOS-LHC and QGSJet-II-04. The signal threshold increases with increasing shower size because of the increased phase space for large signal deposits. The exact scaling, however, is not trivial and depends on the phase space included in the derivation. For each case, the signal threshold is described well using a 3rd order polynomial of the form

$$S_{\text{thr},l} = p_1 \log_{10}^2 S_{125} + p_2 \log_{10} S_{125} + p_3. \quad (6.21)$$

The resulting fit values can be found in Tab. 6.2 The uncertainty bands shown in Fig. 6.9

Table 6.2.: Fit values for the parametrization of the signal threshold.

phase-space coverage	50%	60%	70%	80%	90%	95%
p1	0.252	0.335	0.425	0.533	0.711	0.932
p2	0.033	0.029	0.033	0.070	0.139	0.146
p3	0.045	0.056	0.066	0.066	0.060	0.071

include the statistical uncertainties of the polynomial fits as well as systematic uncertainties derived from spline fits of histograms (as shown in Fig. 6.8) weighted with different cosmic-ray flux models, namely H4a [244], GST [245], and GSF [246]. Both contributions are added in quadrature and fit corresponds to the average of the flux models. With increasing phase-space coverage, the normalization of the parametrization increases toward larger signal thresholds. The parametrizations show only a small dependence on the hadronic interaction model for the entire $\log_{10} S_{125}$ range studied. The magnitude of the hadronic model dependence changes for different phase-space scenarios. In particular, for values of $\log_{10} S_{125} \gtrsim 2$, the parametrization for Sibyll 2.1 consistently lies below the parametrizations for the post-LHC models. This difference is minimal for a threshold of $\sim 70 - 80\%$ for the muon contribution phase-space. Thus, in terms of hadronic model dependence, parametrizations in this range for the muon contribution phase-space are favored. The influence of the composition dependence is visualized in Fig. 6.10, which shows the parametrization for the 70% phase-space inclusion derived with different cosmic-ray flux models. Within the respective statistical uncertainties, the parametrizations are overlapping, suggesting no significant dependence on the applied composition among the studied realistic flux models. To minimize the composition dependence, a threshold of 70% is therefore chosen for the final implementation. The details of the implementation of the large signal regime are discussed at the end of this section.

Small signal regime

In the previous paragraph, it was discussed that the sub-VEM regime of the observed HLC signal distribution is dominated by EM contribution. This is an important constraint that can be implemented into the two-component likelihood to reflect the underlying knowledge about the shower physics. In order to mitigate any further potential model dependence, this *small signal regime* is studied based on burnsample data, specifically 1% of measured IceTop data for the year 2012. This sample comprises ~ 260000 air-shower events. With the measured data, the underlying signal distribution can be studied by comparing the charges measured by the neighboring tanks in triggered HLCs. The general procedure for this is well known from studies of charge fluctuations with IceTop [189] as well as with

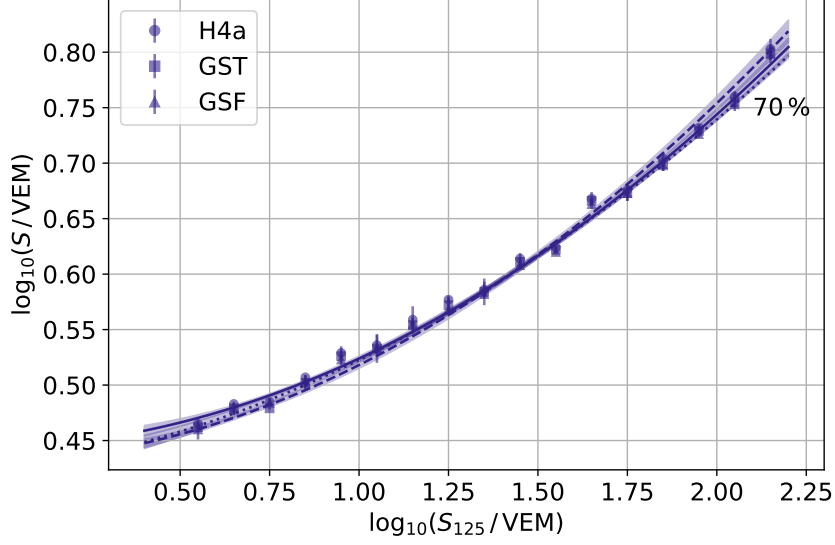


Figure 6.10.: Signal threshold for the inclusion of 70 % of the phase space for the muon contribution to the observed HLC signal distributions as a function of $\log_{10} S_{125}$. Shown are the parametrizations for the hadronic interaction model Sibyll 2.1 for a weighting with the flux models H4a, GST and GSF.

the IceTop-enhancement [194] and the IceCube-Gen2 scintillator array [101]. The motivation for a tank-to-tank charge comparison is the close vicinity of neighboring tanks of ~ 10 m, which, within certain boundary conditions as discussed later, effectively results in an independent double measurement of the same signal expectation value. Typically, the difference of the measured signals is analyzed as basis for a charge fluctuation parametrization. However, since the charge difference is produced by the convolution of the single tank signals, this procedure provides information about the underlying signal distribution. Generally, the HLC distributions can be well approximated as log-normal distributions [189] because the EM component dominates the signal distribution. As discussed in the previous part, however, in the few VEM region single (or a few) muons can have a significant impact on the measured HLC charges. This can result in scenarios where one tank of an HLC station is hit by a muon while the other only measures EM particles. This would result in a significant difference of the measured charge deposit, even though the tanks are situated approximately at the same lateral distance (for near-vertical showers). In these cases, the signal-difference distribution should deviate from a log-normal behavior. Since muons typically cross the ice-Cherenkov tanks and deposit energy along the entire track, small charge deposits are more likely to be produced by EM particles. This fact can be used to derive a small signal threshold condition below which the HLC signal distributions can be approximated as EMally dominated. Fig. 6.11 (top) shows the comparison of the signals, S_a and S_b , of the neighboring tanks in HLC stations for events above the full efficiency threshold, $\log_{10} S_{125} > 0.4$, and for near-vertical showers, $\cos \theta > 0.9$.

As expected, the clear correlation is visible between the signals measured in neighboring tanks, as indicated by the solid black one-to-one correlation line. However, at around $\gtrsim 1$ VEM in S_a or S_b , a wing feature is visible symmetrically around the one-to-one correlation line. This feature is produced in the aforementioned scenario in which a muon hits only one tank in a station. The feature becomes more pronounced when considering the difference distributions of $\log_{10} S_a$ and $\log_{10} S_b$. For this purpose, the distribution is binned orthogonally to the one-to-one correlation line. In each bin, the difference in the log signal is calculated, where the bin average is given by $\log_{10}((S_a + S_b)/2)$. Two example distributions are shown in Fig. 6.11 (bottom). The first bin has an average signal of $\log_{10} \langle S / \text{VEM} \rangle = -0.25$ and is well compatible with a log-normal distribution. For the second bin ($\log_{10} \langle S / \text{VEM} \rangle = -0.05$), a clear deviation from a log-normal is visible. The difference distribution becomes broader and the peak shifts to a plateau-like structure. Both is produced by one tank in a station receiving a muon while the other only measures EM particles. Above mean signals of $\log_{10} \langle S / \text{VEM} \rangle \gtrsim 0.2$ VEM, the distributions slowly transition to the expected log-normal behavior. All distributions are shown in App. B. Within the region of $-0.2 \lesssim \log_{10} \langle S / \text{VEM} \rangle \lesssim 0.3$, the muon contribution therefore has a significant impact on the underlying signal model. In this range, the likelihood calculation should be based on a convolution of EM and muon PDFs. Below mean signals of $\log_{10} \langle S / \text{VEM} \rangle \lesssim -0.2$ VEM, the difference distributions are approximately log-normal and, therefore, dominated by the EM contribution. Since the log-normal signal difference distribution is the result the convolution of the single tank distributions, the latter are log-normal as well (see [189] for details on the theoretical derivation). It should be mentioned, that the zenith angle range included in this study is of high importance as the ratio of muons to EM particles increases with increasing inclination. Also muon track length and therefore the energy deposit of muons inside the tanks changes as discussed in chapter 5. In addition, the approximation of a double measurement of the same signal expectation value becomes less valid due to the increasing projected distance between neighboring tanks. All of these effects and the increasing importance of upstream and downstream regions of the air-shower lead to a modification of the difference distributions. Thus, for the inclusion of more inclined air-showers, the derivation of a low signal regime needs to be re-visited.

SLC signal model

Similar to the histograms used in the procedure for the derivation of the large signal regime in the HLC signal distribution, the SLC signal distributions can be derived as a function of cumulative SLC charge. The resulting distributions for near-vertical showers ($\cos \theta > 0.9$) in multiple bins of $\log_{10} S_{125}$ are shown in Fig. 6.12 for muons, EM particles and hadrons.

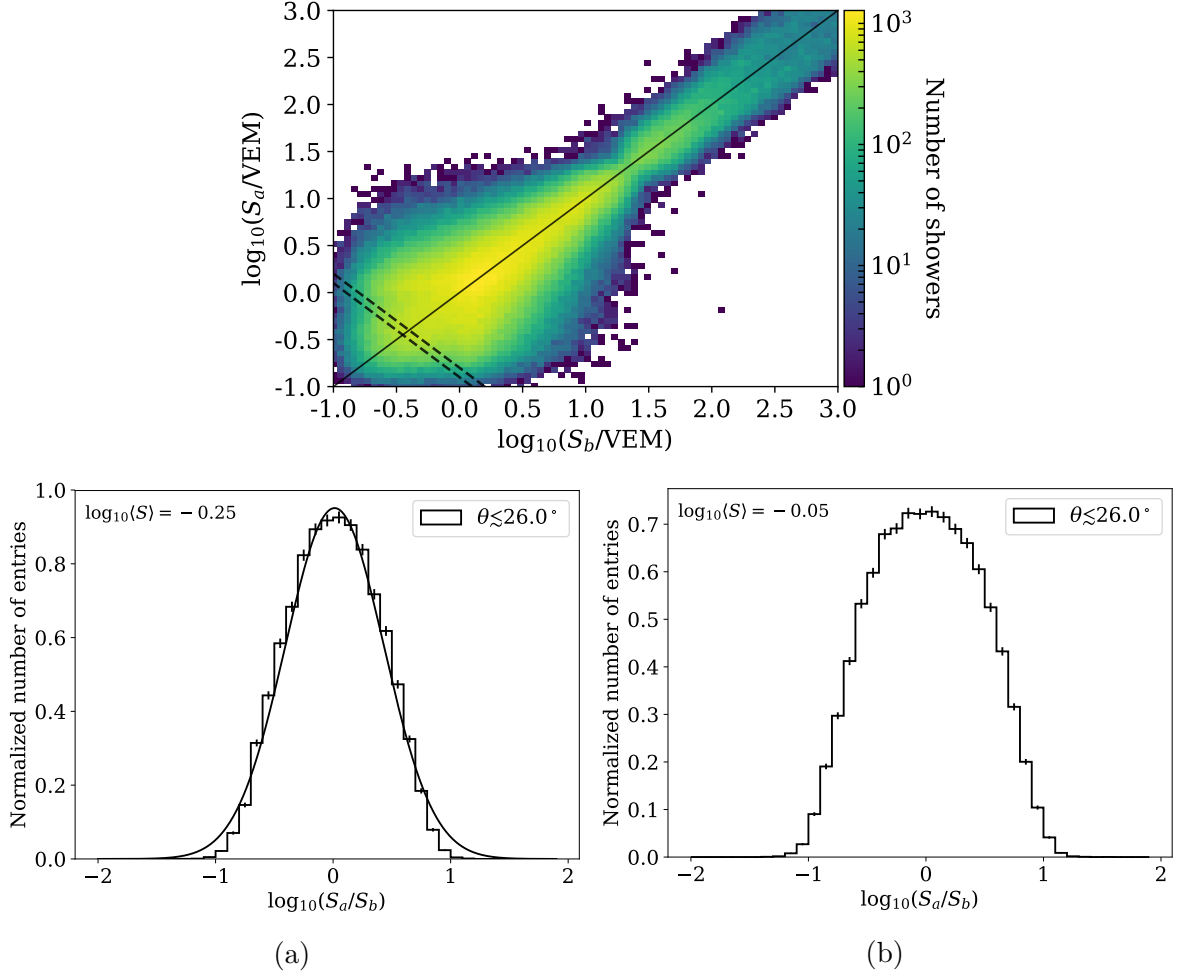


Figure 6.11.: Comparison of signal deposits S_1 and S_2 in neighboring IceTop tanks using 1% of measured data from the year 2012 (top). Included are near-vertical shower with $\theta_{\text{reco}} \lesssim 26^\circ$. The solid black line indicates the one-to-one correlation line. The dashed black lines indicate an example bin orthogonal to the one-to-one correlation line. Resulting signal difference distributions for neighboring HLC tanks in two example bins for an average signal of $\log_{10}\langle S/\text{VEM} \rangle = -0.25$ (a) and $\log_{10}\langle S/\text{VEM} \rangle = -0.05$ (b). While for the first bin the distribution is well approximated by a normal distribution in log space (black line), the distribution in the second bin deviate clearly from a log-normal behavior.

In contrast to HLCs, no large modification as a function of shower size is visible. This is because, by construction, SLCs occur at the edge of the shower front and therefore, to a large part, probe a similar phase space. Additionally, the relative contribution of muons and EM particles to large SLC signals is of a similar order. At smaller signals, the main contribution comes from EM particles, similar to the HLCs. However, for the purpose of the two-component reconstruction, a lower charge cut for SLCs of 0.7 VEM is applied. This cut increases the probability for a given SLC signal to be of muonic origin and is well motivated from [199]. Above SLC values of 0.7 VEM, muons produce a prominent feature

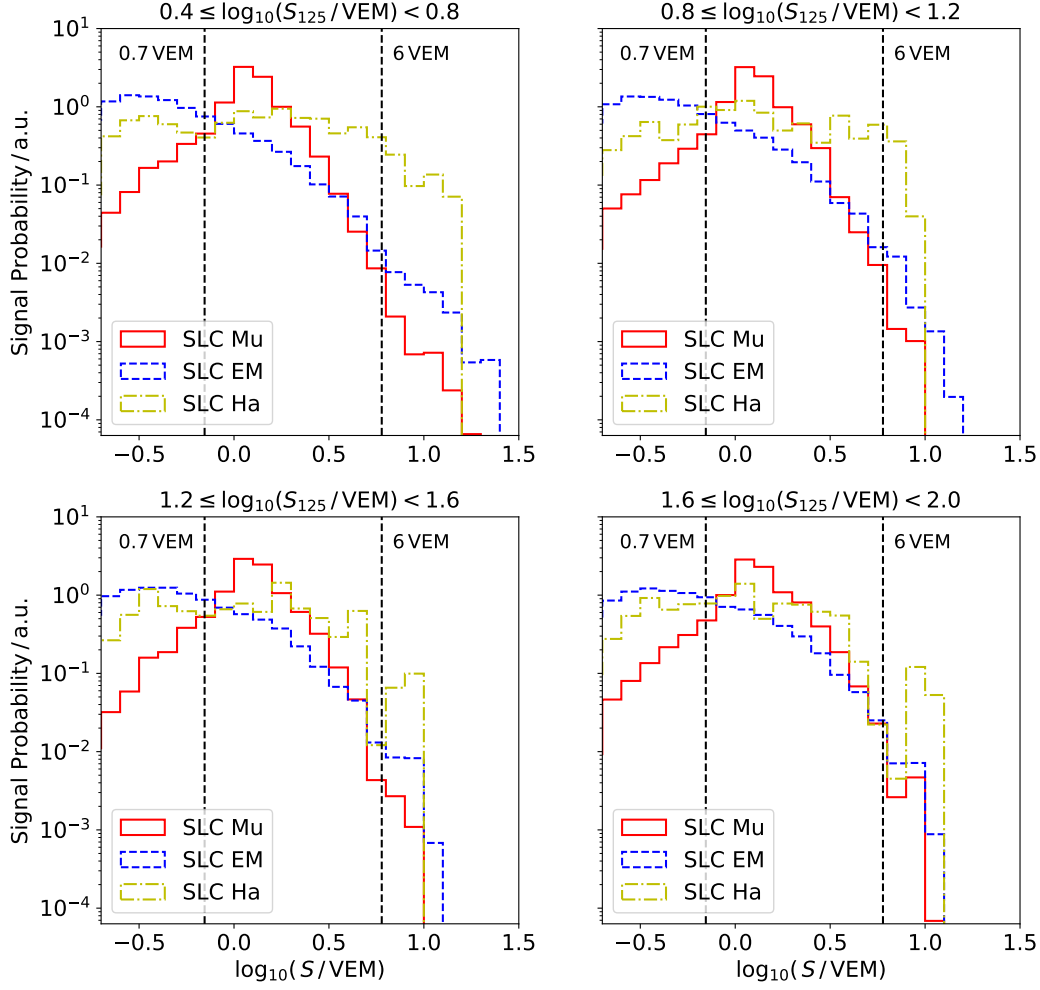


Figure 6.12.: Probability distributions for muons, EM particles and hadrons as a function of the cumulative signal measured in SLCs in bins of $\log_{10} S_{125}$. The distributions are based on air-shower simulations produced with the hadronic interaction model Sibyll 2.1. The two dashed lines bracket the SLC signal range included in the two-component reconstruction.

in measured charge histograms referred to as the muon peak. For smaller charge deposits, muons do not contribute significantly to the muon peak [199] and are sub-dominant to the EM component. Since the muon peak enters the two-component model by means of the muon spline fits, the same cut is applied for the analyses presented in this work. The lower SLC signal cut is illustrated as black dashed line in Fig. 6.12. A second cut on large SLC signals is motivated by the increased relative contribution of hadrons to the measured

signal distributions. In particular, late neutrons can produce large signal deposits far from the shower axis. Since the two-component model is not suited to describe the phase space of such hadronic contributions, an upper signal cut of 6 VEM is chosen for SLC signals included in the reconstruction. The signal cut is illustrated as second black dashed line in Fig. 6.12. Within the SLC signal range defined by both signal cuts, the muon and EM contributions can both be assumed to be significant. Therefore, for all included SLC triggers, a full convolution of EM and muon contribution is applied in the calculation of the corresponding signal likelihood.

Combined Log-Likelihood

With the investigation of the signal models for HLCs and SLCs, the combined signal likelihood can be constructed. For HLCs, different likelihood functions are implemented based on the small and large signal regimes. In the EMally dominated large signal regime, only the EM log-normal PDF is included. The likelihood is then calculated only based on the EM signal, $S - \langle S_\mu \rangle$, during the reconstruction. This procedure is analogous to fixing the muon expectation signal in the calculation of the likelihood. In case of the small signal regime, the cumulative signal measured in HLCs is dominated by EM contribution. Therefore, the likelihood is based on the EM log-normal probability for the measured signal S . For SLCs and for the intermediate signal regime for HLCs, the likelihood comprises a full convolution of the EM and muon signal PDFs. Overall, the HLC and SLC signal likelihoods can be summarized as

$$p_{\text{SLC}}(S|\theta, \langle S_{\text{em}} \rangle, \langle S_\mu \rangle) = \int_0^S p_{\text{em}}(S'_{\text{em}}|\theta, \langle S_{\text{em}} \rangle c_{\text{snow}}) p_\mu(S - S'_{\text{em}}|\theta, \langle N_\mu \rangle) dS'_{\text{em}},$$

$$p_{\text{HLC}}(S|\theta, \langle S_{\text{em}} \rangle, \langle S_\mu \rangle) = \begin{cases} p_{\text{em}}(S - \langle S_\mu \rangle|\theta, \langle S_{\text{em}} \rangle c_{\text{snow}}), & S > S_{\text{thr},1}, \\ p_\mu(0|\theta, \langle N_\mu \rangle) p_{\text{em}}(S|\theta, \langle S_{\text{em}} \rangle c_{\text{snow}}), & \log_{10} S < -0.2, \\ \int_0^S \frac{p_{\text{em}}(S'_{\text{em}}|\theta, \langle S_{\text{em}} \rangle c_{\text{snow}})}{p_\mu(S - S'_{\text{em}}|\theta, \langle N_\mu \rangle)} dS'_{\text{em}}, & \text{else}, \end{cases} \quad (6.22)$$

where the EM signal is attenuated via a snow correction factor, c_{snow} , to account for the snow accumulation. In case of the small signal regime, the log-normal PDF is additionally weighted with the probability, $p_\mu(0|\theta, \langle N_\mu \rangle)$, to not measure any signal contribution from muons. This is necessary because the signal threshold is of $10^{-0.2}$ VEM is applied on the signal strength measured in single HLC tanks. In principle, an application on the average expected total signal, $\langle S_{\text{tot}} \rangle = \langle S_{\text{em}} \rangle + \langle S_\mu \rangle$, is possible. However, this introduces an additional dependence on the model function used for the reconstruction. Additionally, the utilization of the measured signal strength results in a more stable reconstruction procedure.

As discussed in section 6.2, silent detectors are a crucial part of the LDF fit. The quan-

tification of the probability for a detector to not trigger given an expectation value is determined by the no-hit probability, $p_{\text{nohit}} = 1 - p_{\text{hit}}$. Within the convolution regimes, p_{nohit} is given by the convoluted cumulative distribution function of EM and muon PDFs and is therefore determined by the expectation values S_{em} and S_{μ} . Analogous to the HLC signal likelihood, the small signal regime is implemented also in the calculation of the silent likelihood for HLCs. In this case, p_{nohit} is determined solely by the log-normal cumulative distribution function for S_{tot} . The calculation of p_{nohit} can be summarized as

$$\begin{aligned}
 p_{\text{nohit,HLC}} &= \begin{cases} \int_{S_{\text{em}}=0}^{s_{\text{thr,HLC}}} p_{\text{em}}(S'_{\text{em}}|\theta, \langle S_{\text{tot}} \rangle), & \log_{10} \langle S_{\text{tot}} \rangle < -0.2, \\ \sum_{n=0}^{N_{\mu,2\sigma}} \frac{\langle N_{\mu} \rangle^n}{n!} e^{-\langle N_{\mu} \rangle} & \\ \cdot \int_{S_{\mu}=0}^{s_{\text{thr,HLC}}} \int_{S_{\text{em}}=0}^{s_{\text{thr,HLC}} - S_{\mu}} p_{\mu,\text{sig}}(S'_{\mu}|\theta, n) p_{\text{em}}(S'_{\text{em}}|\theta, \langle S_{\text{em}} \rangle c_{\text{snow}}), & \text{else,} \end{cases} \\
 p_{\text{nohit,SLC}} &= \sum_{n=0}^{N_{\mu,2\sigma}} \frac{\langle N_{\mu} \rangle^n}{n!} e^{-\langle N_{\mu} \rangle} \int_{S_{\mu}=0}^{s_{\text{thr,SLC}}} \int_{S_{\text{em}}=0}^{s_{\text{thr,SLC}} - S_{\mu}} p_{\mu,\text{sig}}(S'_{\mu}|\theta, n) p_{\text{em}}(S'_{\text{em}}|\theta, \langle S_{\text{em}} \rangle c_{\text{snow}}),
 \end{aligned} \tag{6.23}$$

where the threshold signals depend on the trigger type. For HLCs, a hardware motivated trigger threshold of $s_{\text{thr,HLC}} = 0.1657$ VEM is assumed similar to the standard reconstruction. In the case of SLCs, the signal threshold of $s_{\text{thr,SLC}} = 0.7$ VEM is motivated by the analysis itself and aims to increase the probability of SLC triggers originating from the muon contribution. The maximum number of muons included in the calculation, $N_{\mu,2\sigma}$, is chosen variably based on the average expected number of muons. Including the 2 sigma interval for the muon multiplicity, it is defined as

$$N_{\mu,2\sigma} = \text{int}(\max(3, N_{\mu} + 2\sqrt{N_{\mu}})), \tag{6.24}$$

with a minimum multiplicity of 3 muons taken into account in the convolution integrals. The saturation probability is determined by a log-normal CDF based on the cumulative expectation signal analogously to the standard reconstruction:

$$p_{\text{sat}} = \int_{s_{\text{thr,sat}}}^{\infty} d\log_{10} S \frac{1}{\sqrt{2\pi}\sigma_{\log_{10}\langle S_{\text{tot}} \rangle}} \exp\left(-\frac{(\log_{10} S - \log_{10}\langle S_{\text{tot}} \rangle)^2}{2\sigma_{\log_{10}\langle S_{\text{tot}} \rangle}^2}\right). \tag{6.25}$$

The combined log likelihood for the two-component fit containing the likelihood functions for triggered, saturated and silent detectors ($\mathcal{L}_{\text{trg}}$, $\mathcal{L}_{\text{sat}}$ and $\mathcal{L}_{\text{sil}}$) can then be summarized

as

$$\mathcal{L}_{\text{tot}} = \sum_i \log(p_{\text{HLC}}) + \sum_i \log(p_{\text{SLC}}) + \sum_i \log(p_{\text{sat}}) + \sum_i \log(1 - p_{\text{hit,HLC}}^2) + \sum_i \log(1 - p_{\text{hit,SLC}}), \quad (6.26)$$

where the sums run over all detectors of the corresponding type. It should be noted, that the inclusion of SLCs in addition to the application of a more flexible function for the description of the time curvature is in development at the time of writing. Further, a two-component time model using different fit functions for the time curvature of the EM and muon component is of interest for future analyses. The arrival time information of the different shower components such a model could provide can give an improved handle on the shower geometry and could hold valuable information for the two-component signal model.

In total, the combined likelihood features a set of 6 fit parameters, $\vec{q}_s$, that are varied to minimize the negative log-likelihood. The two-component LDF $S_{\text{Two-LDF}} = S_{\text{Two-LDF}}(r, \vec{q}_s) = S_{\text{Two-LDF}}(r, \vec{x}_c, S_{\text{em},125}, S_{\mu,550}, \beta_{\text{em}}, \beta_{\mu})$ is a function of the core position, $\vec{x}_c$, the EM and muonic shower size, $S_{\text{em},125}$ and $S_{\mu,550}$, and the corresponding slope parameters, β_{em} and β_{μ} . Here, r is a given lateral distance. The shower direction, which is used in the calculation of the lateral distance, is taken from the standard reconstruction. The two-component reconstruction is build on top of the standard reconstruction and therefore intrinsically has the same minimum HLC multiplicity requirement. However, the pulse cleaning algorithm used for the two-component reconstruction differs from the one used in the standard reconstruction (see section 4.3.1). The latter employs a cleaning based on the time delay with respect to the shower plane reconstructed with the standard reconstruction. While HLCs are required to be within 200 ns and -800 ns relative to the shower plane, the time window for SLCs is 50% smaller with $-500 \text{ ns} \leq t \leq 0 \text{ ns}$. This latter is chosen to minimize the influence of random background hits that are present in data while still including the bulk of the SLC hits with potential muon contribution.

Overall, the two-component reconstruction comprises 6 reconstruction steps. The first 3 steps contain the standard reconstruction described at the beginning of this section. In the different steps, the fit parameters are not varied all at the same time but successively. By that, the amount of free parameters per step is reduced which results in an increased fit stability. An overview of the two-component reconstruction steps along with the corresponding free parameters in each iteration is illustrated in Fig. 6.13. The derivation of initial seeds for the shower geometry and S_{125} is performed before the first step of the standard reconstruction. For β , a fixed value of 2.6 is used as an initial value. All steps in which both LDF and shower front parameters are listed, the combined signal and time likelihood is utilized. After each step, the resulting parameter values are passed to the

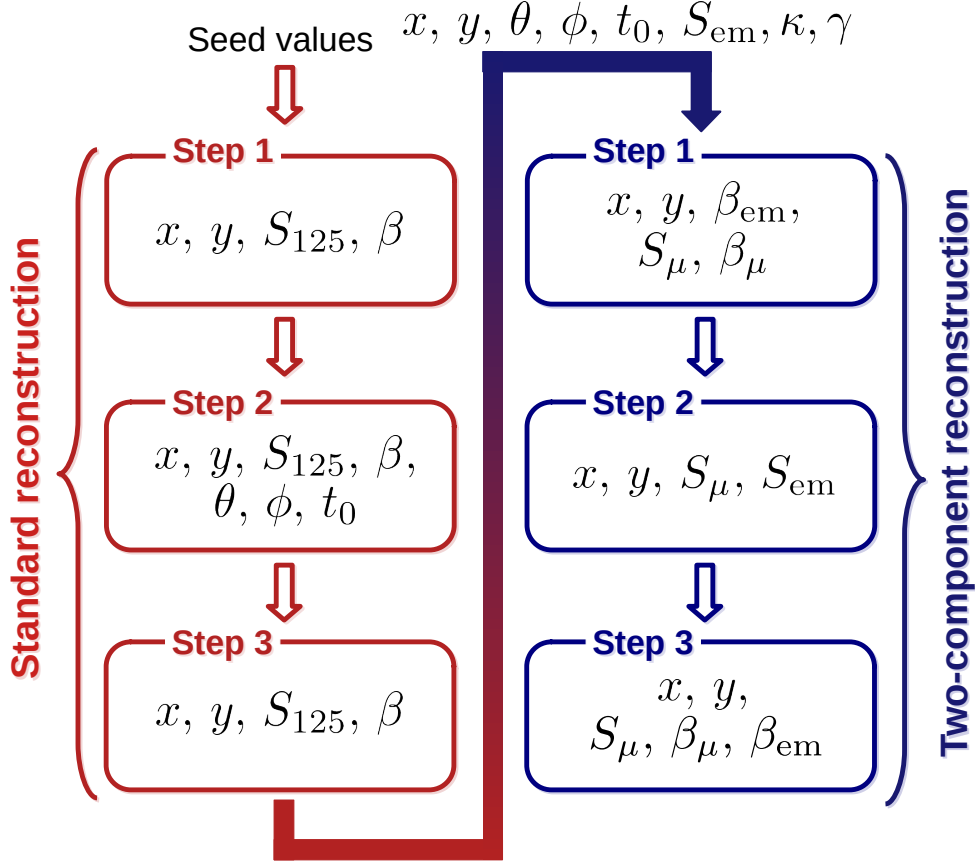


Figure 6.13.: Flow chart of all log-likelihood minimization steps used for the two-component reconstruction. The free parameters in each step are listed inside the boxes. Red color indicates the parts that belong to the standard reconstruction on top of which the two-component reconstruction is built. The steps for the latter are indicated in blue. The output of the standard reconstruction is used as high-quality seeds.

next step. In the standard reconstruction, the first step contains less free parameters and β is tightly bound to values between 2.9 and 3.1 in order to mainly fit the core position and the LDF normalization. The core position is always varied within relative bounds defined as a box around an initial value. In the following step, the signal and time likelihoods are utilized simultaneously for a combined fit of the shower direction and the LDF. For the last step, again only LDF parameters are varied while the direction is fixed. After this step, the reconstructed S_{125} value is used as an initial value for $S_{\text{em},125}$ and to derive initial values for κ and γ . For this purpose, the parametrization of κ and γ derived in section 6.2 for the average of the three hadronic interaction models Sibyll 2.1, EPOS-LHC and QGSJet-II-04 is applied. In the first step of the two-component reconstruction (Step 4), $\vec{x}_c$, $S_{\mu,550}$, β_{μ} and β_{em} are varied while $S_{\text{em},125}$ is fixed to first find the proper phase space for the muon LDF. In the second step, a combined fit of the shower direction, the core position and both LDF normalizations is performed. Lastly, the same parameters as in the first two-component reconstruction step are fit in combination with the shower

Table 6.3.: Settings for the two-component reconstruction steps. For the LDF parameters and the core position, both parameter bounds (given in brackets) and step sizes in each step are listed. In the case of the core position, $\vec{x}_c = (x, y)$, relative bounds defined with respect to an initial value are used.

Parameter	Step 1	Step 2	Step 3	Step 4	Step 5	Step 6
x/m	(-200,200), 10	(-15,15), 2.0	(-45,45), 1.0	(-5,5), 0.1	(-5,5), 0.1	(-5,5), 0.1
y/m	(-200,200), 10	(-15,15), 2.0	(-45,45), 1.0	(-5,5), 0.1	(-5,5), 0.1	(-5,5), 0.1
θ	-	0.01	-	-	-	-
ϕ	-	0.01	-	-	-	-
t_0/ns	-	50	-	-	-	-
β	(2.9,3.1), 0.6	(2.0,4.0), 0.15	(0.0,10.0), 0.15	-	-	-
$\lg S_{125}$	(-3.0,8.0), 1.0	(-3.0,8.0), 0.045	(-3.0,8.0), 0.045	-	-	-
$\lg S_{\text{em},125}$	-	-	-	-	(-3, 8), 0.01	-
$\lg S_{\mu,550}$	-	-	-	(-5.0, 2.0), 0.5	(-5.0, 2.0), 0.2	(-5.0, 2.0), 0.1
β_{em}	-	-	-	(1.0, 8.2), 0.2	-	(1.0, 8.2), 0.1
β_{μ}	-	-	-	(0, 1.8), 0.2	(0, 1.8), 0.05	(0, 1.8), 0.4

direction. In all three steps, the core position is tightly bound in a box of 5 m around the initial value. This is done because the core position reconstructed by the standard reconstruction is already of high quality. However, a small further variation of $\vec{x}_c$ can result in an improved estimate of the shower geometry due to the inclusion of SLCs in the two-component model⁵.

In all steps, the parameter bounds and step sizes vary. For both the standard and two-component reconstruction, the corresponding settings are optimized for showers that are contained within the IceTop array [181]. The settings for all reconstruction steps are

⁵Since the time fit and the LDF fits are entangled, also an additional variation in the parameters of the curvature function could improve the reconstruction of the shower geometry. However, it is found, that the direction resolution becomes slightly worse compared to the standard reconstruction. Therefore, the shower direction is fixed during the two-component reconstruction.

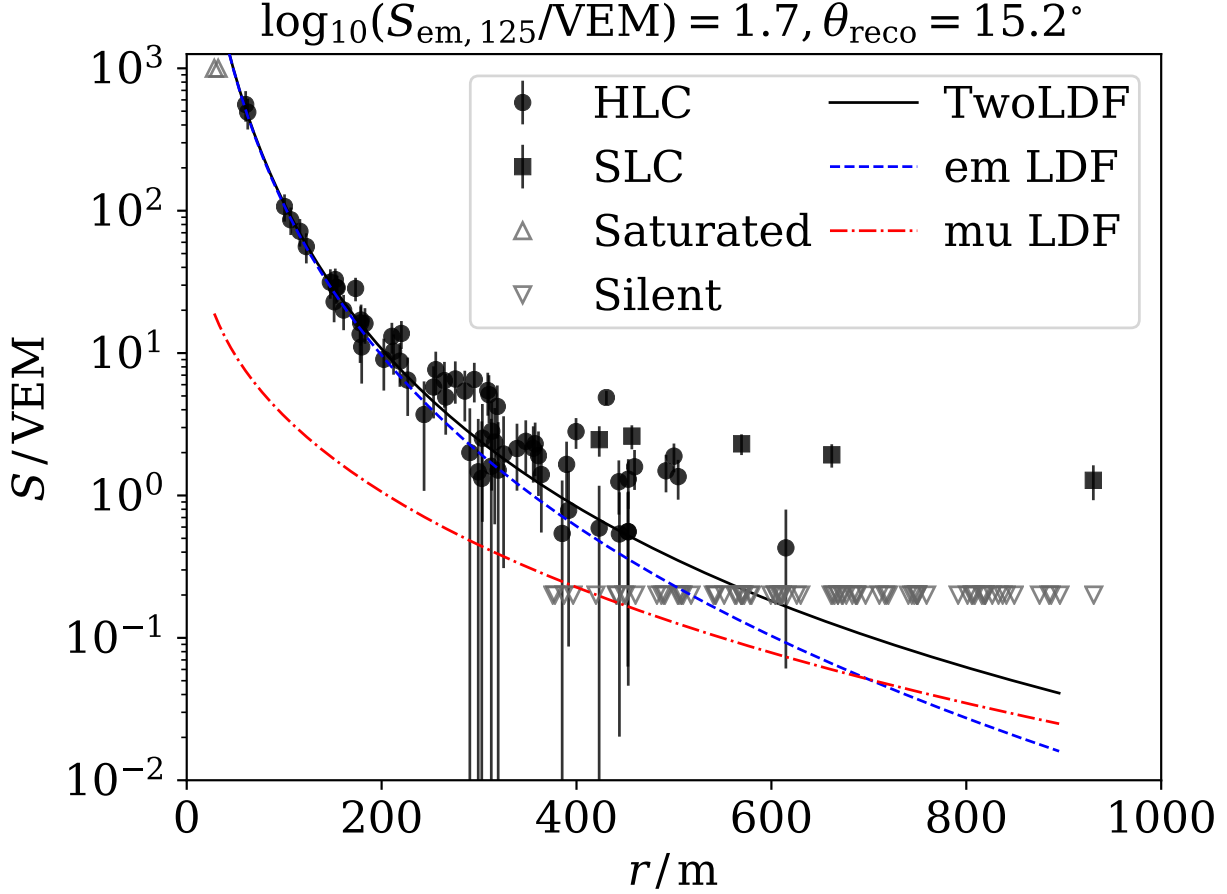


Figure 6.14.: Single event fit obtained after the last step of the two-component reconstruction for a simulated event ($\log_{10}(E_{\text{true}}/\text{eV}) = 16.71$, $\theta_{\text{true}} = 15.24^\circ$). HLCs and SLCs are drawn as circles and squares, respectively. The blue/red line shows the EM/muon LDF, the total LDF (black line) is given by the sum of both. Saturated and silent detectors are illustrated as upward and downward facing triangles and are placed at a fixed value of 1000 VEM and 0.2 VEM, respectively.

listed in Tab. 6.3. The minimization of the negative log-likelihood is performed using the MINUIT algorithm [247] with the SIMPLEX method.

An example two-component fit obtained after the last step for the reconstruction of a single proton initiated air-shower is shown in Fig. 6.14. While the EM LDF well describes the region close to the shower axis, the muon LDF becomes more dominant at large lateral distances, where SLC triggers become more frequent. The uncertainties drawn in Fig. 6.14 are derived by summing up the contributions of the EM and muon components to the total signal uncertainty in quadrature:

$$\sigma_{\text{tot}} = \sqrt{\sigma_{\text{em}}^2 + \sigma_{\mu}^2}, \quad (6.27)$$

where the EM and muon signal uncertainties, σ_{em} and σ_{μ} , are taken from Eq. (6.8) and Eq. (6.18), respectively. To account for the snow accumulation on top of the IceTop tanks,

the EM LDF is attenuated artificially based on the simple snow model. Therefore, the reconstructed total LDF does not line up with the raw measured HLCs and SLCs, which describe the charge deposit after snow attenuation. In Fig. 6.14, the measured signals are therefore corrected for the snow attenuation analogously:

$$S(r) = S'(r) \cdot \left(f_\mu(r) + (1 - f_\mu(r)) \cdot \exp \left[\frac{h_{\text{snow}}}{\lambda_{\text{snow}} \cos(\theta)} \right] \right), \quad (6.28)$$

$$f_\mu(r) = \frac{\langle S_\mu(r) \rangle}{\langle S_{\text{em}}(r) \rangle + \langle S_\mu(r) \rangle}.$$

Here, $S'(r)$ is the measured signal after snow attenuation and $S(r)$ is the corrected signal. Similarly to the two-component reconstruction, only the EM contribution is assumed to be attenuated by the snow. Thus, the muon fraction obtained from the EM and muon expectation values, $\langle S_{\text{em}}(r) \rangle$ and $\langle S_\mu(r) \rangle$, is used to correct the EM signal for a given hit.

Quality Cuts

To improve the reconstruction performance, a series of quality cuts are applied after the full two-component reconstruction. Intrinsically, the event filter removes events that have less than 5 triggered HLC stations⁶ from the analysis presented in this work. Additionally, the reconstruction itself is required to converge. Within the Level 3 processing, parameters that described the topology of events measured with IceTop are produced. These parameters are optimized to filter typical events used in IceTop analyses, i.e., air showers with core position inside of IceTop, energies above the $\sim$ PeV range and inclinations below 40° [42].

To satisfy the first criterion, a series of 4 conditions are required to be fulfilled. Firstly, a cut on the reconstructed core position itself is applied, removing events in which it lies outside of IceTop and too close to the edge of the array. The latter is motivated by the fact that core positions outside of IceTop can be pulled toward the edge of IceTop by the reconstruction algorithm. For this purpose, a so-called IceTop-containment fraction is defined, describing the relative location of the reconstructed core position to the edge of IceTop. Using a polygon that describes the outer edge of the IceTop array, the length of the line between the IceTop center and the reconstructed core location can be compared to the length of the line between the IceTop center and the edge of IceTop to obtain the IceTop-containment fraction:

$$\text{IT}_{\text{cont}} = \frac{D_{\text{it}}}{d_{\text{it}}}. \quad (6.29)$$

⁶It should be mentioned, that an additional small event filter requires only 3 HLC stations which can be used for a simpler version of the standard reconstruction. However, these events are not of interest for the two-component reconstruction and will therefore be neglected.

Here D_{it} and d_{it} are the distance from the center to the core and from the center to the edge, respectively. The value of IT_{cont} is required to be lower than 0.96. Secondly, the

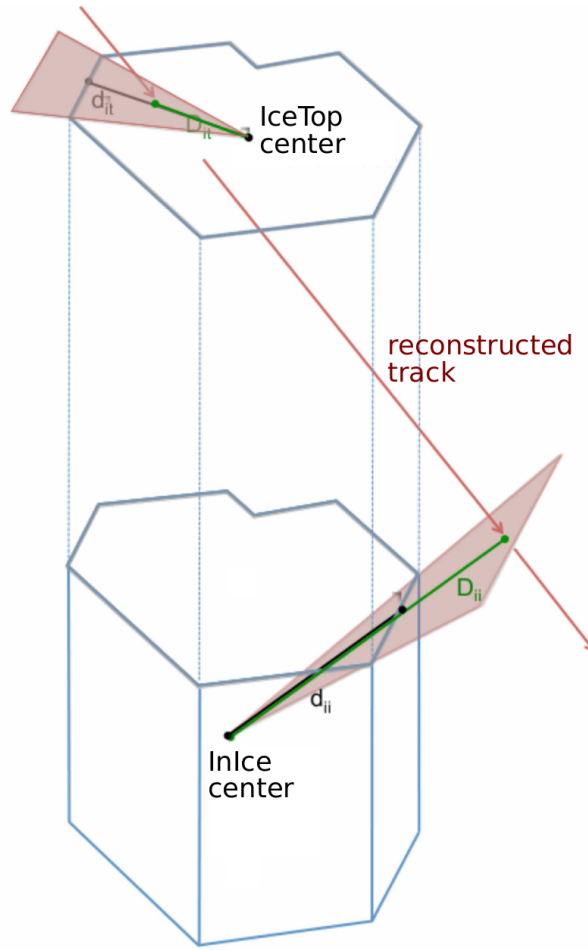


Figure 6.15.: Schematic view of the derivation of the IceTop- and IceCube-containment factors. The reconstructed shower axis is shown as a red arrow. D_{it} and d_{it} are the distances between the center of IceTop and the reconstructed core and between the center and the edge of IceTop, respectively. D_{ii} and d_{ii} describe the corresponding quantities for IceCube, where the smallest distance from the center to the shower axis is used. Figure taken from [42].

HLC tank with the highest charge is not allowed to be on the edge of the array, which mostly tackles events with core not too far outside of IceTop that still have sufficient EM contribution at the edge of IceTop [42]. However, events with core location further outside of IceTop, for which a significant part of the observed footprint is produced by the muon component, the highest charge is not necessarily on the edge. To remove these events, an additional two cuts require the maximum measured HLC signal to be at least 6 VEM as well as its neighboring tank to have a charge deposit of at least 4 VEM, both after correction of the snow attenuation.

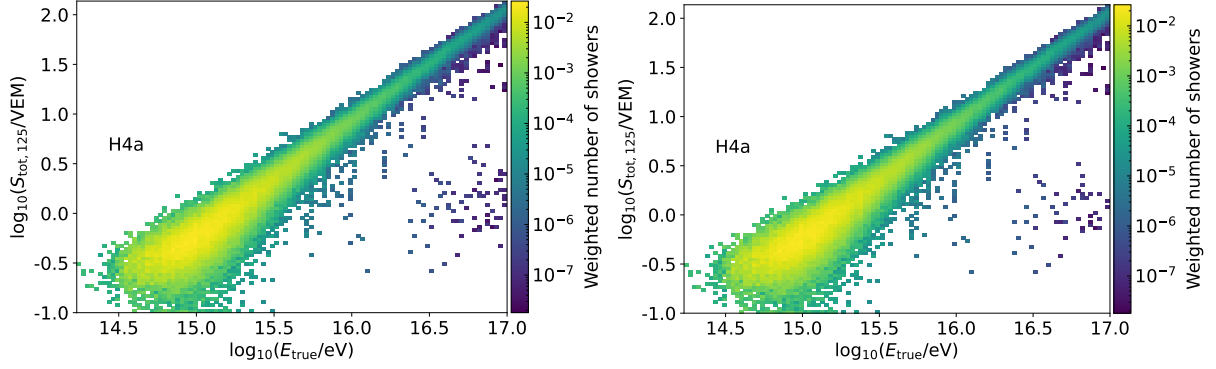


Figure 6.16.: $S_{\text{em},125}$ distribution as a function of the true primary energy derived from the last step of the two-component reconstruction after application of the standard IceTop quality cuts (left) and additionally the $S_{\mu,550}$ dependent cut on β_{em} (right) that removes a significant portion of mis-reconstructed events at high energies.

Further, to remove events with very sparse footprints that are likely produced by muon-rich inclined showers, a cut on the station density and on the reconstructed β value are applied. For the former, the ratio between triggered tanks to the total number of tanks is computed within a circle around the shower COG (Eq. (4.6)), where the radius of the circle is defined by the furthest hit. The station density has to have a value above 0.2. Since such showers produce a very flat charge distribution, the slope of the LDF tends to have small values. Therefore, β must be greater than 1.4.

The resulting relation of the energy proxy, $S_{\text{em},125}$, as a function of the true primary energy after application of these cuts is shown in Fig. 6.16 (left). The distribution contains events for the hadronic interaction model Sibyll 2.1 and is weighted to the H4a flux model. A clear correlation between the energy proxy and the true energy is visible, with the exception of an accumulation of events at high energies that have low values of $\log_{10} S_{\text{em},125}$. These events stem from shower events with true core location outside of the IceTop array that are mis-reconstructed as contained events. To remove a large fraction of these events, an additional two-dimensional quality cut is applied β_{em} as a function of $S_{\mu,550}$:

$$\beta_{\text{em}} > \begin{cases} 4 \log_{10} S_{\mu,550} + 1, & \log_{10} S_{\mu,550} \leq -1.23 \\ 2.5, & \log_{10} S_{\mu,550} > -1.23. \end{cases} \quad (6.30)$$

Since for with shower with true core location outside of IceTop mostly the shower tail is observed, the EM LDF does not have a good handle on the slope of the lateral distribution at small lateral distances and therefore does not provide a reliable estimate of the signal strength close to the shower axis. This results in too small values of β_{em} , i.e., in too flat reconstructed LDFs. However, the muon LDF is more sensitive to the shower tail and provides a sufficient estimate of the shower size even for such uncontained events. It can be noted, that because of this fact the two-component LDF in combination with a

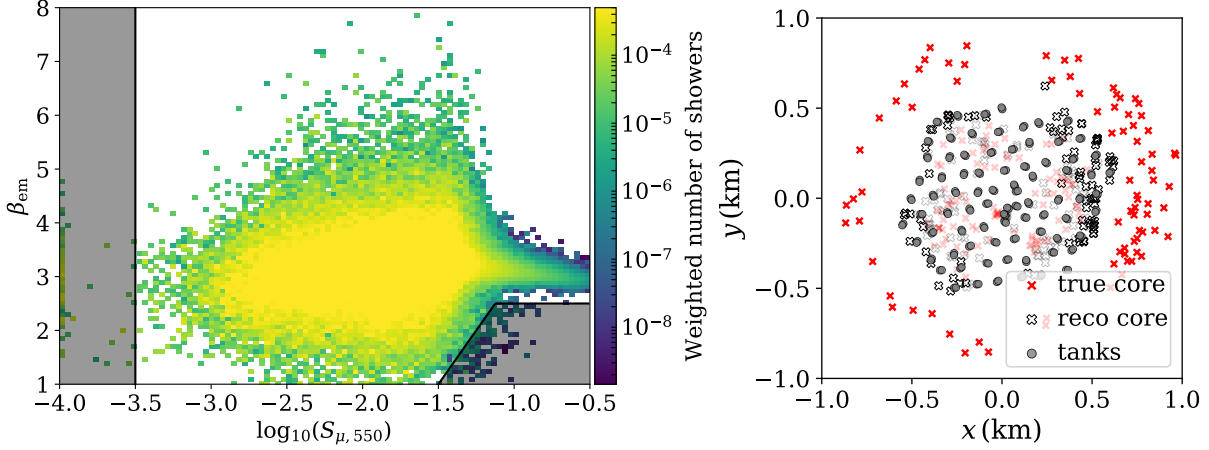


Figure 6.17.: Distribution of the β_{em} as a function of the muon number proxy, $\log_{10} S_{\mu,550}$ (left). The cut on small values of $\log_{10} S_{\mu,550}$ and the two-dimensional cut on β_{em} are illustrated as the left and right black shaded area, respectively. Bird view of IceTop with true and reconstructed core positions for events contained in the right black shaded area in the left figure (right). A large part of events with core outside of IceTop falsely reconstructed inside of the array are contained within this cut area. Some well reconstructed events with energies (< 10 PeV) as indicated by a lower opacity are also removed by the cut.

geometric reconstruction using the in-ice array is of high interest for the reconstruction of IceTop uncontained events⁷. The two-dimensional cut in Eq. (6.30) is visualized in Fig. 6.17 (left) for all three hadronic interaction models as the black shaded lower right corner. The events in this area are depicted in Fig. 6.17 (right). True and reconstructed core positions are shown as red and black crosses, respectively. It can be clearly seen, that a significant portion of events with true core outside of IceTop that are mis-reconstructed as contained within the cut area. Some events that are correctly reconstructed as being contained are removed by the chosen cut as well. However, this is only the case for events below the 10 PeV region. Air showers below the energy region are illustrated with lower opacity. In addition to the two-dimension cut, only events with $\log_{10} S_{\mu,550} > -3.5$ are included for later analyses. This cut removes low energy events with poor reconstruction quality. These events are well isolated from the main distribution as illustrated by the left black shaded area in Fig. 6.17 (left). Overall, the chosen cuts on β_{em} and $\log_{10} S_{\mu,550}$ successfully mitigate the influence of mis-reconstructed uncontained events and removes poorly reconstructed low-energy events. Together, both cuts lead to an event loss of roughly 0.1%.

The combination of standard and two-component quality cuts is summarized in Tab. 6.4.

⁷A reconstruction of air-shower events that are not contained within IceTop can significantly increase the statistics for cosmic-ray studies.

Table 6.4.: Overview of all quality cuts applied for the two-component analysis.

Quality cut	Condition
HLC multiplicity	≥ 5
Signal threshold for hottest HLC and its neighbor	true
Containment of hottest station	true
Station density	> 0.2
Convergence	true
IceTop-containment factor	< 0.96
β	> 1.4
β_{em}	$> \begin{cases} 4 \log_{10} S_{\mu,550} + 1, & \log_{10} S_{\mu,550} \leq -1.23 \\ 2.5, & \log_{10} S_{\mu,550} > -1.23 \end{cases}$
$\log_{10} S_{\mu,550}$	> -3.5

Reconstruction performance

Using the two-component reconstruction, separate LDFs are fit simultaneously to the measured signal distributions of air showers observed with IceTop. The technical details of the likelihood-based approach that is employed to combine both LDFs are discussed in detail in chapter 6. In this chapter, the reconstruction performance of the single-event based two-component model is evaluated. The basic principle of the reconstruction of the primary energy and muon number using the proxy parameters of both LDFs is introduced in section 7.1 and section 7.2, respectively. As discussed in chapter 5, the production of muon PDFs that form the basis of the implementation of the muon LDF within the two-component model requires inherent assumptions for the muon injection. In addition, the signal fluctuation model derived for the standard reconstruction is employed also for the modeling of the EM signal contribution within the two-component reconstruction. For this reason, the impact of these underlying assumptions on the reconstruction performance is tested in section 7.3. Lastly, the final performance in the context of the reconstruction of the shower geometry, the primary energy, and the muon number is quantified in section 7.4 and compared to other modern air-shower arrays within a comparable energy range in section 7.5.

7.1. Energy estimation

The reconstruction of the primary energy is of crucial importance for any cosmic-ray analysis. Due to the limited knowledge about the phase space of high-energy hadronic interactions in the collision of cosmic-rays with the Earth's atmosphere, a significant systematic uncertainty already arises from the choice of the high-energy hadronic interaction model used in simulations which are then compared to measured data to estimate the primary energy. Additionally, in real data no a-priori information about the type of the cosmic-ray is available. An additional systematic uncertainty therefore stems from the differences in the collision of heavy and light nuclei [86], which also have to be extrapolated from collider measurements. In order to minimize the influence of this contribution,

an energy proxy that has a minimal dependence on the primary mass is desirable. This mass dependence should then be balanced with the accuracy in the energy reconstruction such an energy proxy provides.

The approach to use the signal strength at a certain distance from the shower axis as a measure of the shower size and therefore the primary energy was first proposed by Hillas [248]. This *reference signal* taken at a given *reference distance* is determined by the reconstructed LDF. Since the majority of particles in the air-shower events observed with IceTop are electromagnetic, the function in the two-component model which has the highest correlation with the shower size is the electromagnetic LDF. For an accurate reconstruction of the primary energy with minimal mass dependence, the optimization of the reference distance is of crucial importance. The value for the optimal distance for the energy estimation is not expected to differ largely between the standard reconstruction and the two-component reconstruction. The latter is applied successively to the standard reconstruction and has S_{125} as a direct input for $S_{\text{em},125}$ because the standard reconstruction only employs HLCs is therefore mostly affected by the electromagnetic contribution. The reference distance of 125 m of the standard reconstruction has already been optimized to provide a good energy resolution with minimal mass dependence as well as a good fit stability [185]¹. Nevertheless, low-energy muons can have a small contribution to S_{125} . Additionally, the two-component reconstruction is affected by both HLCs and SLCs. Both effects can lead to a small change in the optimal reference distance and is studied by re-processing the two-component reconstruction with different values of the electromagnetic reference distance, R_{em} . For the evaluation of the energy reconstruction performance, two different approaches are chosen. Firstly, $S_{\text{em},125}$ is directly taken as energy proxy and used to derive a conversion function to obtain the reconstructed primary energy. Secondly, the muon contribution to the expected signal at 125 m is included for the energy estimation. In that case, the energy proxy is given by the total expectation signal at 125 m:

$$S_{\text{tot},R_{\text{em}}} = S_{\text{em},R_{\text{em}}} + S_{\mu} \left(\frac{R_{\text{em}}}{R_{\mu}} \right)^{-\beta_{\mu}} \left(\frac{R_{\text{em}} + 320 \text{ m}}{R_{\mu} + 320 \text{ m}} \right)^{-\gamma}, \quad (7.1)$$

where the muon LDF is extrapolated to 125 m using the reconstructed parameters for β_{μ} and S_{μ} on a single-event basis. While a purely electromagnetically based energy estimation is theoretically preferred due to the large fluctuations and model dependence in the muon component, both LDFs within the two-component model are intrinsically

¹Additionally, two further studies have been conducted. A numerical study was performed in [249] by dividing IceTop into two sub-arrays using only one tank in each HLC station and testing the reconstruction stability. An analytical study minimizing the correlation between the energy proxy and the slope of the LDF is presented in [250]. The optimal value of 125 m was independently confirmed by both studies.

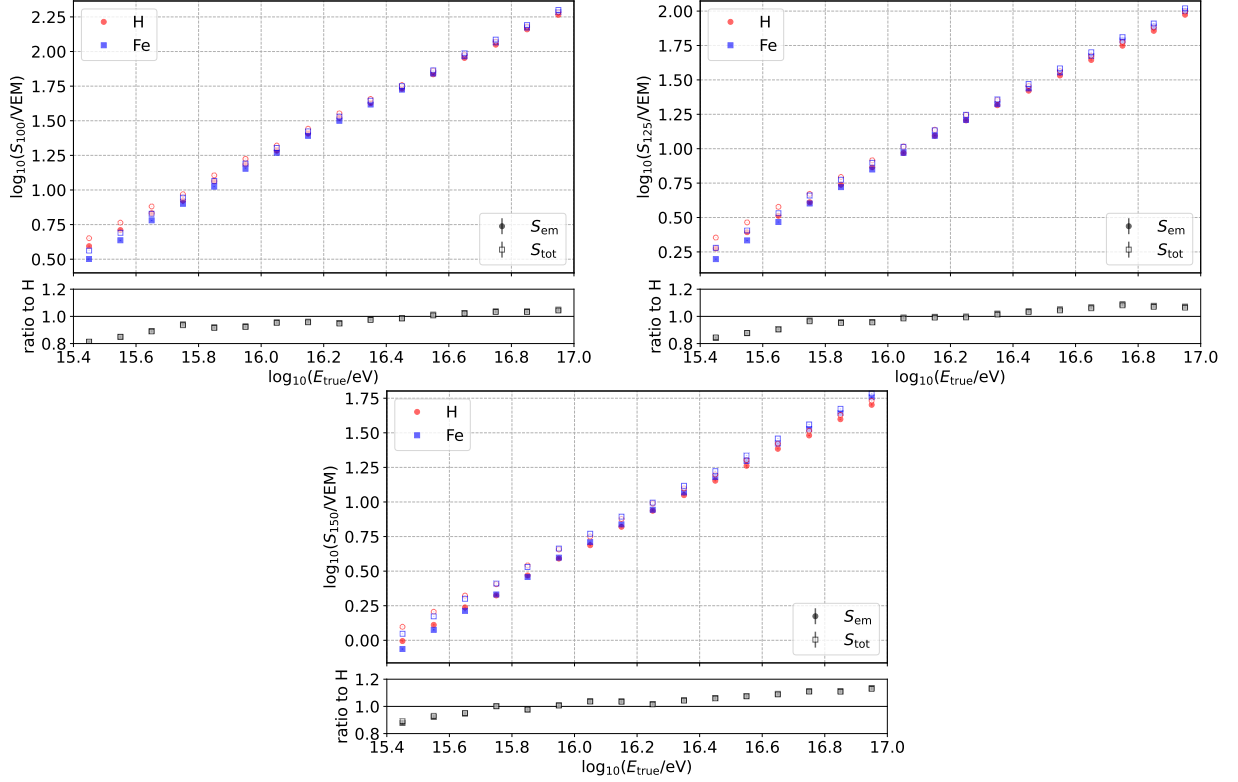


Figure 7.1.: Distribution of $S_{\text{em},125}$, and $S_{\text{tot},125}$ as a function of primary energy for reference distances of 100 m (top left), 125 m (top right), and 150 m (bottom) for near-vertical air-showers ($\cos \theta > 0.9$) produced with Sibyll 2.1 and weighted to the H4a flux model. Lower panels show the ratio between iron and proton.

entangled. A consideration of both components can therefore potentially help with the inclusion of additional information from the SLCs and in the context of fit stability. In particular, for low-energy events that have limited hit multiplicity and are prone to large shower-to-shower fluctuations, additional information provided by the muon LDF could be beneficial for the reconstruction performance. Additionally, while sublinear, the number of muons is strongly correlated with the primary energy.

The relation between both energy proxies and the true primary energy for proton- and iron-initiated showers are shown in Fig. 7.1 for different choices of R_{em} . Generally, in both cases, no large splitting between the proton and iron points is visible. However, the magnitude of the difference between proton and iron is a function of the primary energy. One qualitatively universal feature for all distances is the crossing of the proton and iron points. This is related to the steepness of the electromagnetic LDF. Since the slope of the electromagnetic LDF strongly depends on the primary energy and mass, the lateral distance at which a minimum difference between different primary types is expected also

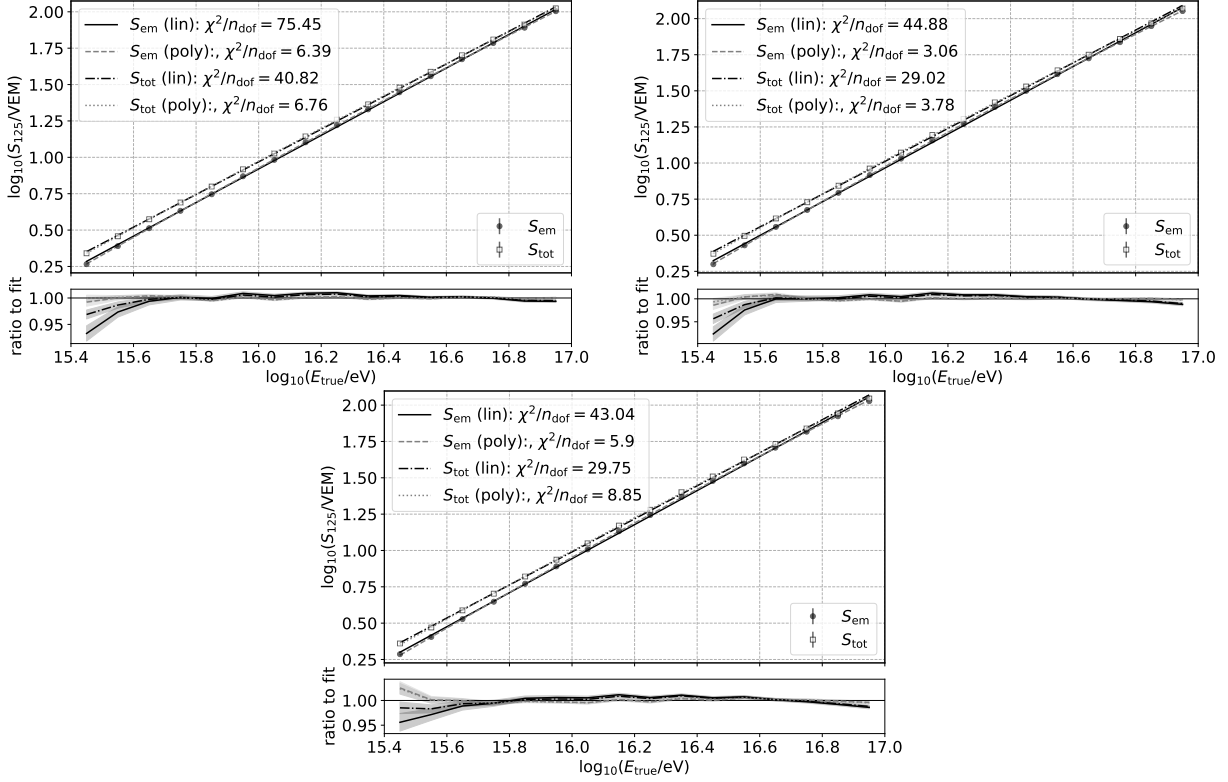


Figure 7.2.: Calibration function fits to the distribution of $S_{\text{em},125}$, and $S_{\text{tot},125}$ as a function of primary energy for a reference distance 125 m for near-vertical air-showers ($\cos \theta > 0.9$) produced with Sibyll 2.1 (top left), EPOS-LHC (top right), and QGSJet-II-04 (bottom). Lower panels show the ratios to the fits. All distributions are weighted to the H4a flux model.

changes as a function of energy². In theory, the optimal reference distance is therefore a function of primary energy. In practice, however, a single reference radius suited for the application within a given energy range is typically preferred. The dependence on R_{em} is clearly visible in the shift of the crossing point between proton and iron, as well as in the increasing separation between both masses for lower and higher primary energies relative to it. In this context, a reference distance of 125 m seems to be well suited for this energy range for both $S_{\text{em},125}$ and $S_{\text{tot},125}$ as the crossing point is located roughly in the center of the energy (and zenith angle) range of interest. The mass dependence in the energy estimation is therefore well balanced for lower energies ($\log_{10}(E_{\text{true}}/\text{eV}) \lesssim 16$) and higher energies ($\log_{10}(E_{\text{true}}/\text{eV}) \gtrsim 16.4$). The offset between $S_{\text{em},125}$ and $S_{\text{tot},125}$ increases with increasing R_{em} . This is due to the increasing influence of the muon contribution at farther distances to the shower axis. However, despite the offset, no significant difference in the mass dependence is visible between both proxy parameters. In the context of the

²Note, that the point of the least fluctuations in the energy proxy is not necessarily similar to the point at which the smallest difference between different primary masses is observed.

Table 7.1.: Parameter values for calibration function (Eq. (7.3)) fits to $S_{\text{em},125}$ and $S_{\text{tot},125}$ as a function of the true primary energy.

hadronic model	$S_{\text{em},125}$			$S_{\text{tot},125}$		
	p_1	p_2	p_3	p_1	p_2	p_3
Sibyll 2.1	-0.0436	1.1925	0.6904	-0.0291	1.1460	0.7457
EPOS-LHC	-0.0591	1.2158	0.7360	-0.0433	1.1687	0.7882
QGSJet-II-04	-0.0566	1.2163	0.7119	-0.0403	1.1683	0.7652

energy reconstruction, a splitting between proton and iron in the energy proxy directly translates to an energy bias since the energy is reconstruction via a single calibration fit. As calibration fits, two different model functions are tested, a linear function and a 2nd order polynomial:

$$\log_{10} S_{\text{em}/\text{tot}} = p_1 \log_{10}(E/\text{eV}) + p_2, \quad (7.2)$$

$$\log_{10} S_{\text{em}/\text{tot}} = p_1 (\log_{10}(E/\text{eV}) - c_E)^2 + p_2 (\log_{10}(E/\text{eV}) - c_E) + p_3, \quad (7.3)$$

where the constant $c_E = 15.8$. The resulting calibration function fits for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 are shown in Fig. 7.2. It is clear that a purely linear calibration function is not well suited for the energy estimation using the two-component reconstruction. Eq. (7.3), however, results in significantly improved χ^2/n_{dof} values and is therefore preferred. This is the case for all included hadronic interaction models. The results for the calibration function fits using Eq. (7.3) are listed in Tab. 7.1.

Using the calibration fits, the energy proxy parameters can be converted to the reconstructed energy. The reconstructed energies are binned along the true energy and for each bin the difference between the true and reconstructed values are calculated. Since differences are normally distributed in logarithmic space, the logarithm of the differences can be modeled using a Gaussian fit in each energy bin. The energy resolution and bias is then given by the standard deviation and the mean of each Gaussian, respectively. The resulting energy-reconstruction resolution and bias is shown in Fig. 7.3 for Sibyll 2.1. For the energy resolution, the preferred value of R_{em} depends on the shower size. While a larger value of R_{em} seems to be beneficial at the highest energies, for region of $\log_{10}(E_{\text{true}}/\text{eV}) \lesssim 16$, the intermediate value of R_{em} are preferred. While the reconstruction accuracy is compatible for S_{em} and S_{tot} at high-energies, the inclusion of the muon contribution at R_{em} leads to a significant improvement in the accuracy at energies below ~ 10 PeV and to a higher stability. At the same time, the change in the reconstruction bias with increasing R_{em} is significantly larger for proton primaries for S_{tot} . Nevertheless, the absolute magnitude of the energy bias is comparable for both energy

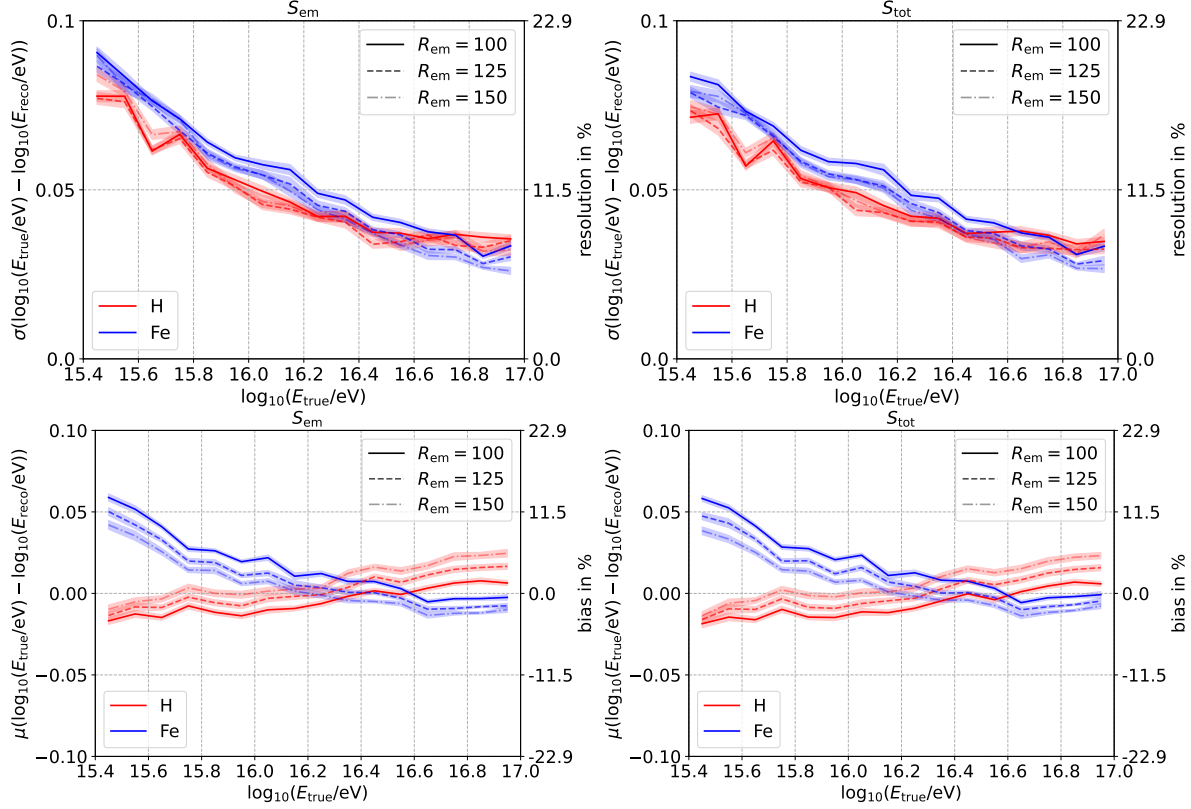


Figure 7.3.: Energy reconstruction resolution (top row) and bias (bottom row) for S_{em} (left column) and S_{tot} (right column) for different reference distances. Included are near-vertical proton and iron showers ($\cos \theta > 0.9$) produced with Sibyll 2.1.

proxies. A value of $R_{\text{em}} = 100$ m, leads to a significantly larger reconstruction bias at lower energies (under-/overestimation of up to $\sim 12\%/8\%$ for iron/proton) and a smaller bias at energies approaching 100 PeV compared to larger values of R_{em} . Together with the energy dependence in the resolution, this suggests that the ideal value of R_{em} may be chosen based on the use case for a specific analysis. In the context of the two-component reconstruction, a balance between a good reconstruction resolution and a small mass dependence is preferred. Since in this regard no significant improvement is visible between the tested reference distances and $R_{\text{em}} = 125$ m, and for consistency reasons with the standard reconstruction and previous analyses, a value of 125 m is chosen as electromagnetic reference distance for the two-component model. To reconstruct the primary energy, an energy proxy utilizing the total expectation signal at the reference distance, $S_{\text{tot},125}$, is preferred. This is likely because of the additional information from SLCs, which improves the energy reconstruction particularly for lower energies. Therefore, for this work, $S_{\text{tot},125}$ is used to derive the primary energy. A more detailed discussion about the final energy reconstruction performance of the two-component model as well as a comparison to the standard reconstruction is given in section 7.4.

7.2. Muon number estimation

Similar to the energy reconstruction in which the electromagnetic LDF is used to derive a proxy for the primary energy, the muon LDF offers a proxy for the muon component in the same air-shower events. As for the energy reconstruction, measured data is compared to the expectation from simulations to derive the muon contribution in real events. This introduces model and mass dependencies. In particular for the reconstruction of the muon component, where different hadronic interaction models exhibit significant differences, an optimization of a corresponding proxy parameter is of high importance. Analogously to the energy reconstruction, the proxy parameter $\log_{10} S_\mu$ of the muon LDF is the muon signal strength at a given reference distance, R_μ . Since the two-component model provides an LDF that is defined over the entire IceTop lateral distance range, the muon proxy parameter can be understood as an overall normalization of the muon LDF and can therefore be used as an estimate for the total muon number in air showers.

Optimal reference distance

To optimize the muon number proxy, different muon reference distances are scanned and used to minimize the dependence of the muon reconstruction on the primary mass. For this purpose, Fig. 7.4 shows the relation between the muon number proxy and the true muon number obtained from CORSIKA simulations for Sibyll 2.1. In the respective figures, the evolution of the average $\log_{10} S_\mu$ for different choices of R_μ as a function of the muon number is shown. For the derivation of the muon number, only muons above an energy of 210 MeV and lateral distances of ≤ 1000 m are counted. The energy threshold is motivated by the minimum muon energy required to produce a signal of 0.7 VEM for the smallest snow coverage on top of the IceTop tanks measured for the year 2012. Due to the geometry of IceTop, hits can have a maximum lateral distance of 1000 m for contained events. Therefore, only muons within this lateral distance range contribute to the measured charge distribution. The scale of $\log_{10} S_\mu$ decreases with increasing muon reference distance, since the muon density decreases with distance to the shower axis. In contrast to the energy proxy, the muon proxy does not exhibit a crossing of the average values for heavy and light primaries. Instead, an energy independent offset between proton and iron is visible. This is likely caused by the flat nature of the muon LDF compared to the electromagnetic LDF. The ordering of this offset changes as a function of R_μ , featuring significantly larger values of S_μ for proton showers compared to iron showers for the same muon number at $R_\mu = 500$ m. This effect is reduced slightly for $R_\mu = 550$ m and nearly vanishes for $R_\mu = 600$ m. In the context of the muon number reconstruction, such a bias will result in an underestimation of the reconstructed muon number for proton showers

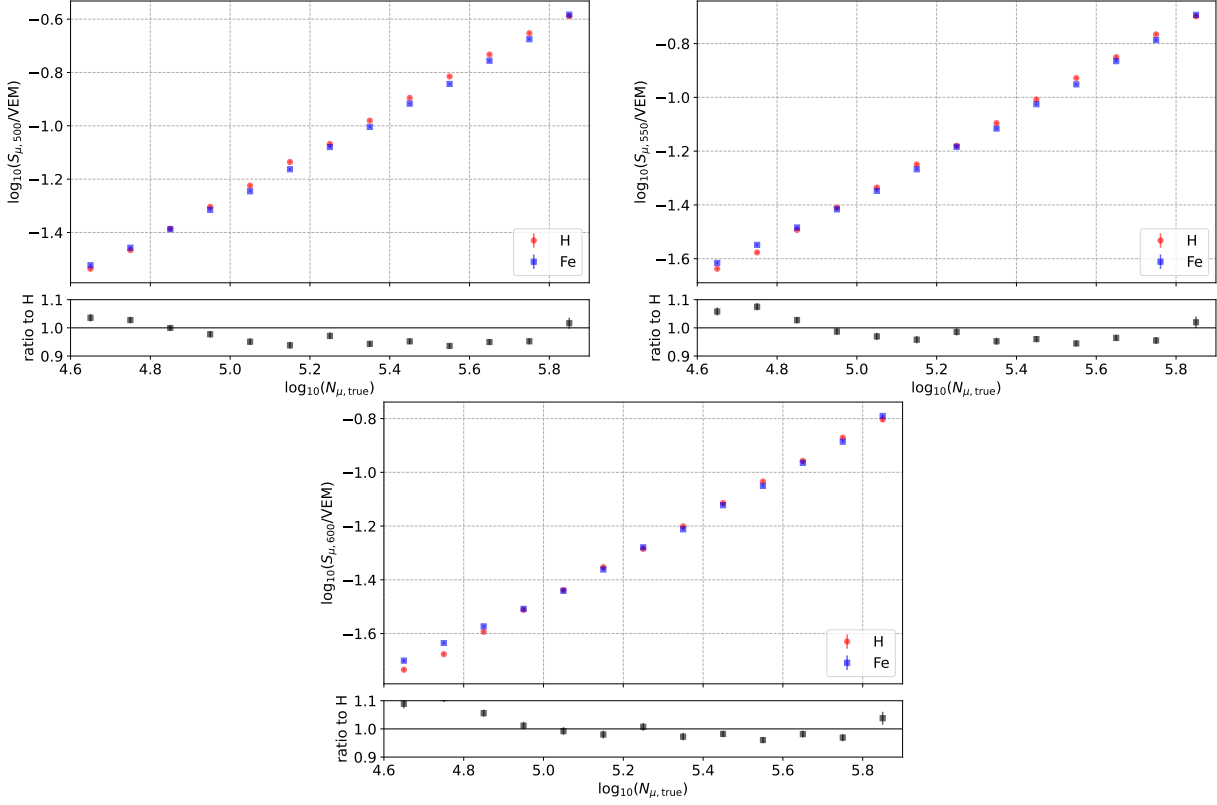


Figure 7.4.: Muon number proxy for the muon reference distances 500 m (top left), 550 m (top right) and 600 m (bottom) as a function of the true muon number in near vertical air-showers ($\cos \theta > 0.9$) derived from CORSIKA. All distributions are based on CORSIKA simulations produced with Sibyll 2.1 and are weighted to the H4a flux model. The lower panels show the ratio between iron and proton.

for $R_\mu = 500$ m. Thus, for the optimization of the mass dependence in the muon number reconstruction, the offset between proton and iron should be minimized. In order to study the differences in the reconstruction performance in more detail, the $\log_{10} S_\mu$ distributions for each R_μ are used to derive calibration functions to convert the muon proxy to the reconstructed muon number. Fig. 7.5 shows the resulting calibration function fits for one muon reference distance ($R_\mu = 550$ m) for the three hadronic interaction models. Two different calibration functions of form

$$\log_{10} S_\mu = p_1 \log_{10} N_\mu + p_2, \quad (7.4)$$

$$\log_{10} S_\mu = p_1 \left(\log_{10} N_\mu - c_{N_\mu} \right)^2 + p_2 \left(\log_{10} N_\mu - c_{N_\mu} \right) + p_3, \quad (7.5)$$

are tested analogously to the energy reconstruction. Here, the constant c_{N_μ} takes the value 4.85 for Sibyll 2.1 and 4.95 for EPOS-LHC and QGSJet-II-04, motivated by the increased muon content of the post-LHC models compared to Sibyll 2.1. While the fit with the simple linear function results in comparably large values for the reduced χ^2 , the curved function Eq. (7.5) results in an improved description of the evolution of S_μ

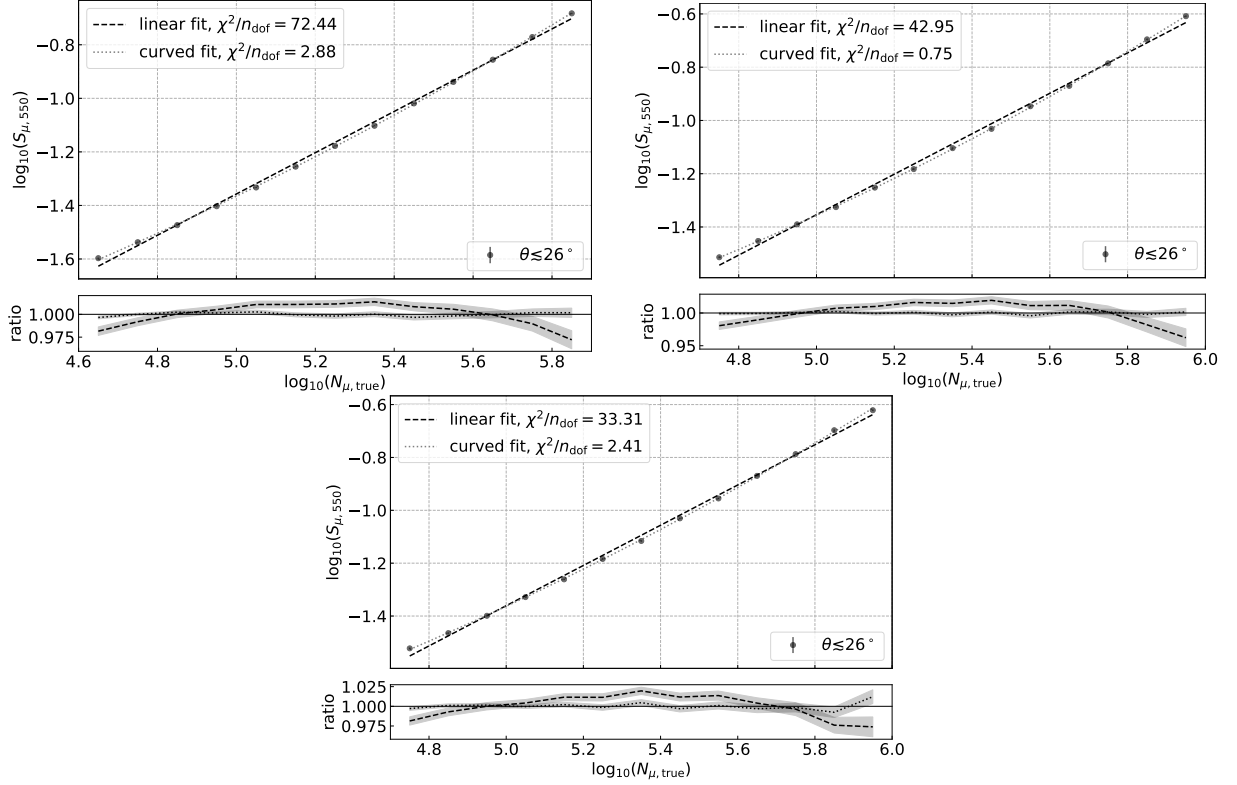


Figure 7.5.: Calibration function fits to the distribution of $S_{\mu,550}$ as a function of the true muon number for the hadronic interaction model Sibyll 2.1 (top left), EPOS-LHC (top right) and QGSJet-II-04 (bottom). All distributions are weighted to the H4a flux model.

with increasing muon number across all three hadronic interaction models. The resulting parameter values for both fits is given in Tab. 7.2. It is interesting to note, that the sign of p_1 is flipped compared to the energy calibration fit. Thus, the curvature of the fit function is concave for the energy calibration and convex for the muon number calibration. This strengthens the assumption that the slight curvature in the distribution of the energy proxy and the muon number proxy as a function of their respective true quantities is a feature of the reconstruction that is caused by the entanglement of the electromagnetic and muon LDF. As for the energy reconstruction, the muon number is reconstructed using a 2nd order polynomial based calibration function. After the calibration fit to the H4a weighted distributions, the distributions of the differences of the true and reconstructed muon number for each primary mass can be used to infer the reconstruction resolution and bias analogously to the energy reconstruction. The distributions of $\log_{10} N_{\mu,true} - \log_{10} N_{\mu, reco}$ in each true muon number bin can be modeled with a Gaussian. The standard deviation and mean of each Gaussian determine the reconstruction resolution and bias, respectively. In Fig. 7.6 (left), the reconstruction resolution is shown for different R_μ for proton and iron initiated showers produced with Sibyll 2.1. A clear trend toward improved resolutions is visible with decreasing R_μ . This is expected, as

Table 7.2.: Parameter values for calibration function (Eq. (7.5)) fits to S_μ as a function of the true muon number.

hadronic model	p_1	p_2	p_3
Sibyll 2.1	0.1059	0.6829	1.4701
EPOS-LHC	0.1272	0.6546	1.3892
QGSJet-II-04	0.1129	0.6704	1.3971

the impact of fluctuations of the particle density decreases closer to the shower axis. For $R_\mu = 500$ m, the reconstruction resolution falls below 20% already for muon numbers of $\log_{10} N_{\mu,\text{true}} = 5.5$ and is better than 15% for the highest energies considered. For all cases, the resolution reaches values of $\lesssim 20\%$, for energies approaching 100 PeV. For large $R_\mu = 600$, however, the resolution becomes worse for $\log_{10} N_{\mu,\text{true}} < 5.0$. Therefore, in terms of reconstruction resolution, a smaller muon reference distance is preferred. However, due to the differences in the average height of the first interaction for different primary masses with the same primary energy, the shower size at the observation level differs accordingly. Therefore, depending on the primary mass, an over- or underestimation of the muon number can occur, leading to a mass dependence in the reconstruction. This systematic shift is represented by the reconstruction bias and is illustrated in Fig. 7.6 (right) for proton and iron showers and for different R_μ . It can be observed that the absolute magnitude of the mass bias is different for proton and iron primaries. This is caused by the application of the H4a flux model in the calibration function fit. Under the assumption of an equal proton/iron composition, the mass bias would be of the same order for both primary types. For $R_\mu = 500$ m, the difference between proton and iron is as large as $\sim 7\%$, where the reconstructed muon number is overestimated for proton and slightly underestimated for iron. A minimum separation is observed for large muon numbers for $R_\mu = 600$ m to a level of a few percent. The magnitude of the separation between proton and iron in the reconstruction bias therefore changes as a function of R_μ . However, at $\log_{10} N_{\mu,\text{true}} \lesssim 4.7$, the mass dependence increases again for large R_μ , which leads to a significant underestimation of the reconstructed muon number for proton. Nevertheless, in terms of mass dependence in the muon number reconstruction, a larger muon reference distance of $R_\mu \sim 600$ m is preferred for Sibyll 2.1. For an optimization of the reconstruction performance, a balance between a good reconstruction resolution and a small bias can be considered. An optimal value could therefore be around $R_\mu \sim 550$ m. In general, however, since the relative importance of the resolution and bias depends on the application, R_μ can be optimized for a specific analysis goal. Due to the large mass dependence in the number of muons in air showers, a higher importance is assigned to a minimization of the mass dependence in the muon number reconstruction in order to

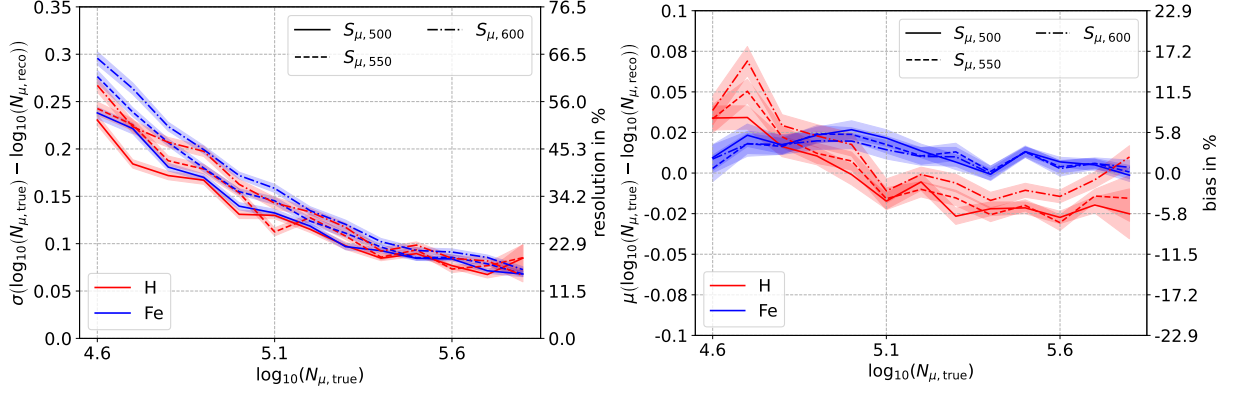


Figure 7.6.: Resolution (left) and bias (right) for the muon number reconstruction using different muon reference distances R_{μ} for proton and iron initiated showers produced with Sibyll 2.1.

reduce the overall mass bias of the two-component reconstruction. Note that the exact reconstruction resolution and bias depends on the hadronic interaction model used in the simulations. To find the optimal R_{μ} that minimizes the mass dependence across the different hadronic interaction models, the absolute systematic shift between proton and iron in the muon number reconstruction is minimized for the entire range of muon numbers considered for each model individually. For computational reasons and because of fluctuations between reconstruction runs, this minimization is performed by extrapolating the signal expectation values of the reconstructed muon LDF at different distances. However, in practice, an extrapolation does not necessarily produce the same result as a complete re-processing of the reconstruction using an adjusted value of R_{μ} . Therefore, this process is repeated for the limited set of R_{μ} shown in Fig. 7.6. The sums of the absolute values of the difference in the reconstruction bias for proton and iron showers are shown in Fig. 7.7 as a function of R_{μ} for all three hadronic interaction models. Here, the reconstruction set that applies $R_{\mu} = 550$ m is used. However, for reconstructions applying different R_{μ} , a similar behavior is observed. The parabolic shape reflects the evolution of the mass splitting of S_{μ} with increasing R_{μ} and exhibits a clear minimum. However, since the post-LHC models generally feature a larger number of muons and exhibits differences in the muon and electromagnetic lateral distributions, the distance at which the minimum mass dependence is obtained differs across the models. Compared to Sibyll 2.1, the optimal R_{μ} shifts toward smaller values. Since EPOS-LHC features the highest muon content of the three models, the corresponding optimal R_{μ} is smallest. To find a suitable R_{μ} that is applicable for all models, a value of $R_{\mu} = 550$ m is chosen as average value of the three models and across the different re-processed reconstructions.

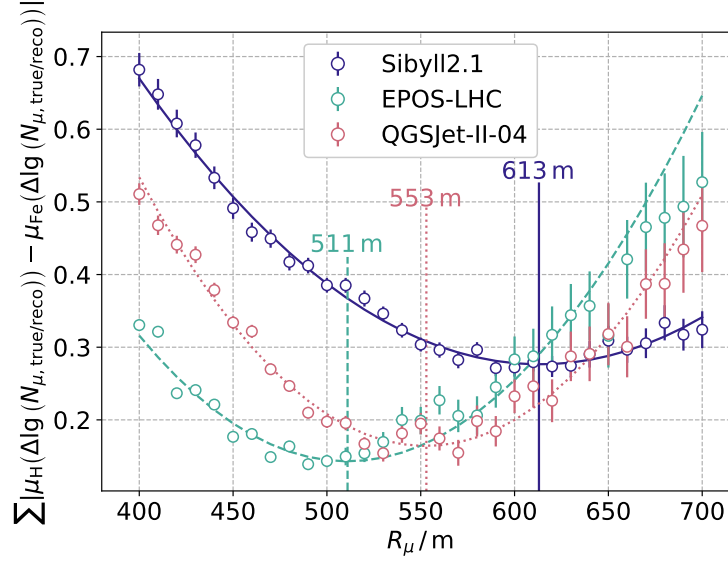


Figure 7.7.: Sum of the absolute reconstruction bias difference for proton and iron initiated showers as a function of the muon reference distance, R_μ , for the hadronic interaction models Sibyll 2.1, EPOS-LHC and QGSJet-II-04.

7.3. Validity tests

For a further optimization of the two-component reconstruction, the underlying assumptions implemented in the model can be tested and evaluated in the context of reconstruction performance. Firstly, the parametrization of the large signal regime derived in section 6.3, defining the phase space for the muon contribution included in the two-component model influences its performance. Secondly, utilizing the primary zenith angle in the evaluation of the muon PDFs within the reconstruction implies the assumption that the direction of muons coincides with the shower axis. The validity of this assumption and its impact on the reconstruction performance is studied in this section. Further, the derivation of the muon PDFs requires an assumption about the energy of the muons injected for IceTop tank response simulations. The impact of the different muon PDFs obtained in chapter 5 on the two-component reconstruction is tested.

7.3.1. Muon angular spread

One of the main simplifying assumptions for the muon number reconstruction using the two-component LDF is the alignment of the zenith angles of the individual muons with the primary zenith angle. In reality, muons from cosmic-ray air showers can manifest a significant spread with respect to the primary direction. The magnitude of this spread depends on multiple factors, such as the properties of the primary particle and the de-

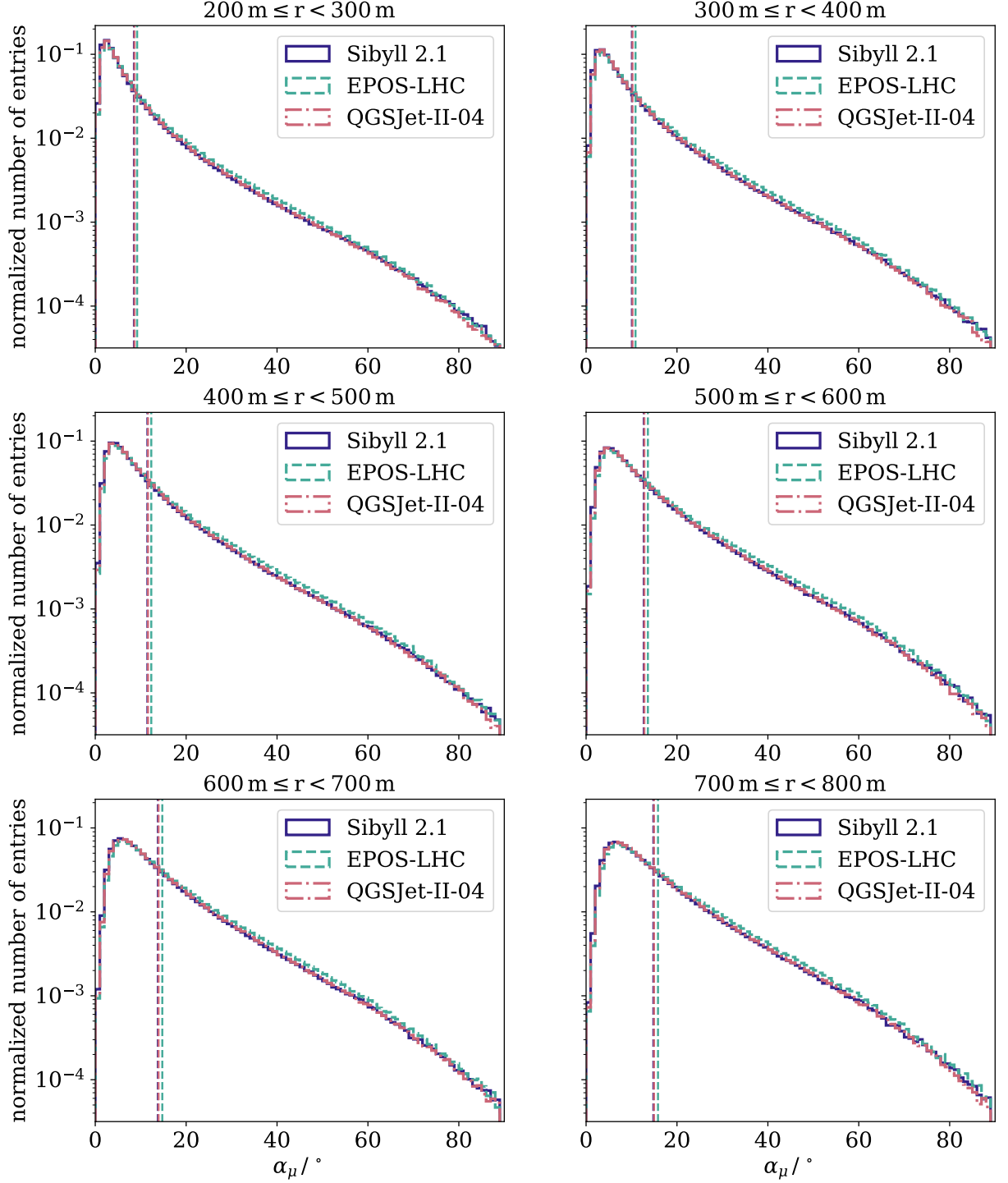


Figure 7.8.: Muon space angle distributions with respect to the primary direction for near-vertical events ($\cos\theta > 0.9$) derived for CORSIKA showers produced with Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 in bins of lateral distance. Vertical lines indicate the average values of the distributions.

tails of the shower development. The transverse momentum relative to the primary axis

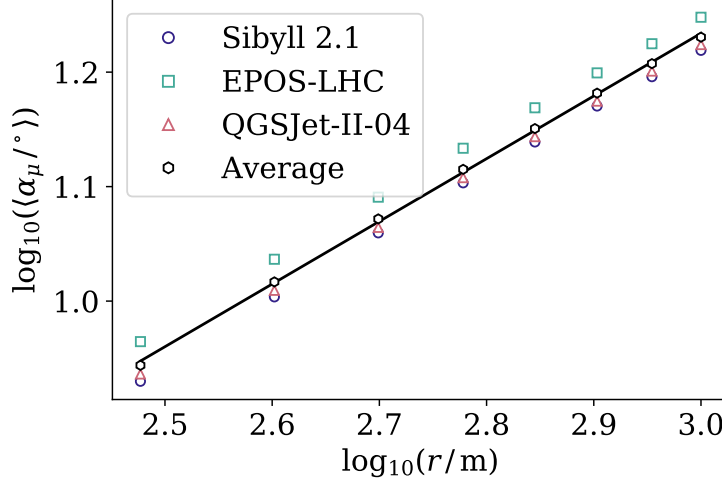


Figure 7.9.: Average muon opening angle with respect to the shower axis as a function of lateral distance for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 as well as for the average of all three models. The latter is described by a linear fit in log-log space (black line).

inherited by a muon in a hadronic decay is one main source of the angular spread [61]:

$$\sin(\alpha) \simeq \frac{cp_t}{E_i}, \quad (7.6)$$

in the approximation $cp \simeq E_i$. Here, α , p_t , and E_i describe the muon angle relative to the axis, the muon transverse momentum and the muon energy, respectively. For typical muon energies of GeV, the resulting angular spread is of the order of 10° .

The transverse momentum transferred to the muons translates into a lateral separation with respect to the shower axis, which in turn depends on the length of the muon trajectories. The trajectories can, in first order, be approximated by a straight line from the production point to the ground level, along which the muons propagate with the speed of light. Therefore, the lateral separation of muons from the shower axis depends on the muon production height. In addition to multiple Coulomb scattering, also geomagnetic deflection can further enhance the muon separation, since they can cause deviations from the straight-line approximation of the muon propagation. Both effects are stronger for low-energy muons and increase with increasing shower inclination. To study the influence of the muon separation on the two-component reconstruction, the muon angle with respect to the shower axis can be obtained from CORSIKA simulations. For this purpose, a small set of 100 showers per bin in $\log_{10} E_{\text{true}}$ with a bin width of 0.1 is used for the Sibyll 2.1, EPOS-LHC and QGSJet-II-04. To derive a preliminary parametrization of the muon angular separation, only shower with $\cos \theta > 0.9$ are included to match the zenith range used for the optimization of the two-component model. Since the angular spread depends on the muon energy which is unknown in measured data, instead, the angular distributions are binned in lateral distance. The resulting distributions for the different hadronic interaction models are shown in Fig. 7.8. The average values of the distributions

are indicated as vertical lines. The bulk of the muons observed with IceTop have a spread around the shower axis smaller than 10° . Considering the muon spline fits derived in section 5.2, such a shift in the muon inclination results in a change in the contribution of corner-clipping muons and the width of the muon PDFs. Therefore, the muon signal uncertainty changes accordingly. Additionally, the expected average track length of muons changes as a function of the muon zenith angle. This results in a difference in the average muon signal expectation value. The muon signal expectation value is of particular importance to determine the average expected number of muons used in the calculation of the Poisson terms in Eq. (6.17). To estimate the influence of the muon angular spread on the reconstruction performance, the average values in each lateral distance bin are used to derive a parametrization of the muon opening angle. Fig. 7.9 shows the average muon opening angles as a function of lateral distance. Due to the differences in the muon energy spectrum and the number of low-energy muons at the observation level across the different hadronic interaction models, the exact magnitude of the muon spread differs as well. Since EPOS-LHC features the highest number of low-energy muons out of the three models, the average muon spread is largest. Therefore, any parametrization of the muon spread introduced in the reconstruction leads to an additional model dependence. As a preliminary parametrization, a linear fit in log-log space to the average of the three hadronic interaction models is used:

$$\alpha_\mu = 10^{0.544 \log_{10}(r/m) - 0.390} \quad (7.7)$$

Using Eq. (7.7), the expected muon zenith angle can be modified during the reconstruction with respect to the primary zenith angle. However, the change in the muon zenith angle has to be adjusted depending on the relative location of a given detector with respect to the shower axis. In this context, the *upstream* and *downstream* regions on the arriving air-shower event must be distinguished. As illustrated in Fig. 7.10, the relative orientation of a given detector with respect to the shower geometry can be described by an angle ψ and the lateral distance, r . In this context, ψ is defined to be 0 along the downward projection of the shower axis onto the shower plane (orange line in Fig. 7.10). The region in the shower plane on the right-hand/left-hand side of the shower axis ($\cos \psi > 0 / \cos \psi < 0$, respectively) is defined as the upstream/downstream regions. If the projection of a given detector position in the shower plane of an inclined shower is in the upstream/downstream region, the average muon zenith angle is therefore smaller/larger with respect to the primary zenith. To modify the muon zenith expectation for each detector during the reconstruction, ψ can be defined as [252]

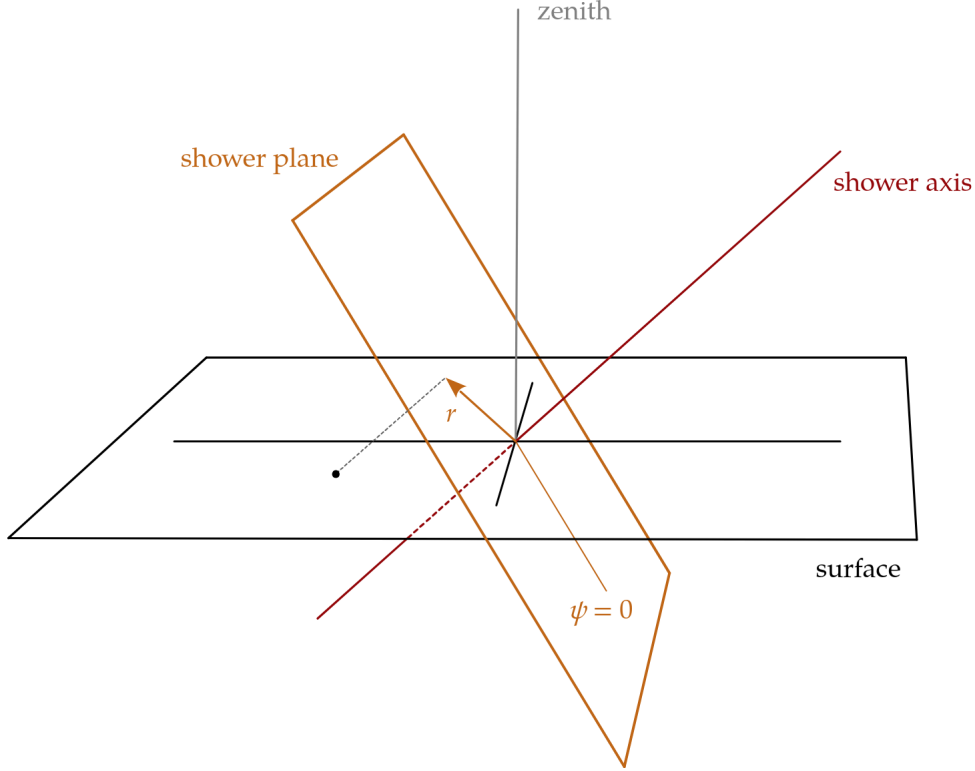


Figure 7.10.: Depiction of the geometry of an arriving air-shower event. The shower axis is defined by the arrival direction of the incident primary. Surface plane and shower plane are illustrated in black and orange, respectively. The lateral distance, r , of a given detector (black point) is defined in the shower plane perpendicular to the shower axis. The angle ψ defines the upstream ($\cos \psi > 0$) and downstream ($\cos \psi < 0$) regions. Figure taken from [251].

$$\vec{x}_{\text{proj}} = \begin{pmatrix} x_c \\ y_c \\ z_c \end{pmatrix} + |\vec{x}_c - \vec{x}_d| \cdot \begin{pmatrix} \cos \phi \\ \sin \phi \\ 0 \end{pmatrix}, \quad (7.8)$$

$$\psi = \arccos \left(1 - \frac{|\vec{x}_{\text{proj}} - \vec{x}_d|^2}{2|\vec{x}_c - \vec{x}_d|^2} \right), \quad (7.9)$$

with the core position, $\vec{x}_c = (x_c, y_c, z_c)^T$, the detector position, $\vec{x}_d = (x_d, y_d, z_d)^T$ and the downward projection of the shower axis onto the surface plane, $\vec{x}_{\text{proj}}$. The change in the muon zenith angle is then given by

$$\theta_\mu = \theta + \alpha_\mu \cos \psi, \quad (7.10)$$

where θ is the primary zenith angle. With the expected muon zenith angle, also the shape of the muon signal PDF changes. Fig. 7.11 shows a single two-component fit derived from a reconstruction employing the muon angular separation. Since the muon spread differs depending on the relative location of a detector to the shower axis, the

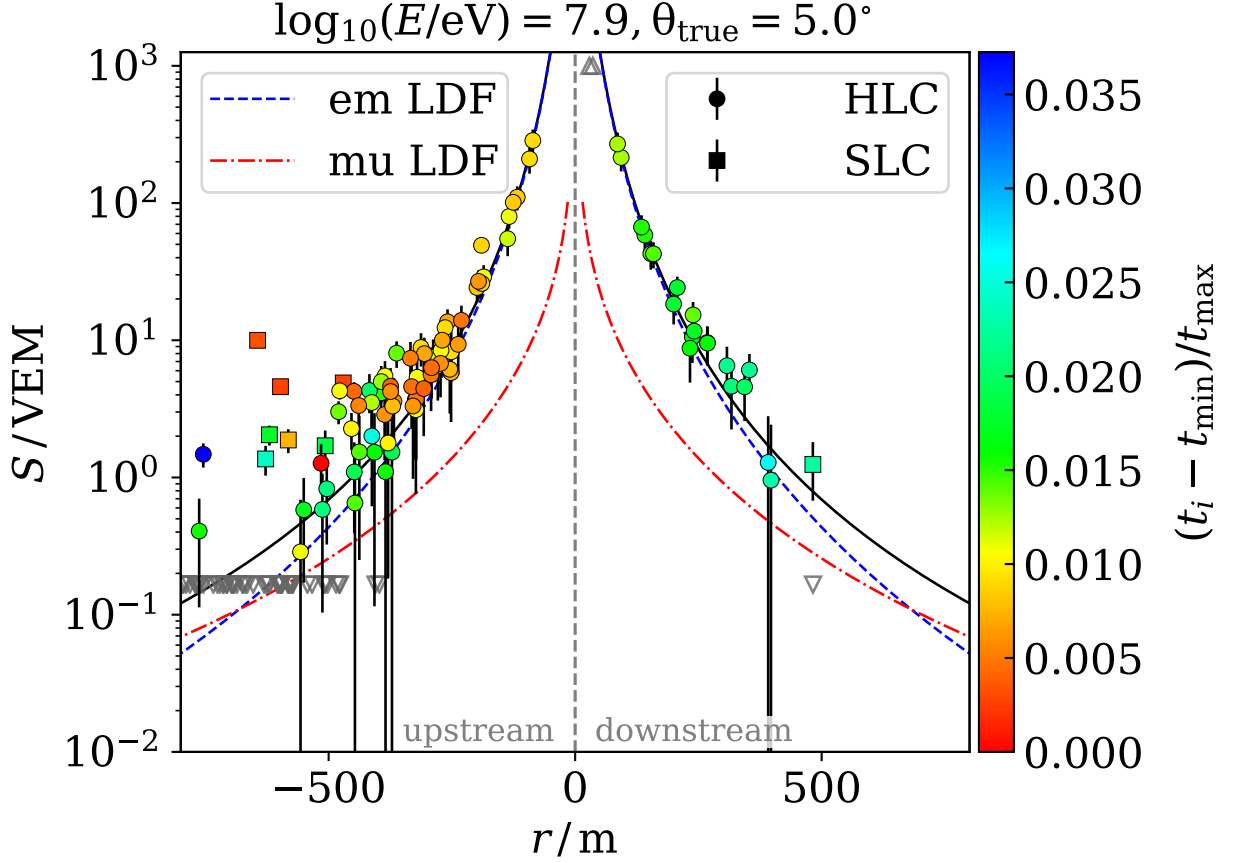


Figure 7.11.: Example single two-component fit for a simulated event ($\log_{10}(E_{\text{true}}/\text{eV}) = 7.9$, $\theta = 5.0^\circ$) with the inclusion of the upstream/downstream regions by means of a modification of the expected muon zenith angle. The blue/red line shows the electromagnetic/muon LDF, the total LDF (black line) is given by the sum of both. Saturated and silent detectors are illustrated as upward and downward facing triangles and are placed at a fixed value of 1000 VEM and 0.2 VEM, respectively. The color coding represents the measured detector times from early (red) to late (blue) hits.

fit is shown for the upstream and downstream regions separately. The impact on the reconstruction performance is estimated by comparing a reconstruction run in which the muon angular separation is implemented to a reference run that assumes a coherent muon and primary zenith angle. Since the muon LDF is potentially influenced most by the underlying assumption about the muon spread, the muon number reconstruction performance is compared for both runs. Fig. 7.12 shows the muon number resolution and bias for proton and iron primaries for Sibyll 2.1. Only near-vertical showers with $\cos \theta > 0.9$ are included. Since both runs exhibit differences that are contained within the statistical uncertainties, no significant influence of the tested assumptions about the muon angular spread are observed. For the further analysis presented in this work, the muon zenith angle is therefore assumed to follow the primary zenith angle. This simplification is

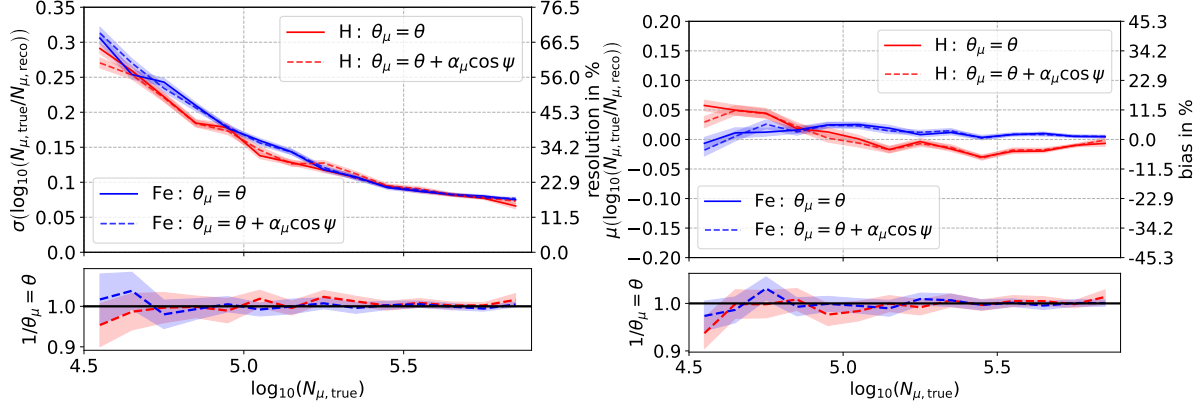


Figure 7.12.: Muon number reconstruction resolution (left) and bias (right) for the incorporation of the muon angular spread (dashed lines) as compared to the assumption of a coherent primary and muon zenith angle (solid lines) for proton and iron primaries with $\cos \theta > 0.9$ produced with Sibyll 2.1. The lower panels show the ratio between both runs. Statistical uncertainties are shown as shaded bands.

chosen to mitigate any model dependence that is introduced with a parametrization of the muon angular separation. It should be noted, however, that a realistic parametrization of the muon spread becomes increasingly important for the study of more recent data, since differences in the path lengths through large snow overburdens can cause significant differences in the muon attenuation and consequently in the muon signal PDFs. Since, the muon energy threshold to cross the entire detector increases with increasing snow height, the muon angular spread should be parametrized including an energy threshold dependence. Additionally, future studies should incorporate a primary zenith dependence of the muon angular separation. Since the particles in an inclined shower need to traverse more atmosphere to reach the ground, muon attenuation effectively increases the muon energy threshold to reach the detector level. However, as the muon spread increases with decreasing muon energy according to Eq. (7.6), the average muon angular separation decreases as a function of the primary zenith angle (see Fig. B.6). For the reconstruction of more inclined events with the two-component model, the impact of the muon spread on the reconstruction performance should therefore be studied in more detail.

7.3.2. Muon spline fits

To test the influence of the assumed muon energy in the tank response simulations introduced in chapter 5, the muon number reconstruction performance is evaluated for a two-component reconstruction utilizing muon PDFs derived from an injection spectrum (see Figs. 5.3 and 5.4) and compared with the baseline reconstruction using 1 GeV muons. The impact of the underlying assumption on the muon proxy as a function of the true

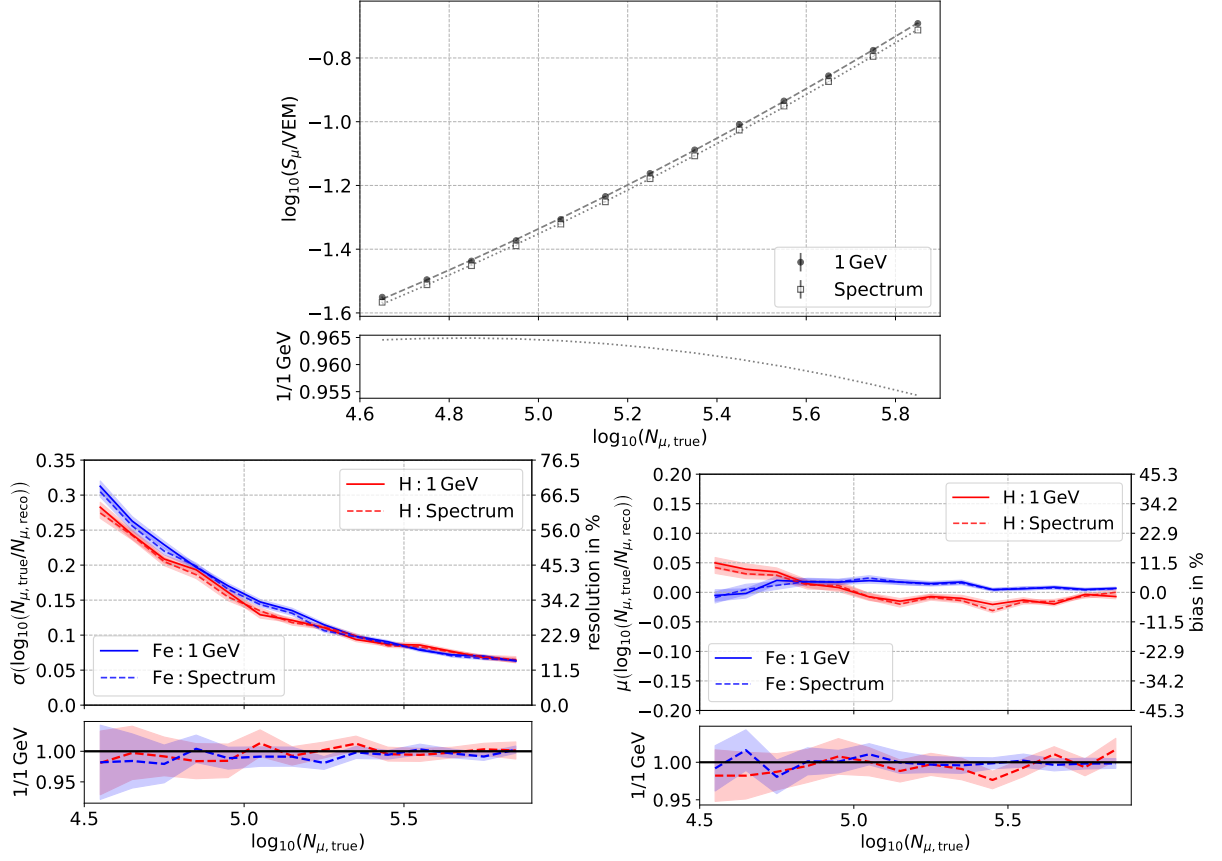


Figure 7.13.: Comparison of the muon number calibration fit for reconstructions using muon spline fits based on 1 GeV muons (dashed line) and the muon-energy spectrum (dotted line) shown in Fig. 5.4 (top). Corresponding muon number reconstruction resolution (bottom left) and bias (bottom right) for proton and iron primaries with $\cos \theta > 0.9$ produced with Sibyll 2.1. The lower panels show the ratio between both runs. Statistical uncertainties are shown as shaded bands.

muon number is shown in Fig. 7.13 (top) for Sibyll 2.1. Generally, the application of spectrum weighted muon PDFs results in muon proxy that is slightly shifted toward smaller values (with an average shift of $\sim 4\%$) due to the increased average expectation signal (see Fig. 5.8). Fig. 7.13 (bottom) shows the resulting muon number resolution and bias for both reconstructions and for proton- and iron-induced showers produced with Sibyll 2.1. Since the application of a calibration function used for the conversion of the muon proxy to the reconstructed muon number compensates for the visible offset in the muon proxy between both reconstructions, they are well compatible within the statistical uncertainties. Therefore, the application of spectrum-weighted muon PDFs does not lead to significant improvements compared to the baseline reconstruction. Thus, muon PDFs based on the injection of 1 GeV muons are chosen for this work, as assumptions about the muon energy spectrum used for the production of spectrum-weighted muon PDFs additionally lead to an intrinsic dependence on a specific hadronic interaction model.

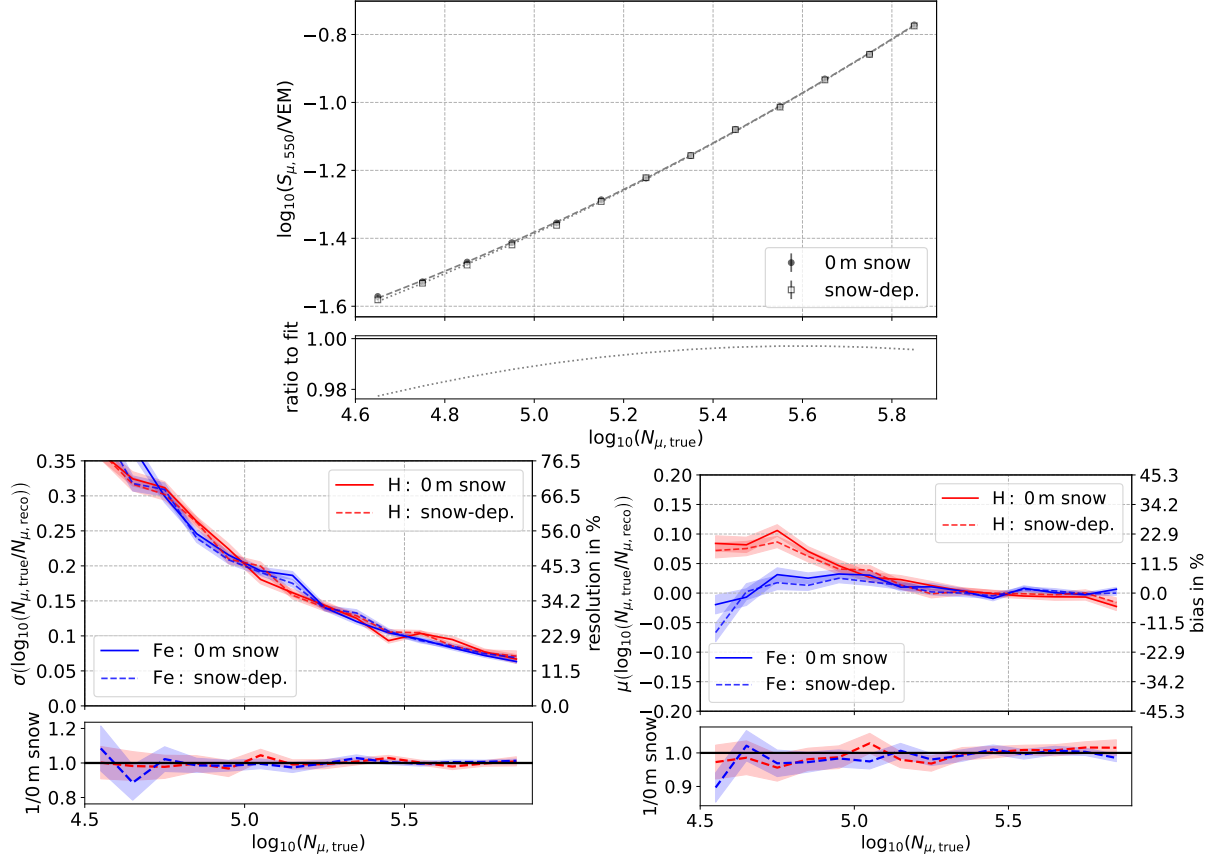


Figure 7.14.: Comparison of the muon number calibration fit for reconstructions using muon spline fits without (dashed line) and with (dotted line) dependence on the snow height (top). Corresponding muon number reconstruction resolution (bottom left) and bias (bottom right) for proton and iron primaries with $\cos\theta > 0.9$ produced with Sibyll 2.1. The lower panels show the ratio between both runs. Statistical uncertainties are shown as shaded bands.

Moreover, the influence of the assumption of negligible impact of muon attenuation through snow accumulation on top of the IceTop tanks is tested. For this purpose, the snow-dependent muon spline fits produced in chapter 5 (see also Fig. 5.5) are used in the two-component reconstruction. For comparison with the baseline reconstruction, the same spline fits are used and a constant snow height of 0 m is used in their evaluation. This is done to ensure a fair comparison between both scenarios, as the application of snow-dependent spline fits is found to be less stable at low energies compared to the two-dimensional spline fits³. The difference of both scenarios in the obtained muon number proxy is shown in Fig. 7.14 (top) for Sibyll 2.1. Generally, the muon number proxy exhibits a maximum difference of 2% for the lowest primary energies considered. The difference decreases to the sub-percent level toward higher energies. Since snow attenua-

³Possible reasons for the lower stability are still under investigation.

tion causes a shift in the average expectation signals toward slightly smaller values, the muon proxy is expected to decrease slightly if the snow attenuation is of relevance. This effect is not observed (for the considered snow accumulations), suggesting that the small observed differences are likely due to statistical variations. Fig. 7.13 (bottom) shows the resulting muon number resolution and bias for both reconstructions and for proton- and iron-induced showers produced with Sibyll 2.1. For both cases, the reconstruction resolution and bias are well compatible within the statistical uncertainties. Consequently, snow attenuation is concluded to have a negligible impact on the two-component reconstruction of snow accumulation relevant for this work.

7.3.3. Electromagnetic signal uncertainty

The electromagnetic PDF (Eq. (6.14)) used in the two-component reconstruction is based on the parametrization derived for the standard reconstruction. In particular, the signal uncertainty is derived in [189] from dedicated simulations of the detector response in a ring-like array geometry. Vertical proton-initiated air showers of different energies are injected onto the center of an array that comprises IceTop tanks located in circles in a distance of 10 m from each other. Details on the exact tank placement can be found in [189]. This procedure has the advantage of allowing for the same signal expectation value in all tank of the same ring, since they are placed at the exact same lateral distance. For the measured charge footprints, the observed charge values in each tank of the same ring can then be compared to estimate the signal fluctuations. However, as mentioned in section 6.3, also low-energy muons are part of these simulations and can potentially bias the resulting parametrization of the signal uncertainty. To gauge the impact of the muon contribution, a new parametrization based only on the electromagnetic signal contribution as obtained from CORSIKA is derived and tested within the two-component model. For this purpose, the electromagnetic contribution to the HLC signal distribution is used to compared the signals measured in neighboring tanks⁴, $S_{\text{em,a}}$ and $S_{\text{em,b}}$. Similarly to the derivation of the *small signal regime* in section 6.3, only air-shower events with $\log_{10} S_{125} > 0.4$ and $\cos \theta > 0.9$ are included. To ensure significant electromagnetic contribution to measured HLC signals, at least 10% of each HLC signal must be produced by electromagnetic particles. Further, an artificial signal threshold of 0.2 VEM is applied for all HLC signals. This is done to unify the threshold in all tanks, since the exact discriminator threshold differs for each DOM. For large signals close to the shower axis, the approximation of a similar signal expectation value for neighboring HLC tanks

⁴As mentioned in section 6.3, due to the close proximity (~ 10 m) of tanks in the same station, the signal in neighboring tanks can be approximated as independent double measurement of the same signal expectation value if the tanks are not located too close to the shower axis.

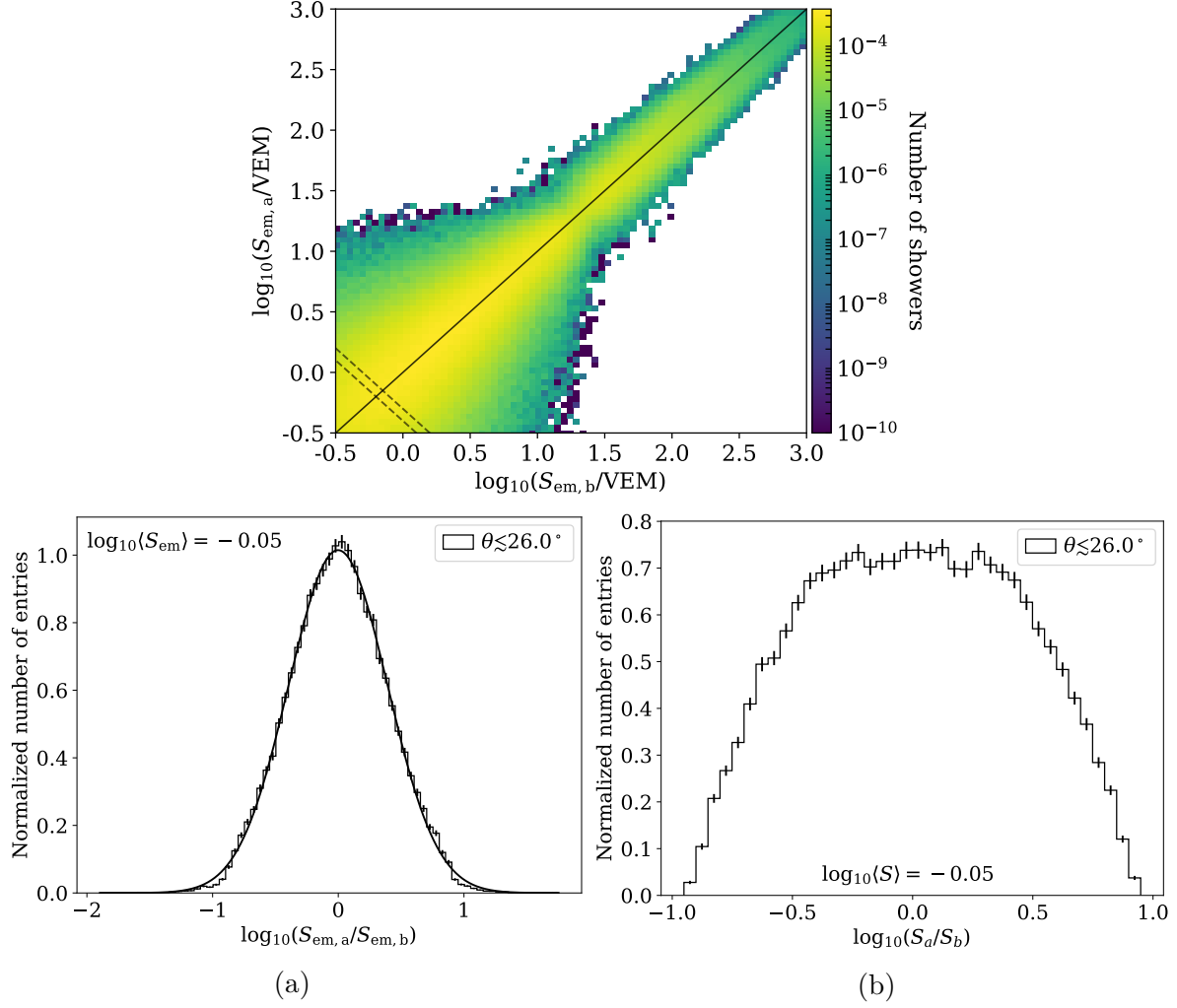


Figure 7.15.: Comparison of signal deposits $S_{\text{em},a}$ and $S_{\text{em},b}$ in neighboring IceTop tanks using simulations of near-vertical shower with $\theta_{\text{reco}} \lesssim 26^\circ$ weighted with H4a (top). The solid black line indicates the one-to-one correlation line. The dashed black lines indicate an example bin orthogonal to the one-to-one correlation line. Electromagnetic signal difference distribution for neighboring HLC tanks for an average signal of $\log_{10}\langle S_{\text{em}}/\text{VEM} \rangle = -0.05$ (bottom left) and the same bin including the contribution of muons (bottom right). The distribution in the latter clearly deviates from a log-normal behavior due to the influence of muons.

does no longer hold. Therefore, only HLCs with lateral distances below 40 m are included in this analysis. Additionally, the events are required to pass the standard quality cuts introduced in section 6.3. Fig. 7.15 (top) shows the distribution of electromagnetic signal deposits in neighboring IceTop tanks weighted to the H4a flux model. Although no large differences are expected between the different hadronic interaction models for the electromagnetic signal fluctuations, the entire simulation sets for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 are included. A clear correlation between the signals measured

in neighboring detectors is visible, as indicated by the black one-to-one correlation line. To visualize the impact of muons on the distribution, two example bins with the same average signal are shown in the bottom left and right of Fig. 7.15. While the former shows the difference distribution of $\log_{10} S_{\text{em},a}$ and $\log_{10} S_{\text{em},b}$ for an average signal of $\langle \log_{10} S_{\text{em}} \rangle = \log_{10}((S_{\text{em},a} + S_{\text{em},b})/2) = -0.05$ obtained from pure electromagnetic response, the latter shows the same distribution in the same bin but with the inclusion of the muon contribution. For the pure electromagnetic contribution, the difference distribution is well modeled by a Gaussian in logarithmic space. The contribution of muons clearly leads to a deviation from the log-normal behavior. To derive a parametrization of the electromagnetic signal fluctuations, the difference distribution in each bin along the one-to-one correlation line is obtained and modeled with a Gaussian. Since the difference distributions follow a Gaussian in logarithmic space, the single tank distributions are also log-normal since the former is a result of the convolution of the single tank distributions⁵. The signal differences describe the relative signal fluctuations between the neighboring tanks [253]

$$\Delta S_{\text{rel}} = \frac{\log_{10} S_{\text{em},a} - \log_{10} S_{\text{em},b}}{\sqrt{2}}. \quad (7.11)$$

Due to the convolution of the single tank distributions, the width of the difference distribution is $\sqrt{2}\sigma_{\text{em}}$ with the single tank standard deviation σ_{em} . To obtain the signal fluctuations of a single tank as a function of the average signal strength, the width of the Gaussian fit in each bin is extracted and divided by a factor of $\sqrt{2}$. The resulting distribution of electromagnetic signal fluctuations as a function of the average signal is shown in Fig. 7.16 (top left). The pure electromagnetic signal uncertainty aligns well with the default parametrization (see section 4.3.1) used in the standard reconstruction and in the two-component model in the few VEM regime. Above $\sim 10\text{VEM}$, a decrease and a successive increase of the signal fluctuations is visible. This is caused by nonlinearities in the VEM calibration in the transition from the high- to low-gain DOMs. This region is not included in the derivation of a preliminary parametrization of the electromagnetic signal fluctuations but should be studied in more detail in the future. It should be noted, that in the region above an average signal of 1 VEM, the electromagnetic fluctuations lie below the default parametrization. This is the region in which the influence of single muons is most prominent due to the scenario in which one tank in an HLC station receives a muon, while the other one only measured electromagnetic contribution. In the sub-VEM regime, an apparent decrease in fluctuations is also visible caused by the influence of the applied signal threshold of $S_{\text{thr}} = 0.2\text{VEM}$, which effectively restricts the phase space for signal fluctuations. To correct for this effect, an analytical threshold model based on [254] can be derived. The probability of an IceTop tank not to trigger is given by the integral of the signal PDF up to the threshold signal

⁵For a detailed derivation see [190]

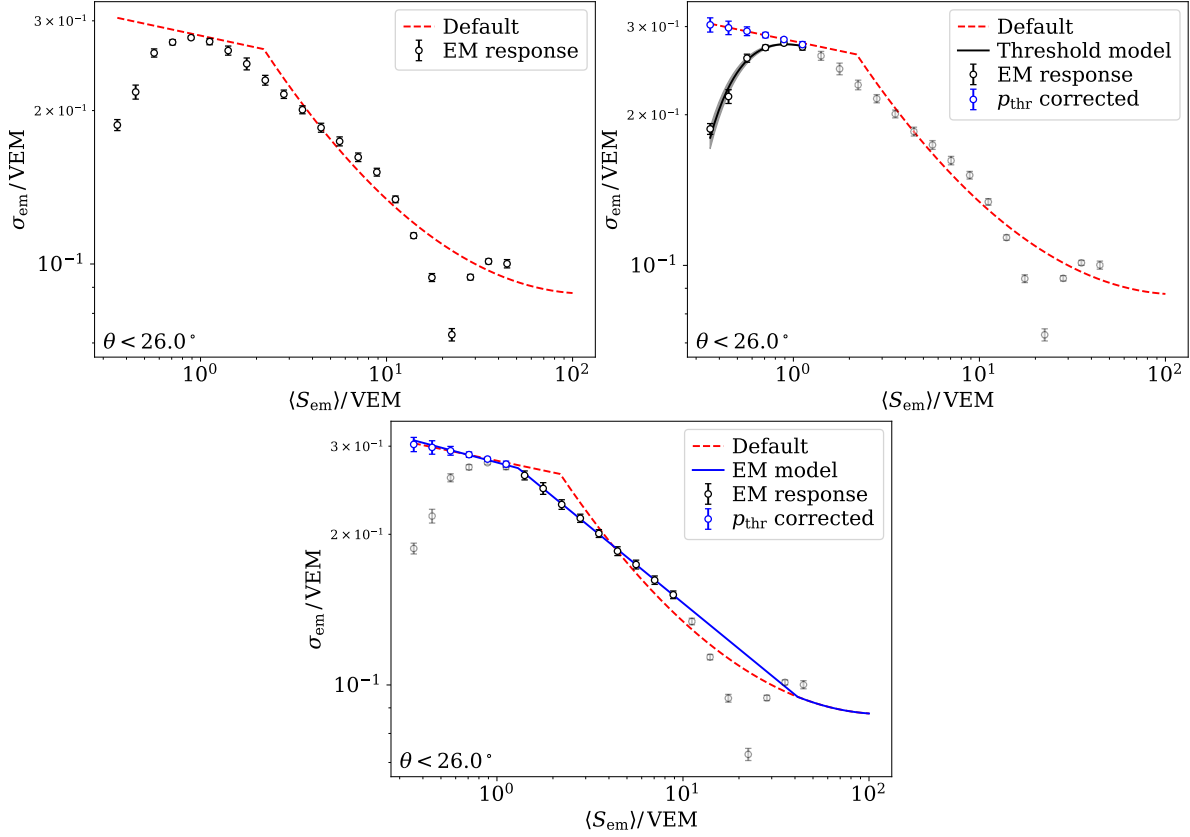


Figure 7.16.: Electromagnetic signal uncertainty as a function of the average signal compared to the default parametrization (top left). The measured fluctuations can be corrected for the influence of the signal threshold by means of a fit with a corresponding threshold model (top right). The final parametrization of the electromagnetic signal uncertainty derived from a fit to the threshold corrected points is shown in the bottom. The pure electromagnetic parametrization transitions back to the default parametrization for large signal deposits.

$$P(\langle S_{\text{em}} \rangle < S_{\text{thr}}) = \frac{1}{\sigma_{\text{em}} \sqrt{2\pi}} \int_{-\infty}^{S_{\text{thr}}} \exp \left(-\frac{(\log_{10} S' - \log_{10} \langle S_{\text{em}} \rangle)^2}{2\sigma_{\text{em}}^2} \right) d \log_{10} S', \quad (7.12)$$

where $\sigma_{\text{em}} = p_{\sigma,1} \sqrt{\langle S_{\text{em}} \rangle} + p_{\sigma,2}$ is assumed to follow a Poisson-like model with an additional free constant. As both tanks in a station are required to trigger to be included in the sample, the probability that both tanks in an HLC station measure a signal above the threshold is

$$P'(\langle S_{\text{em}} \rangle) = 1 - 2P(\langle S_{\text{em}} \rangle < S_{\text{thr}}). \quad (7.13)$$

Therefore, the threshold effect can be described analytically by

$$\sigma'_{\text{em}} = \sigma_{\text{em}} \cdot P'(\langle S_{\text{em}} \rangle). \quad (7.14)$$

This threshold model is fit to the observed electromagnetic signal fluctuations to obtain $p_{\sigma,1} = -0.057 \pm 0.033$ and $p_{\sigma,2} = 0.337 \pm 0.032$. Fig. 7.16 (top right) shows the resulting threshold model fit including the 1σ uncertainty band. The data points included in the fit are highlighted in black with a high opacity. The model shows a good agreement with the measured points within the statistical uncertainty. Since the threshold model does not describe the signal fluctuations over the entire signal range, it is used to modify the points influenced by the threshold effect by multiplication with the correction factor

$$c_{\text{thr}}(\langle S_{\text{em}} \rangle) = 1/P'(\langle S_{\text{em}} \rangle) \quad (7.15)$$

to obtain the threshold-corrected electromagnetic signal fluctuation indicated as blue points. The corrected points can now be used to derive a parametrization for the electromagnetic signal uncertainty. A suitable model is found to comprise a combination of two linear functions in double logarithmic space that transitions to the default parametrization for $\log_{10} \langle S_{\text{em}} \rangle \geq 1.614$:

$$\sigma_{\log_{10} \langle S_{\text{em}} \rangle} = \begin{cases} -0.099 - 0.555 \log_{10} \langle S_{\text{em}} \rangle & , \log_{10} \langle S_{\text{em}} \rangle < 0.113 \\ -0.304 - 0.532 \log_{10} \langle S_{\text{em}} \rangle & , 0.113 \leq \log_{10} \langle S_{\text{em}} \rangle < 1.614 \\ -0.373 - 0.658 \log_{10} \langle S_{\text{em}} \rangle + 0.158 \log_{10}^2 \langle S_{\text{em}} \rangle & , 0.340 \leq \log_{10} \langle S_{\text{em}} \rangle < 2.077 \\ -1.058 & , 2.077 \leq \log_{10} \langle S_{\text{em}} \rangle . \end{cases} \quad (7.16)$$

The cross over points are chosen to provide a smooth transition between the signal regions. Fig. 7.16 (bottom) shows a visualization of Eq. (7.16) compared to the default parametrization. The data points included in the fit are highlighted with high opacity. The reason for the transition to the default parametrization is its higher accuracy at large signal deposits. This is because in the derivation of the default model, only vertical showers are sampled in the center of a ring-based array geometry, leading to the same signal expectation value for all tanks on a ring. For the pure electromagnetic model, the steep rise of the LDF close to the shower axis can lead to significant differences in the signal expectation of tanks within the same station.

To estimate the influence of the assumption about the underlying signal fluctuation model used in the two-component model, the reconstruction is processed with Eq. (7.16) implemented as a new signal fluctuation model and compared to the base line reconstruction. Fig. 7.17 shows the resulting reconstruction performance for both reconstruction runs. The preliminary version of the purely electromagnetic based signal fluctuation model does not show a significant improvement with respect to the base line reconstruction using the standard parametrization for the signal uncertainty over the entire considered energy and muon number range. Based on this observation, it can be concluded that the small differences between both signal uncertainty models does not have a significant impact on the two-component reconstruction. This is likely due to the fact that the default

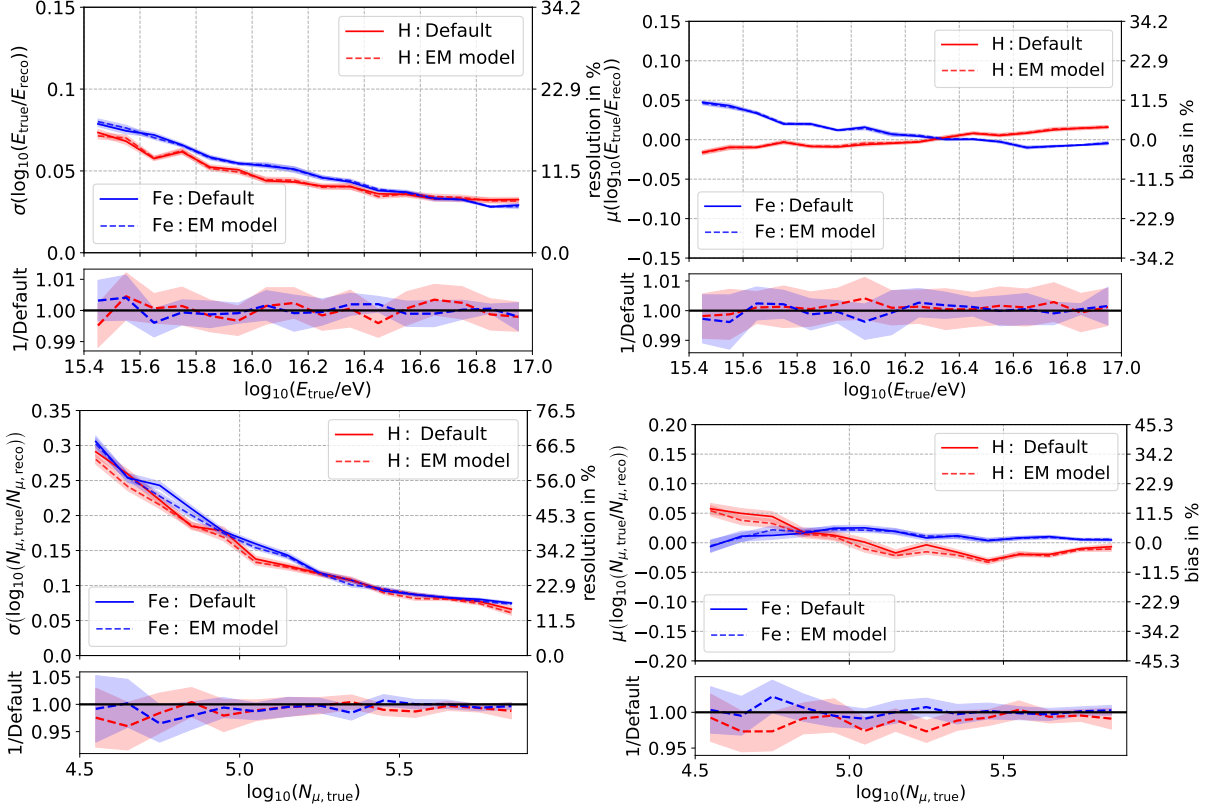


Figure 7.17.: Energy (top row) and muon number (bottom row) resolution (left) and bias (right) for the two-component reconstruction using the electromagnetic signal fluctuation model (Eq. (7.16)) (dashed lines) and the default model (Eq. (4.13)) (solid lines). The distributions are derived for simulations of proton and iron initiated air-showers with $\cos\theta > 0.9$ produced with Sibyll 2.1. The lower panels show the ratio between both reconstruction runs. Statistical uncertainties are shown as shaded bands.

parametrization also only includes HLCs and is therefore, by construction, dominated by the electromagnetic component. The default model therefore seems to describe the electromagnetic signal fluctuations sufficiently well. Thus, for consistency reasons, the default parametrization is also applied as the standard model for the two-component reconstruction.

Due to the contribution of the intrinsic shower fluctuations, the observed signal fluctuations can depend on the distance of the HLCs to the shower axis in addition to their dependence on the signal strength. For this reason, a preliminary study on the lateral distance dependence on σ_{em} is performed (see App. B). While a slight over-/underestimation of σ_{em} is found for detectors close/far away from the shower axis, no lateral distance dependence is introduced. This is because a corresponding parametrization would result in the introduction of a significant mass dependence. Additionally, due to the difference in the amount of atmosphere inclined air-showers have to traverse to reach the observation level compared to near-vertical showers, σ_{em} is expected to increase with increasing zenith

angle. Additionally, the projected difference between neighboring detectors increases with shower inclination, decreasing the validity of the underlying assumption of this method. For the inclusion of more inclined events, the parameterization of σ_{em} should be revisited. The lateral dependence of σ_{em} as well as a possible zenith dependence should therefore be part of more sophisticated studies.

7.4. Reconstruction performance

For the final quantification of the reconstruction performance, the full simulation set for the year 2012 introduced in section 4.4 is used, where the quality cuts listed in Tab. 6.4 are applied. This includes only near-vertical events with $\cos \theta > 0.9$ and only events with reconstructed core position inside of IceTop. It should be noted, that an extension of the energy and zenith angle range as well as a inclusion of IceTop uncontained events in future analyses requires the re-optimization of the parametrizations implemented within the two-component model.

Shower geometry

The shower geometry is described by the primary direction and the position of the shower core at the observation level. The latter is of high importance for the reconstruction of the shower front as well as the LDF. However, since both signal and time likelihoods are minimized in a combined manner in the reconstruction, the shower front fit has a direct and indirect influence on all shower observables. Since the, both, reconstruction stability and accuracy are strongly dependent on the hit multiplicity, the reconstruction performance of the shower geometry is expected to improve as a function of energy. An example single event reconstruction of the lateral distribution and the shower front is shown in Fig. 7.18. An accurate reconstruction of shower geometry leads to a small difference in the location of the true and reconstructed points. For quantification of the accuracy of the core position reconstruction, the difference of the true and reconstructed distance of the shower core perpendicular to the shower axis, $\Delta r(\text{true}, \text{reco})$, is calculated⁶. This approach is chosen to account for the high sensitivity to changes in the reconstructed shower axis, which influences the difference of the reconstructed and true core position in the surface plane proportional to $\sec \theta$ [101]. The differences are derived in bins of the true energy. For each bin, the 68th percentile is used to quantify the core position reso-

⁶In principle, for the near-vertical events studied in this work, the difference of the reconstructed and true core position can be calculated simply in the surface plane. However, for more inclined events, this distinction becomes relevant and can therefore be adopted for future studies.

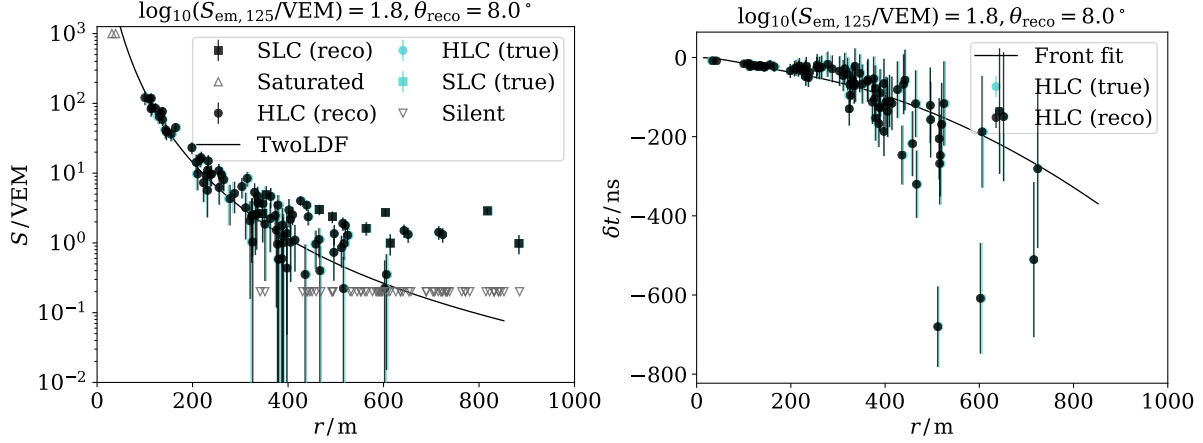


Figure 7.18.: Example event of an air shower reconstruction for a simulated proton shower with roughly 52 PeV true primary energy and $\approx 31^\circ$ and $\approx 268^\circ$ primary zenith and azimuth angle, respectively. The signal as well as time distributions are shown on the left and right, respectively. Cyan points show the MC data with corresponding uncertainties (Eq. (6.27)) indicated by the error bars. The reconstructed distribution and the reconstructed fit are illustrated in black.

lution. Fig. 7.19 (left) shows the resulting core position resolution of the two-component reconstruction compared to the standard reconstruction for Sibyll 2.1 as a function of true energy. Compared to the standard reconstruction, the core position resolution is significantly improved by the two-component model for energies above a few PeV. For energies above the 10 PeV region, the core position is reconstructed with an accuracy of $\lesssim 7$ m and well below 5 m at the highest energies. Note that the physical dimension of an IceTop tank itself becomes a relevant factor with such high accuracies. This effect, in combination with detector saturation, leads to a flattening of the resolution at the highest energies. For the energies around a few PeV, the resolution is of the order of ~ 10 m, which roughly corresponds to the difference between neighboring IceTop tanks. Generally, the resolution is best for light primaries since they produce a larger hit multiplicity compared to heavy primaries. This effect is more pronounced for low primary energies. To quantify the angular resolution, the space angle $\phi(\text{true}, \text{reco})$ between the true and reconstructed primary direction is determined in bins of the primary energy. The resolution is then given as the 68th percentile in each energy bin. The resulting distribution for Sibyll 2.1 is shown in Fig. 7.19 (right). Generally, the accuracy improves as a function of energy, since the curvature of the shower front (and therefore of the time distribution) increases with increasing energy. This leads to a more precise description of the time distribution by the model function for the shower front. Over the entire energy range, sub-degree resolutions are observed for near-vertical showers. At the highest energies, the shower direction can be determined with an accuracy of $< 0.4^\circ$. It should be noted, that a potential improvement of the angular resolution can be achieved by introducing a

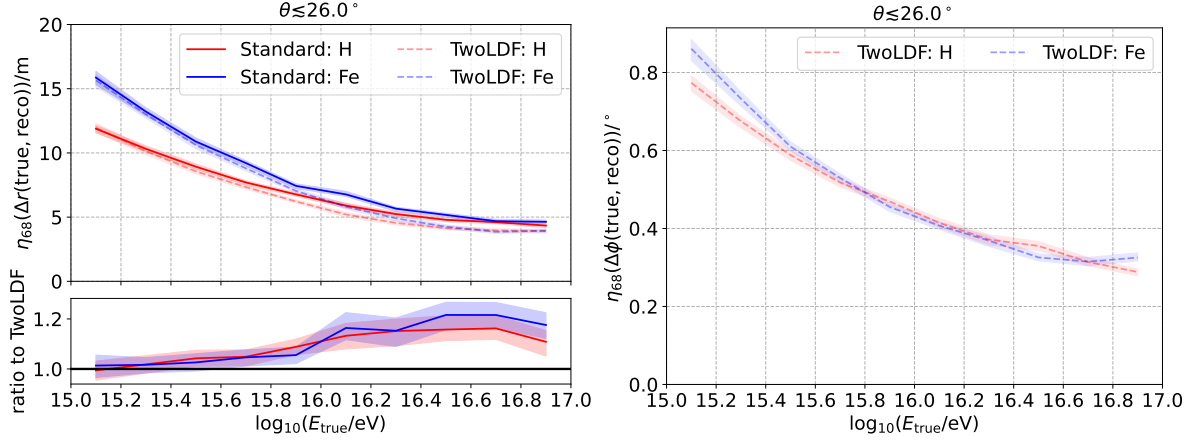


Figure 7.19.: Core position (left) and direction (right) resolution for near-vertical ($\cos \theta > 0.9$) proton- and iron-initiated showers produced with Sibyll 2.1. The uncertainty band reflects the 95 % bootstrap confidence interval.

two-component model for the arrival time distribution that separates the expected arrival times of the electromagnetic component from the muons. Such a model could make use of additional information contributed by SLCs⁷.

Energy

The optimization of the optimal reference distance at which the energy proxy is determined is detailed in section 7.1. The resulting distribution of $S_{\text{tot},125}$ as a function of primary energy is shown in Fig. 7.20 (top left). The reconstructed energy is obtained via the calibration function Eq. (7.3) using the parameters listed in Tab. 7.1. The resulting reconstruction performance (resolution and bias) for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 is shown in Fig. 7.20 for the entire simulation set after all quality cuts in Tab. 6.4 are applied. For near-vertical showers above ~ 20 PeV, the primary energy can be reconstructed with a resolution of $< 10\%$ for all models and independent of the primary mass. At lower energies, the resolution becomes worse to a level of $\lesssim 20\%$ as the shower size decreases. Because of the difference in the average value of X_{max} for different primary masses but same primary energy, the shower size and therefore the energy estimate can show a mass dependence. This energy bias is minimized with the optimization study discussed in section 7.1 and exhibits a maximum mass bias of $\sim 10\%$. While for lower energies the reconstructed energy is over-/underestimated for light and heavy primaries⁸, the opposite behavior is observed for high energies. The absolute magnitude

⁷An new description of the shower front employing an improved likelihood model that is suited for the inclusion of SLCs is currently in development [192].

⁸Intermediate primaries (for Sibyll 2.1) show an energy bias that does not interpolate between proton and iron. This behavior might be related to X_{max} being below the observation level for a significant

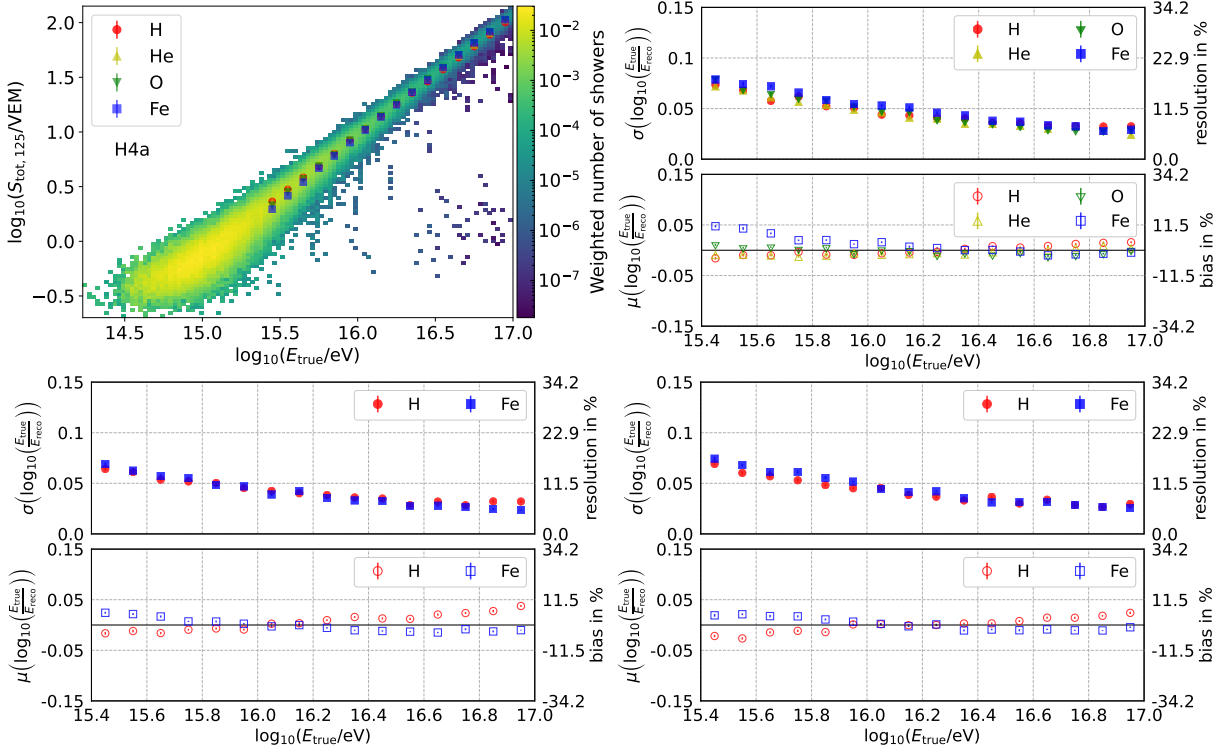


Figure 7.20.: Distribution of the energy proxy, $S_{\text{tot},125}$, as a function of true primary energy for near-vertical showers $\theta_{\text{reco}} \lesssim 26^\circ$ produced with Sibyll 2.1 and weighted to H4a (top left). Average values for different species are shown above the regime where the two-component reconstruction reaches full efficiency. The reconstruction resolution and bias for Sibyll 2.1 (top right), EPOS-LHC (bottom left), and QGSJet-II-04 (bottom right) are shown in the upper and lower panels, respectively.

of this bias is a function of energy. Since the mass dependence in the energy estimation using the signal strength at a given distance depends on the differences in the respective LDF slopes, which in turn are strongly connected to X_{max} , the exact evolution of the energy bias depends on the hadronic interaction model.

The energy resolution and bias obtained with the two-component reconstruction is compared to the standard reconstruction in Fig. 7.21. The two-component model outperforms the standard reconstruction in terms of reconstruction resolution for energies above ~ 10 PeV by $> 12\%$ for both proton and iron primaries. Conversely, at energies of a few PeV, the standard reconstruction is better by $\sim 7\%$ for proton. In the case of iron primaries, both reconstructions show a compatible performance in the few PeV scale. The reconstruction bias of the two-component reconstruction exhibits a larger mass depen-

fraction of events in the observed energy range. The mass dependence of the energy bias has a distinct effect on the analysis presented in chapter 9. However, no clear correlation is found between the energy bias for proton and parameters that contain information about X_{max} . This should be studied in more detail in the future.

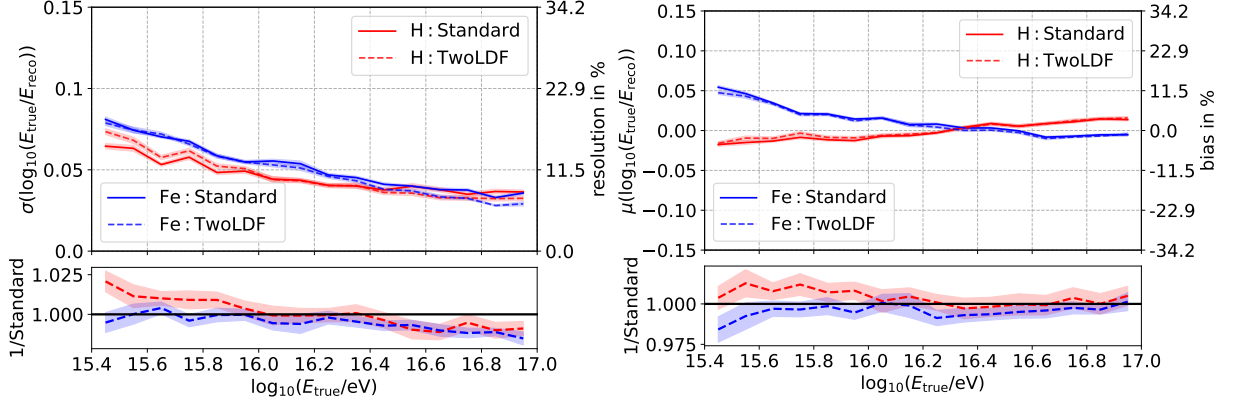


Figure 7.21.: Energy resolution (left) and bias (right) obtained for the two-component model compared to the standard reconstruction for proton- and iron-initiated showers produced with Sibyll 2.1. The ratios to the standard reconstruction are shown in the lower panels.

dence on the few percent level for high energies and a $\sim 10\%$ smaller mass dependence for low energies for both iron and proton primaries. Overall, the two-component fit results in a slightly improved energy reconstruction compared to the standard IceTop reconstruction.

Muon number

After optimizing the muon reference distance, R_μ , in section 7.2, the final reconstruction performance of the number of muons can be determined. The distribution of $S_{\mu,550}$ as a function of the true muon number obtained from CORSIKA is shown in Fig. 7.22 (top left). Only muons above energies of 420 MeV and lateral distances of below 1 km are included in the muon multiplicity. The average values of $S_{\mu,550}$ for each primary mass are shown roughly above the full efficiency threshold for the two-component reconstruction. Note, that this threshold is different for Sibyll 2.1 ($\log_{10} N_\mu \sim 4.6$) and the post-LHC models ($\log_{10} N_\mu \sim 4.7$) as the average amount of muons for a given primary energy differs significantly between the models. For the same reason, the maximum bin of the observed number of muons is larger for EPOS-LHC and QGSJet-II-04 ($\log_{10} N_\mu \lesssim 6.0$) compared to Sibyll 2.1 ($\log_{10} N_\mu \lesssim 5.9$). The reconstructed muon number is obtained via the calibration function Eq. (7.5) using the parameters listed in Tab. 7.2. The resulting reconstruction resolution and bias for the three models is shown in Fig. 7.22 for the entire simulation set after all quality cuts in Tab. 6.4 are applied. The muon number can be reconstructed with a resolution of $\lesssim 20\%$ for all hadronic models and primary masses for the highest energies. However, the resolution is on the $\sim 20\%$ level already for muon numbers of $\log_{10} N_\mu \gtrsim 5.4$. A resolution of 20% is in particular promising when

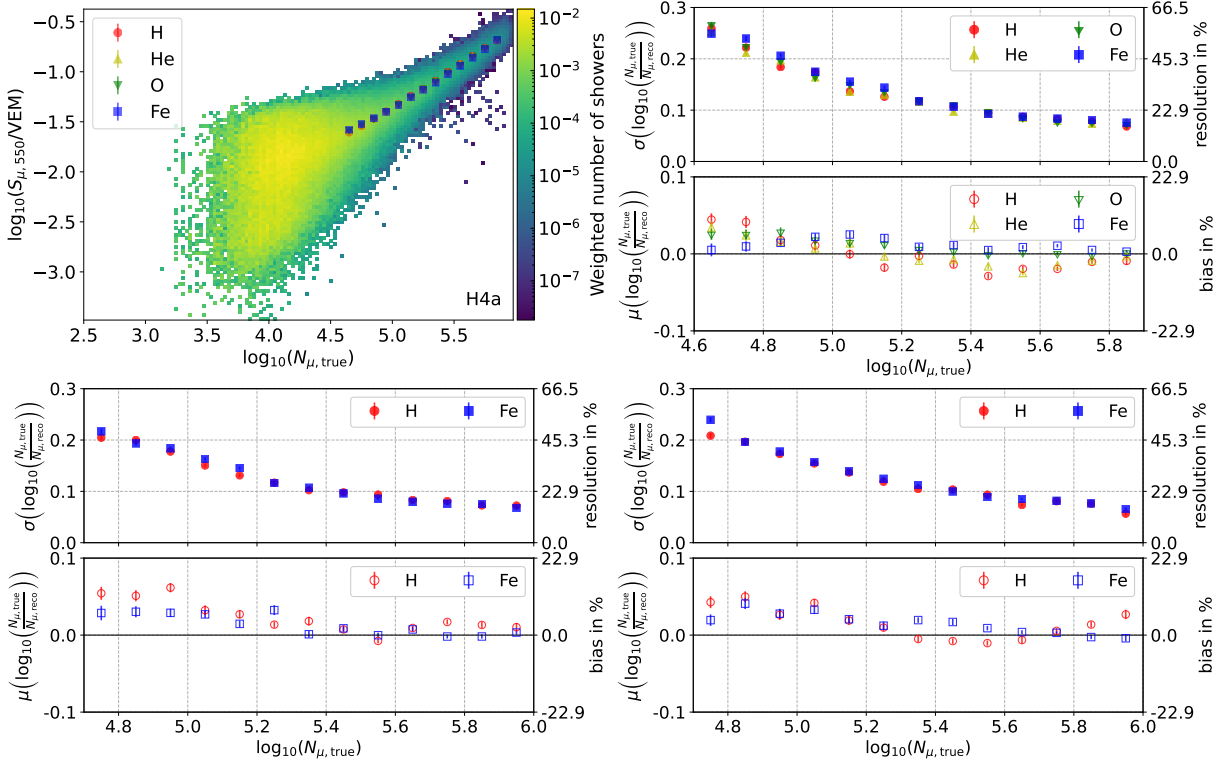


Figure 7.22.: Distribution of the muon number proxy, $S_{\mu,550}$, as a function of true muon number ($E_{\mu} \geq 420$ MeV, $r_{\mu} \leq 1$ km) for near-vertical showers $\theta_{\text{reco}} \lesssim 26^{\circ}$ produced with Sibyll 2.1 and weighted to H4a (top left). Average values for different species are shown approximately in the regime where the two-component reconstruction reaches full efficiency. The reconstruction resolution and bias for Sibyll 2.1 (top right), EPOS-LHC (bottom left), and QGSJet-II-04 (bottom right) are shown in the upper and lower panels, respectively.

considering the difference in the average muon number between proton and iron, which is around 40% (see section 3.6). For the lowest observed energies, the resolution worsens to a level of $\sim 50\%$. The reference radius is chosen to minimize the mass dependence in the muon number estimation across all models. Therefore, the muon number bias exhibits a comparably small mass dependence on the few percent level. The mass dependence is largest for Sibyll 2.1, as the optimal reference distance for the pre-LHC model is largest due to its lower muon content compared to the post-LHC models.

Reconstruction Efficiency

The reconstruction efficiency is of high importance for the any cosmic-ray analysis, as it defines the application range and stability of a reconstruction procedure. Particularly, the energy range above which the reconstruction efficiency is independent of the primary mass

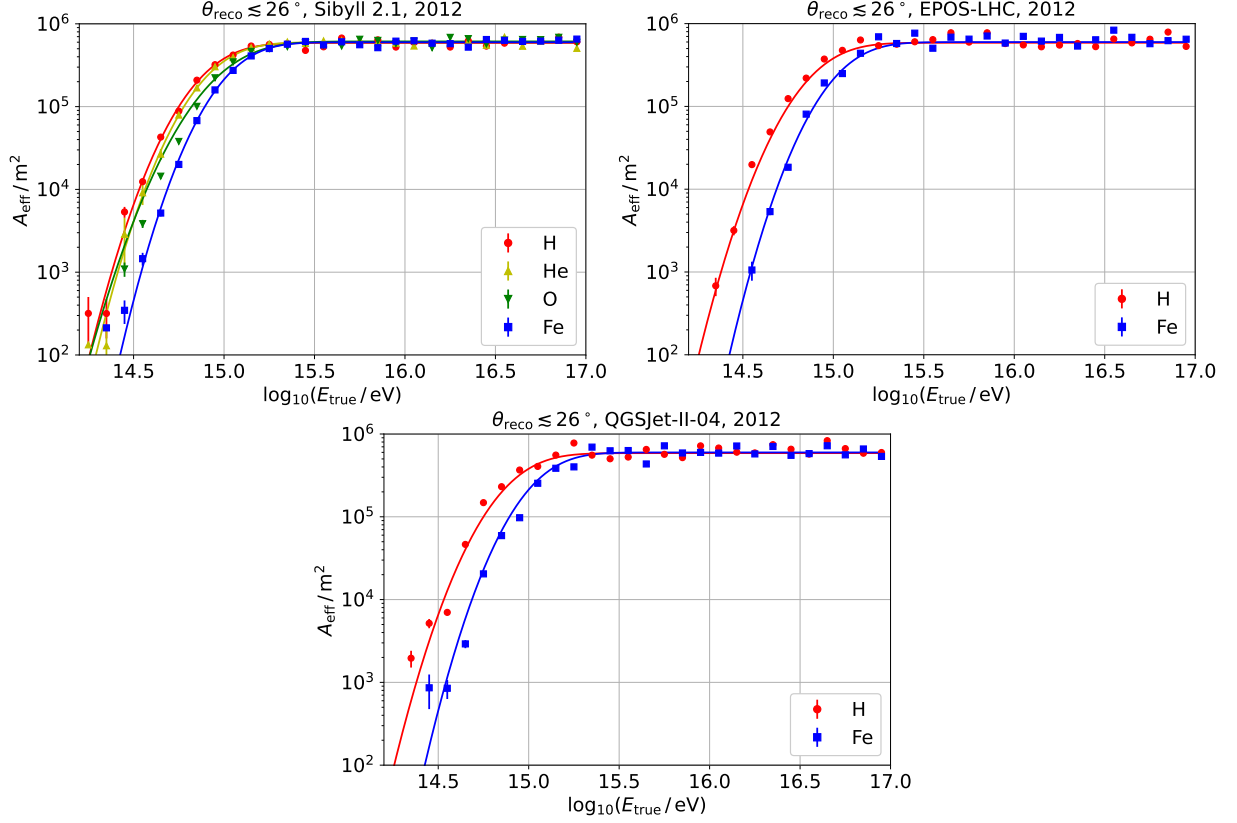


Figure 7.23.: Effective area for the two-component reconstruction as a function of primary energy after application of quality cuts for Sibyll 2.1 (top left), EPOS-LHC (top right), and QGSJet-II-04 (bottom). Solid lines show fits with Eq. (7.18) used to quantify the region in which the

is crucial, since in this range analyses are not effected by selection effects. To quantify the reconstruction efficiency, the *effective area*, A_{eff} , of IceTop defined as

$$A_{\text{eff}}(E) = A_{\text{tot}}(E)\epsilon(E)\frac{\cos\theta_{\min} + \cos\theta_{\max}}{2}, \quad (7.17)$$

$$\epsilon(E) = \frac{N_{\text{sel}}}{N_{\text{tot}}},$$

is calculated⁹. The total area over which CORSIKA showers are injected for the IceTop response simulation is given as A_{tot} . The zenith angle range included for this work corresponds to $\cos\theta_{\min} = 1$ and $\cos\theta_{\max} = 0.9$. Finally, the reconstruction efficiency, ϵ , is determined by the number of events after application of all quality cuts and with a reconstructed zenith angle within this bin, N_{sel} , divided by the total number of generated showers, N_{tot} , in each bin. As an estimate of the uncertainty of A_{eff} , a simple Poisson error is assumed for N_{sel} . To quantify the region of full efficiency, the effective area is

⁹The effective area is calculated using the *SimWeights* python module within the IceCube software (see <https://github.com/icecube/simweights> for details).

modeled via an error function of form

$$f_{A_{\text{eff}}} = p_1 \left(1 + \text{erf} \left(\frac{x - p_2}{\sqrt{2p_3^2}} \right) \right). \quad (7.18)$$

The resulting distributions of A_{eff} and the corresponding fits with Eq. (7.18) are shown in Fig. 7.23 for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04. Note, that the maximum value of A_{eff} is restricted by the containment cut which requires the shower core to be located well inside IceTop. Therefore, the A_{eff} is always smaller than the physical area of IceTop. The threshold effect can be observed at around a PeV in primary energy. This effect is clearly mass dependent and would lead to a corresponding selection bias when included. Thus, the region of full efficiency is defined for energies above which the integral of the fit with Eq. (7.18) for a given model and mass reaches 97%¹⁰ of its maximum value. Since heavy primaries produces the lowest hit multiplicities at low energies, this threshold is reached latest for iron. For all models and masses, the two-component reconstruction is found to be fully efficient above $\log_{10}(E/\text{eV}) \sim 15.4$. This is consistent with the full efficiency threshold of the standard IceTop reconstruction [181]. Therefore, the same energy threshold as used for the standard reconstruction can be applied for analyses using the two-component reconstruction¹¹.

7.5. Comparison to other experiments

In section 7.4, the reconstruction performance obtained for the two-component model is compared to the standard reconstruction introduced in section 4.3.1. To put the reconstruction performance in a more general context, it can be compared to other modern air-shower observatories that operate in a comparable primary energy range.

The LHAASO observatory [20] is situated at ~ 4400 m above sea level (~ 600 g/cm²) and is comprised of ~ 5200 scintillation detectors distributed over an area of 1.3 km² (KM2A), ~ 1200 buried water-Cherenkov detectors that act as muon detectors, a central water-Cherenkov detector array (WCDA) covering 78000 m², and a *Wide Field-of-view air Cherenkov/fluorescence Telescope Array* (WFCTA) with 18 telescopes [255]. With this instrumentation, LHAASO can measure cosmic rays in a large energy range from GeV to a few EeV. With a combination of the detection of Cherenkov light and the measurement of the number of muons, a resolution of $\sim 10\%$ is reached already around 1 PeV in primary energy with small biases within 3%. The resolution improves to well below 10% at ~ 10 PeV. With the KM2A alone, an energy resolution of $\gtrsim 15\%$ is reached around 3 PeV for light primaries [256]. In the same energy range, angular resolutions of $\sim 0.2^\circ$

¹⁰This specific value has been chosen for consistency reasons with previous studies.

¹¹For studies of more inclined air-showers, the full efficiency region has to be adjusted accordingly.

and core position resolutions of a few meters are achieved [257]. The values are obtained for showers with zenith angles below 45° . It should be noted, that the detector spacing within the KM2A is around 15 m and therefore almost an order of magnitude smaller compared to the station spacing of IceTop. The core position resolution of IceTop using the two-component LDF reaches ~ 10 m around a few PeV and decreases to ~ 5 m at 100 PeV for near-vertical showers and for all primaries. The angular resolution is below 0.6° already at a few PeV. In terms of the energy reconstruction, resolutions of around 15% are achieved at the few PeV scale which improve to well below 10% at a few tens of PeV. Despite the significantly higher detector coverage of LHAASO and its hybrid detection, IceTop achieves a reconstruction performance that is close to that of LHAASO.

The low-energy extension of the Telescope Array, TALE [258], operates in the PeV to EeV region and consists of 10 fluorescence telescopes and 80 plastic scintillation detectors that are spaced with distances of 400 m and 800 m [259]. In terms of angular reconstruction, TALE reaches sub-degree resolutions between $\sim 20 - 200$ PeV for zenith angles between $28^\circ - 65^\circ$ [260]. The reconstruction accuracy in the primary energy of TALE in the same zenith range is below 17% up to ~ 200 PeV [260]. For IceTop, sub-degree resolutions are reached in the few PeV region, however, for zenith angles $\lesssim 36^\circ$. The primary energy for near-vertical showers is below 10% with the two-component LDF. The resolution for more inclined events is currently under investigation. However, based on [171], it is not expected to worsen significantly at energies $\lesssim 100$ PeV.

The *Auger Muons and Infill for the Ground Array* (AMIGA) detector features stations of water-Cherenkov tanks and buried scintillation detectors with a spacing of 750 m that are arranged in a hexagonal grid. For energies of 3 PeV and zenith angles up to 55° , it can reach angular resolutions in the sub-degree range [261]. In [262] the muon number resolution in different bins of lateral distance based on different likelihood approaches is reported. For showers in the EeV range and 30° in zenith produced with EPOS-LHC, the muon number is reconstructed with $\sim 6\%$ and $\sim 10\%$ resolution at ~ 450 m and ~ 800 m in lateral distance. It should be noted, however, that since the resolution is determined for lateral distance bins and via the comparison of the reconstructed muon number to the average over all simulated showers, it is not directly comparable with the approach presented in this work.

The KASCADE-Grande detector [33] comprises the KASCADE array [32], which covers $200 \times 200 \text{ m}^2$ and features unshielded and shielded scintillation detectors, muon tracking detectors, and a central hadron calorimeter, and a total area of $700 \times 700 \text{ m}^2$ instrumented with scintillation detectors. KASCADE-Grande operated in the 10 PeV to EeV energy range [263], where core position resolutions of ~ 5 m and direction resolutions in the sub-degree range were achieved for vertical showers [264]. Using the shielded scintillation detectors, muon number resolutions of $\lesssim 15\%$ and $\lesssim 20\%$ are reached for near-vertical showers ($\theta \leq 18^\circ$) at 10 PeV and 2 EeV, respectively [263]. At 10 PeV, a muon number

resolution of around 20% is reached with IceTop using the two-component model. However, the resolution improves with increasing energy and is well below 20% at $\lesssim 100$ PeV. The Tunka-Grande array [265] in Siberia is part of the TAIGA Gamma Observatory [266] and comprises 19 scintillation stations, where each features a surface and an underground component. Each station consists of 12 scintillation counters that were part of KASCADE-Grande and EAS-TOP [92]. Eight similar detectors act as underground muon detectors. Tunka-Grande operates in the 10 PeV to EeV energy range. For zenith up to $\sim 35^\circ$, its core position and angular resolution are ≤ 26 m and $\leq 2.6^\circ$, respectively, above 10 PeV, while the energy resolution is $\leq 36\%$ [265]. These values improve to ~ 17 m, $\sim 1.4^\circ$, and $\sim 20\%$ at 100 PeV [267]. At 100 PeV, muon number resolution reached with Tunka-Grande is $\sim 25\%$.

Considering the fact that IceTop is not a hybrid cosmic-ray air shower observatory and does not feature dedicated muon detectors, its performance in the reconstruction of various observables using the two-component LDF is well compatible with other modern air-shower observatories.

Consistency tests of hadronic interaction models

In section 3.6, the challenges connected to the interpretation of measured air-shower data introduced by uncertainties in the simulations through hadronic interaction models are discussed. In this chapter, different hadronic interaction models are tested for their ability to provide a self-consistent interpretation in their prediction of the average composition based on different mass-sensitive observables. For this purpose, both, established mass-sensitive parameters from previous analyses from IceTop and the in-ice array as well as the new parameters derived from the two-component reconstruction discussed in the previous chapter are analyzed. The method of comparing different observables is based on a previous analysis presented in [241] and is discussed in detail in the following. The data set used for the analysis presented in chapter is given in section 4.4.

Since studies including SLCs are more prone to the influence of accidental background hits produced mainly by small showers that are present in experimental data but not taken into account in the standard IceTop processing introduced in section 4.3.1, firstly, in section 8.1, a simplified method for the injection of random background coincidences is presented. This method is based on studies described in [199], and will be utilized to consider background hits in the analysis presented in this work. Before analyzing the measured data, the general agreement between the data and the simulations for all two-component LDF parameters is studied in section 8.2. In addition, in section 8.3, all mass-sensitive observables are introduced and the corresponding composition prediction is derived for different hadronic interaction models. Lastly, a discussion of the implications of the results is given in section 8.4.

8.1. Coincidence background

For the interpretation of measured data, small air-shower events that occur in coincidence with the main event can lead to a bias by producing additional tank triggers. Such ran-

dom coincident background hits are not part of the simulation chain and therefore have to be accounted for separately. The simulation of background hits is highly non-trivial since coincident hits produced by small showers are not uncorrelated. However, to gauge the impact of background triggers on the two-component reconstruction, a simplified simulation of random background coincidences is performed in a similar manner as for the statistical analysis of low-energy muons measured with IceTop described in [199]. Using an off-time window of $7.5\,\mu\text{s}$ with respect to the shower plane in measured data for the years 2010-2012, the rate of accidental coincidence triggers is found to be 1470 Hz on a single-DOM basis. From this study, the signal probability distribution for coincident hits was obtained and can be used as the basis for the simulation of background hits. Fig. 8.1 (left) shows the resulting signal probability distribution function of accidental background events and the corresponding distribution produced from the background simulation as a consistency test.

For each simulated air-shower event used for the analysis presented in this chapter and in chapter 9, a simulation of the coincident background is performed. For this purpose, coincident hits are generated with a fixed rate of 1470 Hz for each IceTop tank. For each background hit, the trigger time is randomly sampled from a uniform distribution within the time window of a given event. The measured charge is sampled from the signal PDF shown in Fig. 8.1 (left). In case a background hit is generated for a DOM that already has a signal, the sum of both signals is used instead if both hits occur within 427 ns. If the two signals are generated within the dead time of a DOM¹, the later signal is removed. Since the coincident background is added after the classification of local coincidences, HLCs and SLCs have to be reassigned. On the one hand, if a background signal is generated in the neighboring tank of an existing SLC within $1\,\mu\text{s}$ of the SLC trigger, the whole station is reclassified as HLC. On the other hand, the dead time window can lead to the removal of one tank trigger within an HLC station, leading to a reclassification as SLC. Injection of background hits is performed as an additional step after the standard processing, and a successive track-based² cleaning is applied on the modified HLC and SLC hits. To minimize the potential impact of accidental coincidence signals while still considering the bulk of the arriving shower front, the time window for SLCs is chosen to be $-500\,\text{ns} \leq \Delta t \leq 0\,\text{ns}$ with respect to the reconstructed shower plane. For the track-based cleaning of HLCs, the default time window of $-800\,\text{ns} \leq \Delta t \leq 200\,\text{ns}$ is used. Fig. 8.1 (right) shows the rate of coincident background hits³ in different shower size bins as a function of lateral distance. The contribution of background hits increases significantly for decreasing primary energy and for increasing distance to the shower axis. Therefore, it is

¹The minimum time between successive hits in a DOM was shown to be $\sim 1.65\,\mu\text{s}$ [199].

²See section 4.3.1 for details.

³Note that the signal window used here is with $4.5\,\mu\text{s}$ significantly larger compared to the one applied in this work. However, it is sufficient for the purpose of this discussion.

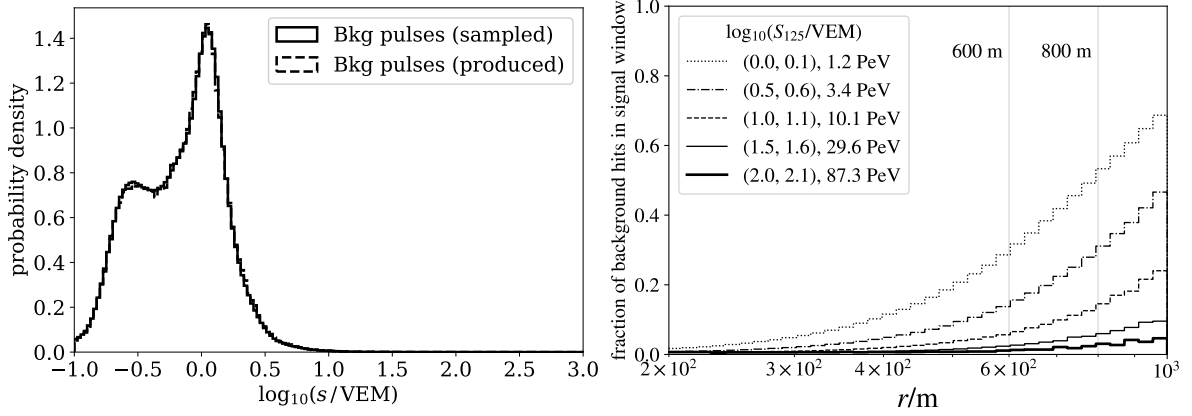


Figure 8.1.: Signal probability distribution function determined from experimental data (see [199] for details) in an off-time window (left). Fraction of accidental background hits in a signal window of $4.5 \mu\text{s}$ in bins of $\log_{10} S_{125}$ and as a function of lateral distance (right). Figure taken from [199].

expected that the influence of the background on the muon number reconstruction using the two-component LDF is larger for low-energy showers while for high-energy showers the sheer size of the events reduced the influence of coincident hits. It should be noted, that ideally the background rate should be estimated based only on the measured events that are included in the analysis to ensure that both the background in the time window of the event and in the off-time window are effected by systematics in the same way. In particular, the background rate decreases over the years due to the increasing snow accumulation on top of the IceTop tanks. However, since the background rate used for this analysis is estimated using data from 2010-2012, while only events from 2012 are considered for the two-component reconstruction, the background rate can be viewed as a conservative estimate for the analysis presented in this chapter.

The distribution of background SLCs produced (which represent the majority of background hits) over the entire trigger window for each event is shown in Fig. 8.2. While the number of background SLCs comprises multiplicities of up to ~ 20 over the entire trigger window, typically only about 0-2 coincident background SLCs per air-shower event are contained within the signal time window of 500 ns. After injection of background coincidences and subsequent event cleaning, the two-component reconstruction is performed and the quality cuts derived in section 6.3 are applied. To gauge the impact of background coincidences on the parameters of the two-component reconstruction, reconstructions including background simulations are compared to reference reconstructions without background in App. C. For the lowest energies considered, the relative influence of background coincidences is on the $\lesssim 2\%$ level, which decreases toward $\sim 0.1\%$ for increasing primary energy.

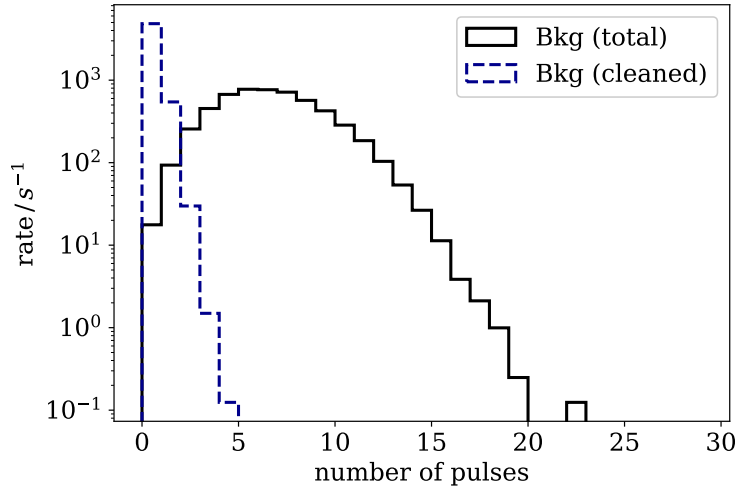


Figure 8.2.: Distribution of the number of injected background SLCs during the event time window compared to the number of background events after the arrival time based cleaning of SLC pulses (see section 4.3.1).

8.2. Data-MC comparison

Before experimental data can be included in the analysis, it is important to test its consistency compared to MC simulations in order to ensure reasonable behavior of the two-component reconstruction. For this purpose, the corresponding high-level parameter distributions derived in the previous chapter are compared to the results obtained for experimental data. Since the true composition is unknown, a realistic cosmic-ray composition model has to be assumed for such comparisons. While it is not meaningful to compare the exact composition obtained from data to a given composition assumption due to its large uncertainties, the parameter distributions from experimental data should be bracketed within the extreme cases of a pure proton and pure iron composition. Therefore, the data distributions are compared to pure proton and iron simulations weighted to the all-particle flux for a specific flux model.

Fig. 8.3 shows the parameter distributions of $S_{\text{tot},125}$, β_{em} , β_{μ} , and $S_{\mu,550}$ obtained from 1% of the experimental data of the year 2012 compared to the corresponding MC distributions for proton and iron primaries weighted to H4a. After application of the quality cuts listed in Tab. 6.4, this data set contains ~ 260000 events. In comparisons of low-level distributions, it is found that the event rate distributions for simulations weighted with H4a need to be increased by 25% to match the data rates [41]. This shift is also applied to the high-level distributions shown in Fig. 8.3.

For all parameters, the data distributions are reasonably well within the pure proton and iron expectations and within the statistical uncertainties. In general, a higher event rate is observed for data at the highest and lowest energies, which is mainly produced by

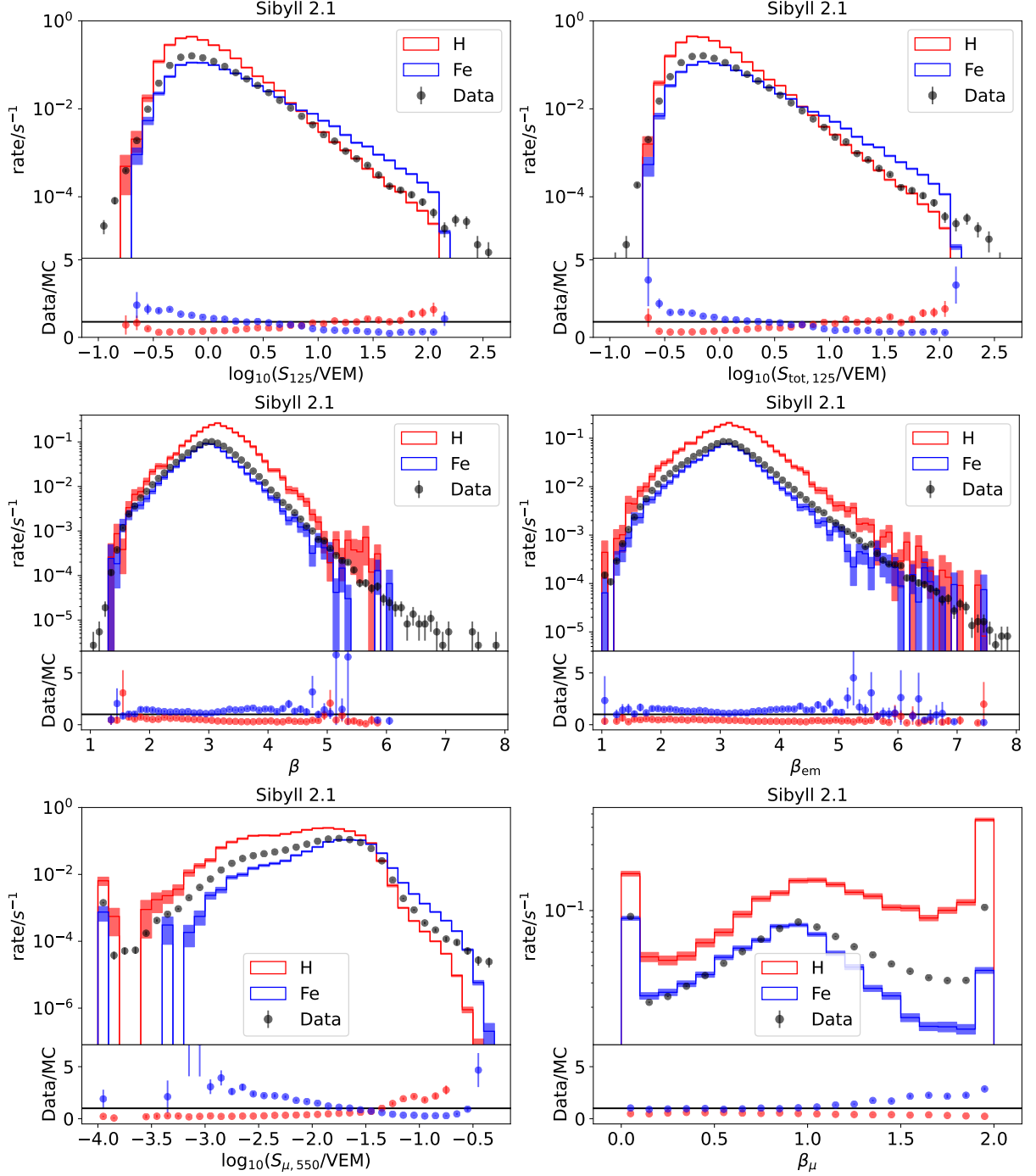


Figure 8.3.: Parameter distributions of $S_{\text{tot},125}$, β_{em} , β_{μ} , and $S_{\mu,550}$ obtained for the application of the two-component reconstruction on experimental data and simulations for Sibyll 2.1. For comparison, also the parameter distributions for S_{125} and β derived from the standard reconstruction are shown. For all distributions, the quality cuts listed in Tab. 6.4 are applied.

showers with primary energies that are not part of the simulation set. Small deviations from this behavior as observed, e.g., between values of $\sim 0.5 - 1 \text{ VEM}$ in $\log_{10} S_{\text{tot},125}$

and between -1.6 to -1.4 in $\log_{10} S_{\mu,550}$ are not unexpected, since the energy spectra assumed in a specific flux model can differ from the true one. However, various parameters can differ in their scaling between the pure proton and iron assumptions depending on the hadronic interaction model, leading to a different interpretation of the measured data. For instance, a composition-sensitive parameter such as β_{μ} is closer to the proton expectation for post-LHC models compared to Sibyll 2.1 due to their larger content of low-energy muons. The respective data-MC comparisons for EPOS-LHC and QGSJet-II-04 are shown in Figs. C.2 and C.3.

For an additional consistency test, Fig. 8.3 also shows the distributions for the parameters S_{125} and β of the standard reconstruction as their respective data-MC agreement should, by construction⁴, be roughly comparable to that of $S_{\text{tot},125}$ and β_{em} . In fact, no significant differences are observed for $\log_{10} S_{\text{tot},125}$ and $\log_{10} S_{125}$ when comparing the MC expectation for proton and iron with the experimental data, which is expected since both include mainly EM and a small muon contribution. The distributions of β_{em} shows an increase in the number of events at small and large values compared to β , which is likely due to the energy-dependent parametrization of κ in the two-component model and the steeper shape of the EM LDF compared to the LDF described by β .

8.3. Internal consistency

For the interpretation of cosmic-ray air shower events, accurate simulations of the shower evolution are necessary. In this context, the description of the generation of the high-energy hadronic component as the backbone of the entire EAS development via hadronic interaction models constitutes one main part of the systematic uncertainty.

The IceCube Neutrino Observatory has the unique capability to measure the electromagnetic and low-energy muon part of air-shower events with IceTop, and the high-energy muon content with its deep in-ice array. This enables the study of muons in two vastly different energy regimes, which probes the corresponding hadronic processes at different stages of the shower development. Overall, this is an ideal setup for tests of the validity of hadronic interaction models. Additionally, the multitude of different cosmic-ray mass-sensitive parameters provided by measurements with IceTop and the in-ice array can be used to perform consistency checks among the different parameters. The two-component reconstructions adds additional parameters that can be used in this context. In this section, different hadronic interaction models are tested for internal consistency using the new composition-sensitive parameters of the two-component LDF based on a previous

⁴As discussed previously, both, S_{125} and β , are dominated by electromagnetic contribution with a small contribution of low-energy muons.

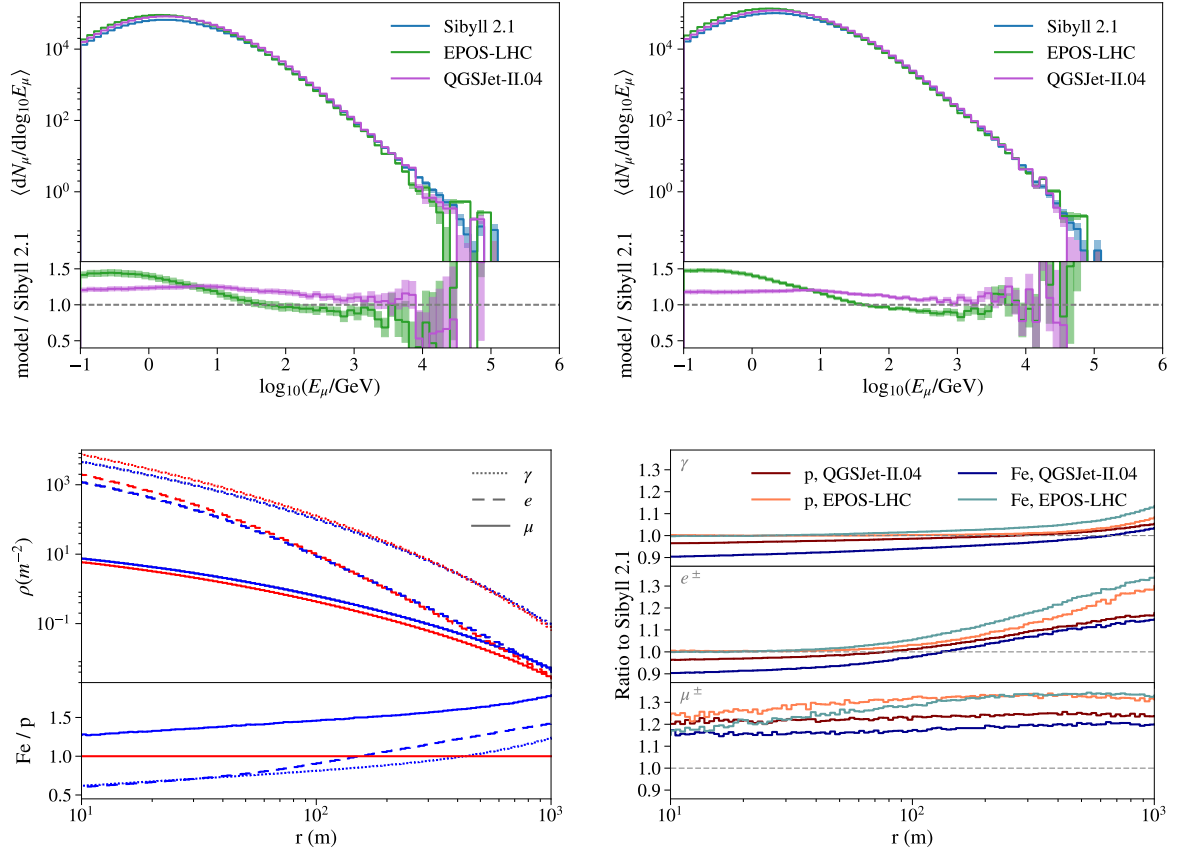


Figure 8.4.: Muon-energy spectra for vertical proton- (top left) and iron-initiated (top right) showers with primary energy around 10 PeV for Sibyll 2.1, EPOS-LHC, and QGSJet-II.04. Average lateral distributions of electromagnetic particles (electrons and photons) and muons for vertical proton- and iron-initiated showers around 10 PeV obtained from CORSIKA simulations produced with Sibyll 2.1 and corresponding distributions for EPOS-LHC and QGSJet-II-04 compared to Sibyll 2.1 are shown in the bottom left and right, respectively. Figures taken from [41].

study presented in [241, 41] and compared to established parameters from IceTop and the in-ice detector.

8.3.1. MC expectations

Before describing all reconstructed composition-sensitive parameters in more detail and testing different hadronic interaction models for self-consistency in their prediction, it is important to have a closer look at the corresponding MC expectations for the different models. Firstly, the average muon energy spectra for vertical proton- and iron-initiated air showers of 10 PeV in primary energy are shown in Fig. 8.4 (top row) for Sibyll 2.1,

EPOS-LHC, and QGSJet-II-04. While the post-LHC models feature a larger number of low-energy muons, the QGSJet-II-04 has the highest number of high-energy muons, followed by Sibyll 2.1 and then EPOS-LHC. Generally, the difference in the high-energy muon content between the models is smaller compared to the low-energy muons, which exhibits differences up to 50%. Consequently, the spectral slopes differ significantly between the models depending on the muon energies. This strongly motivates the study of correlations between low- and high-energy muons with IceTop and the in-ice detector to derive strong constraints on hadronic interaction models. The bottom row of Fig. 8.4 illustrates the average lateral distributions of electromagnetic particles and muons for vertical air-showers with ~ 10 PeV primary energy for proton and iron primaries as well as the ratios of the corresponding distributions of the post-LHC models to Sibyll 2.1. Naturally, the total muon content in iron-initiated showers is larger compared to proton due to the larger hadronic contribution. This difference increases as a function of the lateral distance, as the average muon energy decreases. Overall, the LDFs of both electromagnetic particles and muons are steeper for proton-initiated showers because of their earlier development for the same primary energy. Comparing the post-LHC models to Sibyll 2.1, the most eminent difference is visible in the muon content, which is significantly larger for the post-LHC models over the entire lateral distance range. This difference increases to over 30%/20% for large lateral distances for proton and iron, respectively. In case of the electromagnetic distribution, a steeper distribution is visible for the post-LHC models compared to Sibyll 2.1. This is an interesting observation, as the average value of X_{max} is in fact larger for the post-LHC models, which results in a smaller shower age at the observation level, i.e., in a steeper distribution. The fact that the opposite behavior is observed can be explained by the high observation level of IceTop, which is located around the position of X_{max} in the observed energy range for light primaries. Since the particle content along the longitudinal shower-development depends on the location relative to X_{max} , the steeper distributions in Sibyll 2.1 could be caused by the sampling of the air shower around X_{max} [240].

8.3.2. Composition sensitive parameters

Tests of the consistency of hadronic interaction models using a combination of different parameters sensitive to the primary mass were first studied in [268, 269, 270] with KASCADE and in [42] with IceCube. In general, different composition-sensitive parameters should describe the data in a self-consistent way, i.e., they should agree in their mass prediction as they observe the same composition. In a subsequent study presented in [241, 41], this study was further enhanced and expanded with new mass-sensitive parameters. Since the IceCube Neutrino Observatory provides surface and in-ice information, mass-

sensitive parameters are used for both detector components. Firstly, by reconstruction air-shower events with IceTop with the standard reconstruction, the reconstructed slope parameter, β , provides information about the primary mass. Additionally, in a statistical analysis detailed in section 4.3.2, the low-energy muon density at large distances from the shower axis (600 m and 800 m) can be obtained. Lastly, using the measurement of high-energy muons above several hundred GeV with the in-ice detector, the muon bundle loss parameter, dE/dX_{1500} , can be used as a composition-sensitive parameter. These parameters are developed in previous analyses and will be introduced in more detail in the following as they are used in section 8.3.5.

Using the two-component reconstruction, three new parameters can be included, namely, the electromagnetic slope, β_{em} , the muon slope, β_{μ} , and the expected muon signal strength, $S_{\mu,550}$ at a distance of 550 m from the shower axis.

Standard LDF slope, β

The LDF slope of the standard reconstruction introduced in section 4.3.1 is sensitive mainly to the electromagnetic component, but is also influenced by the contribution of low-energy muons [41]. The sensitivity of the LDF slope to the primary mass stems from both contributions. Firstly, heavier primaries, on average, interact earlier in the atmosphere for the same primary energy and therefore have a higher shower age. As a result, the shower particles are more spread out compared to light primaries, leading to a flatter lateral distribution. Secondly, heavy primaries have a higher low-energy muon content, which have a flatter lateral distribution compared to the electromagnetic component. Both effects result in a flatter lateral distribution for heavy primaries, i.e., in a smaller value of β . Example distributions for proton- and iron-initiated showers produced with Sibyll 2.1 are shown in Fig. 8.5 (top left).

Two-component LDF electromagnetic slope, β_{em}

For the electromagnetic slope parameter of the two-component reconstruction, the composition dependence is produced from the differences in the average values of X_{max} , similar to β . An example distribution of β_{em} for Sibyll 2.1 is shown in Fig. 8.5 (top right). It is visible, that the values of β_{em} are shifted slightly toward larger values compared to β , suggesting that the electromagnetic contribution of β is successfully disentangled by the two-component reconstruction and extracted in β_{em} . The evolution of $\langle\beta_{\text{em}}\rangle$ as a function of primary energy for proton- and iron-initiated showers produced with different hadronic interaction models is shown in Fig. 8.6 (top left). As expected from Fig. 8.4, the

average electromagnetic LDF is slightly flatter (smaller values of β_{em}) for the post-LHC models by only $\sim 2\%$. It should be noted, that the distributions of β and β_{em} can not be directly compared, since the values of the LDF curvature, κ , are different in the standard reconstruction compared to the two-component model. For the latter, κ is parametrized as a function of S_{125} and increases with increasing primary energy, i.e., the LDF becomes steeper. For this reason, $\langle\beta_{\text{em}}\rangle$ is decreasing as a function of energy. Overall, however, the reconstructed electromagnetic LDF is steeper compared to the LDF of the standard reconstruction, which is consistent with the fact that β is significantly influenced by low-energy muons. This has been proven in [41] by studying the evolution of β when fixing either N_μ or X_{max} . For a fixed X_{max} , β is found to become smaller (flatter LDF slope) with increasing N_μ . Conversely, when fixing N_μ , the LDF slope becomes steeper (larger values of β) with increasing X_{max} . Since the number of muons and X_{max} are highly correlated with the primary energy, this is consistent with the observed behavior of β_{em} .

Two-component LDF muon slope, β_μ

The two-component reconstruction not only provides the slope of one LDF describing mostly the electromagnetic contribution, which typically drives the LDF fit due to its large signal deposits close to the shower axis, but also the slope of the muon LDF. The latter describes the slope of the muon lateral distribution, which is significantly flatter than the electromagnetic LDF. This is because muons are less affected by attenuation and therefore can travel farther from the shower axis compared to electromagnetic particles [42]. Although the maximum of the longitudinal muon distribution, $X_{\mu,\text{max}}$, arises from different shower physics compared to the electromagnetically dominated X_{max} [199], both are intrinsically linked through the fundamental properties of the shower development and the primary particle that initiated the cascade⁵. Thus, the composition sensitivity of β_μ can be explained analogously to β_{em} . Since, on average, $X_{\mu,\text{max}}$ is more shallow for heavy primaries for the same primary energy, the slope of the muon LDF is expected to be more flat (smaller values of β_μ) compared to light primaries. In addition, heavy primaries produce a larger number of low-energy muons for the same primary energy, contributing further to a more flat muon distribution. An example distribution of β_μ for proton- and iron-initiated air showers is shown in Fig. 8.5 (bottom left) for Sibyll 2.1. Since the muon component in air showers is subject to larger fluctuations compared to the electromagnetic component, the spread of the β_μ distributions is larger compared to β and β_{em} . Fig. 8.6 (top right) illustrates the evolution of $\langle\beta_\mu\rangle$ as a function of primary energy for proton-

⁵The height of maximum muon production, $X_{\mu,\text{max}}$, is more shallow than X_{max} . Since the difference between both, $X_{\text{max}} - X_{\mu,\text{max}}$, is by construction independent of the height of the first interaction [271] and therefore does not depend much on the primary particle [272].

and iron-initiated showers produced with Sibyll 2.1, EPOS-LHC, and QGSJet-II-04. The post-LHC models, on average, show a $\sim 10\%$ (up to 20% at the highest energies) flatter muon LDF (smaller values of β_μ) compared to Sibyll 2.1. This is consistent with the higher low-energy muon content in the post-LHC models. It should be noted, that the reason for the decreasing $\langle\beta_\mu\rangle$ as a function of energy is the parametrization of the second muon slope parameter, γ , which increases with increasing energy. Overall, the muon LDF becomes slightly steeper with increasing energy, which can be explained by the increase in $X_{\mu,\max}$ as a function of energy.

GeV muon density, ρ_μ^{600} and ρ_μ^{800}

The reconstruction of the density of GeV muons with IceTop using at large distances to the shower axis is introduced in detail in section 4.3.2. It should be mentioned, that this method is based on a statistical analysis applied on the entire set of observed showers. In contrast to that, all other parameters used in this section are obtained on a single-event basis. Nevertheless, this method utilized the distinct tank response to muons similarly to the two-component reconstruction. For this, two lateral distance bins, 600 m and 800 m, are used to derive the corresponding muon densities, ρ_μ^{600} and ρ_μ^{800} . For the comparison of the muon density with the other composition-sensitive parameters, two conceptual differences with respect to the method described in section 4.3.2 are derived in [241, 41]. Firstly, the energy conversion function used in [199] is updated to the IC86.2012 detector configuration also used for the work presented in this thesis. Secondly, the correction factors used to correct for the differences between the true and reconstructed muon densities are applied as a function of S_{125} . The corresponding systematic uncertainties introduced by this adjustment are taken into account by means of a systematic uncertainty [41]. Since the muon content in air showers strongly depends on the hadronic component and therefore on the primary mass, the muon density is a valuable parameter to derive the cosmic-ray composition. The dependence of ρ_μ^{600} and ρ_μ^{800} on the primary mass is shown in [241, 41].

Two-component LDF normalization, $S_{\mu,550}$

The muon estimator, $S_{\mu,550}$, of the two-component model is shown to be sensitive to the number of muons in air showers measured with IceTop in section 7.2. Similarly to the muon density at large distances from the shower axis, the total number of muons (above 420 MeV) is sensitive to the composition due to the difference in the muon content of different primary masses with the same primary energy. An example distribution of $\log_{10} S_{\mu,550}$ for Sibyll 2.1 is shown in Fig. 8.5 (bottom right). The muon proxy exhibits

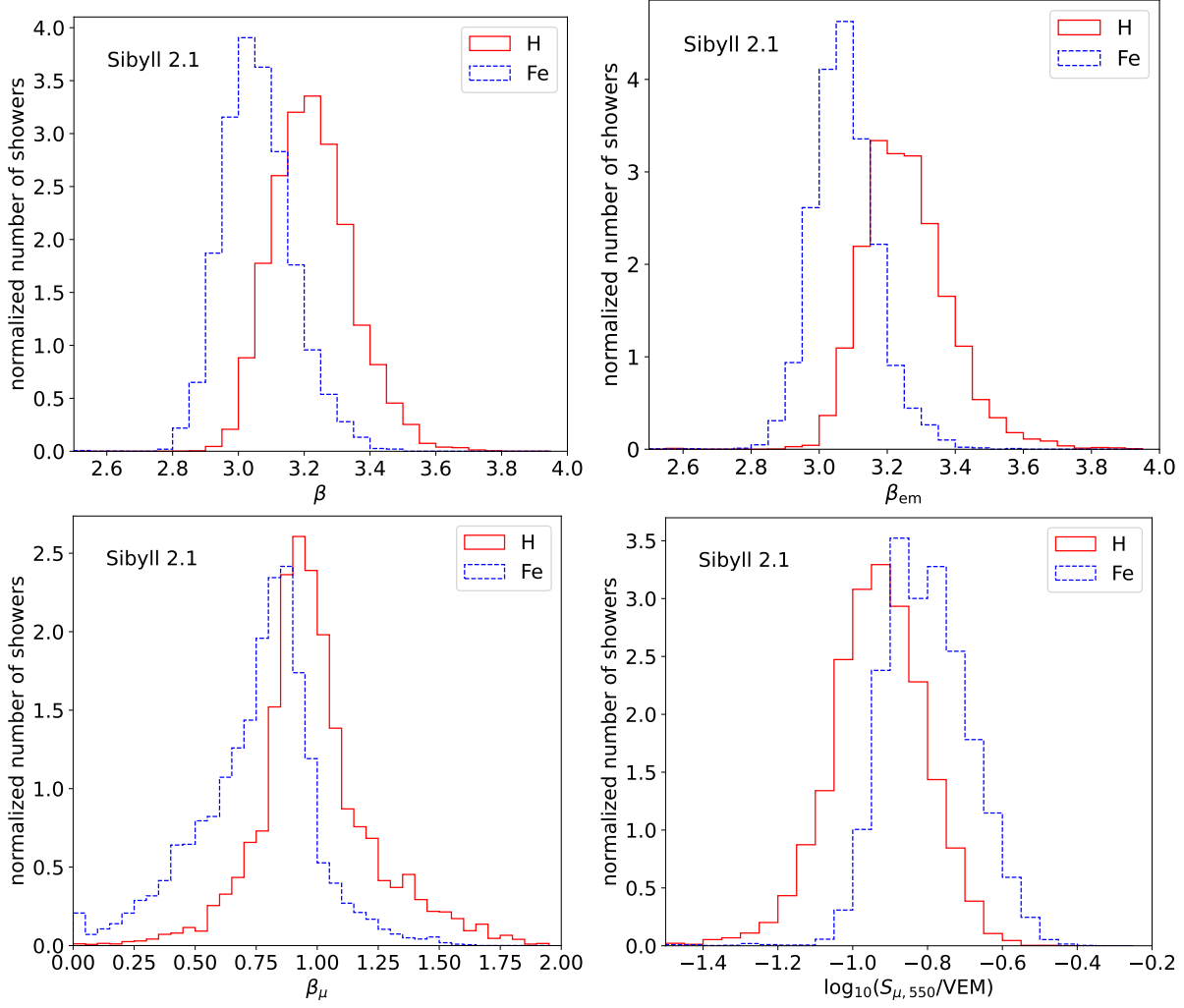


Figure 8.5.: Distributions of different mass-sensitive parameters, β , β_{em} , β_μ , and $S_{\mu,550}$, for air showers with primary energies of $16.6 < \log_{10}(E_{true}/\text{eV}) \leq 17.0$ produced with Sibyll 2.1. Near-vertical showers ($\cos\theta > 0.9$) produced by proton and iron primaries are shown as solid red and dashed blue lines, respectively.

smaller values for proton primaries compared to iron initiated air-showers consistent with the smaller muon content for light primaries. Fig. 8.6 (bottom left) illustrates the evolution of $S_{\mu,550}$ as a function of primary energy for proton- and iron-initiated showers produced with Sibyll 2.1, EPOS-LHC, and QGSJet-II-04. For all energies, the clear separation between proton and iron primaries is visible. Consistent with the increased muon content in EPOS-LHC and QGSJet-II-04 compared to Sibyll 2.1, the average values of the muon number proxy are larger for the post-LHC models over the entire energy range by around 20%. Since the muon content is largest for EPOS-LHC, the values of QGSJet-II-04 are lower by a few percent.

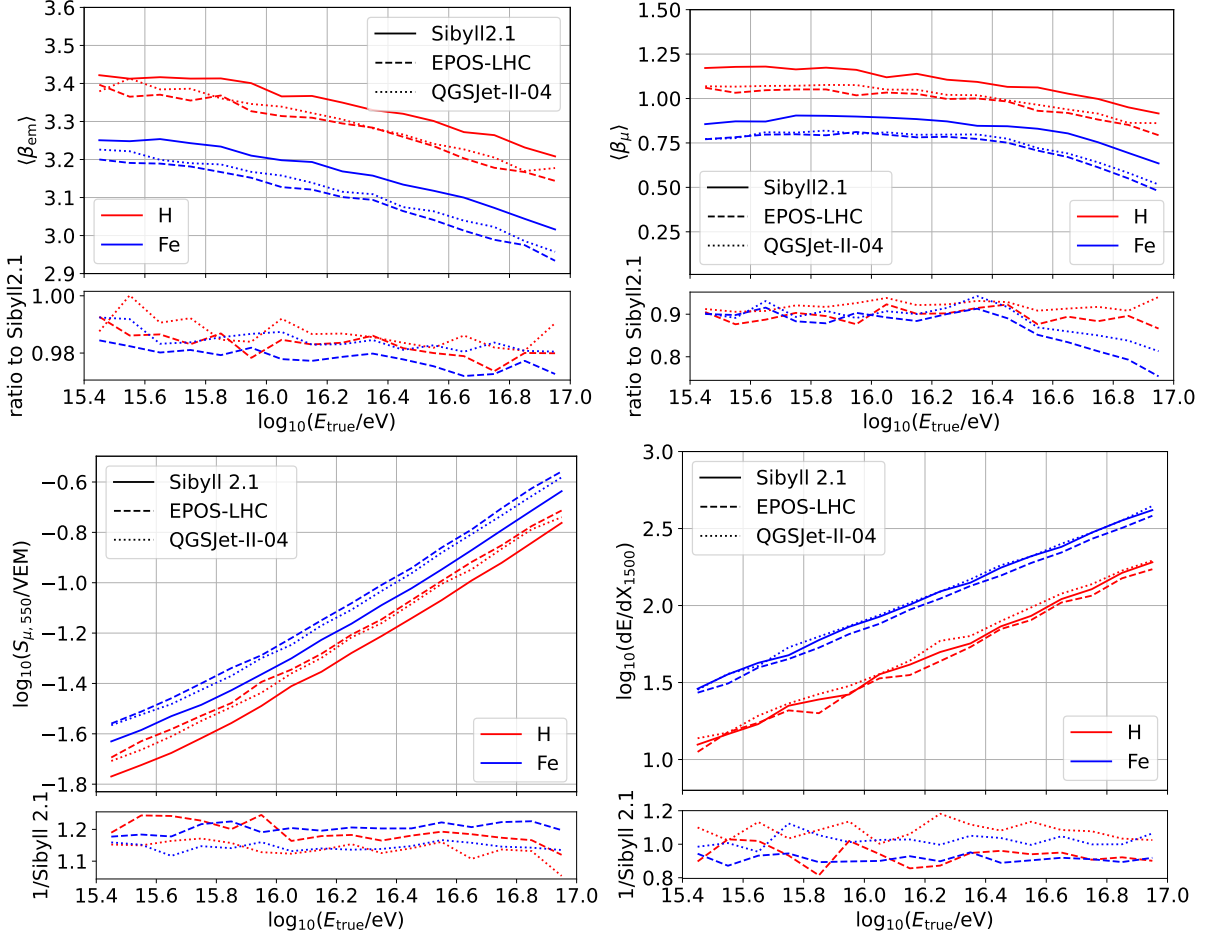


Figure 8.6.: Average values of the electromagnetic and muon slope parameters, β_{em} and β_{μ} , the muon number proxy $S_{\mu,550}$ of the two-component LDF, and dE/dX_{1500} as a function of primary energy for near-vertical ($\cos\theta > 0.9$) proton- and iron-initiated showers for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04.

Energy loss of the muon bundle, dE/dX_{1500}

The only mass-sensitive parameter reconstructed with the in-ice detector included in this analysis is the energy loss of the high-energy muon bundle, dE/dX_{1500} . High-energy muons are produced early in the shower development and closely follow the primary direction. The energy threshold of muons reaching the in-ice array is around a few hundred GeV. The so selected high-energy muons probe a different stage of the shower development compared to the low-energy muons and are therefore of high interest for hadronic model tests. Since the energy loss of the muon bundle is strongly correlated with the muon multiplicity, dE/dX_{1500} is sensitive to the number of high-energy muons. As the muon multiplicity depends on the primary mass, dE/dX_{1500} is a valuable composition-sensitive parameter [187]. The evolution of dE/dX_{1500} as a function of primary energy for proton- and iron-initiated showers produced with Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 is

shown in Fig. 8.6 (bottom right). Compared to Sibyll 2.1, the post-LHC model QGSJet-II-04 predicts higher values of dE/dX_{1500} by $\sim 10\%$ for proton and by a few percent for iron. Conversely, EPOS-LHC leads to $\sim 10\%$ smaller values compared to Sibyll 2.1 for both proton and iron.

8.3.3. Systematic uncertainty

To interpret the measured data in a meaningful way, the systematic uncertainties of the reconstruction methods and the detectors need to be estimated for each of the considered parameters. For the known composition-sensitive parameters, β , ρ_μ^{600} , ρ_μ^{800} , and dE/dX_{1500} , the systematic uncertainties are adapted from previous studies. In the case of β , this comprises the systematic uncertainties on the VEM calibration of 3% and the on the snow attenuation factor, λ_{snow} (see section 4.3.1), of 0.2 m. For both cases, the standard IceTop reconstruction is processed with shifted VEM charges by $\pm 3\%$ and an adjusted value of λ_{snow} by ± 0.2 m. These changes have a significant impact on the reconstructed LDF and therefore on β and S_{125} . The resulting differences of the average β values to the nominal values from the initial reconstruction are taken as systematic uncertainties and added up in quadrature. For the muon densities, significant systematic uncertainties arise from the reconstruction procedure itself in the form of an average correction factor that includes statistical uncertainties, uncertainties from the unknown cosmic-ray composition, and of the finite energy resolution. Additionally, the assumed shape of the electromagnetic contribution as well as the energy estimation cause significant systematic uncertainties (see [199] for details). In the case of dE/dX_{1500} , the main part of the systematic uncertainty originates from the ice model used in the reconstruction which has a large influence on the total light yield. This includes uncertainties on absorption, DOM efficiency, and scattering, yielding a total light yield uncertainty of $+9.6\%/ -12.5\%$ [187]. Additionally, to derive the $\langle dE/dX_{1500} \rangle$ as a function of S_{125} , also the systematics introduced by the uncertainties in λ_{snow} and in the VEM calibration are taken into account [41].

Similarly, the two-component reconstruction is influenced by the snow attenuation and the VEM calibration. Therefore, the reconstruction is re-processed for shifted values of λ_{snow} and the VEM definition. Again, the differences of the resulting average values of β_{em} , β_μ , and $S_{\mu,550}$ to the nominal values are taken as systematic uncertainties and added in quadrature to obtain the total systematic uncertainty. It should be mentioned, that the presence of random coincidence background in measured data produces an additional bias. The influence of coincident background hits increases as a function of lateral distance and therefore has to be included for the reconstruction of the muon density at large lateral distances and for the two-component reconstruction. Since the simulation of background

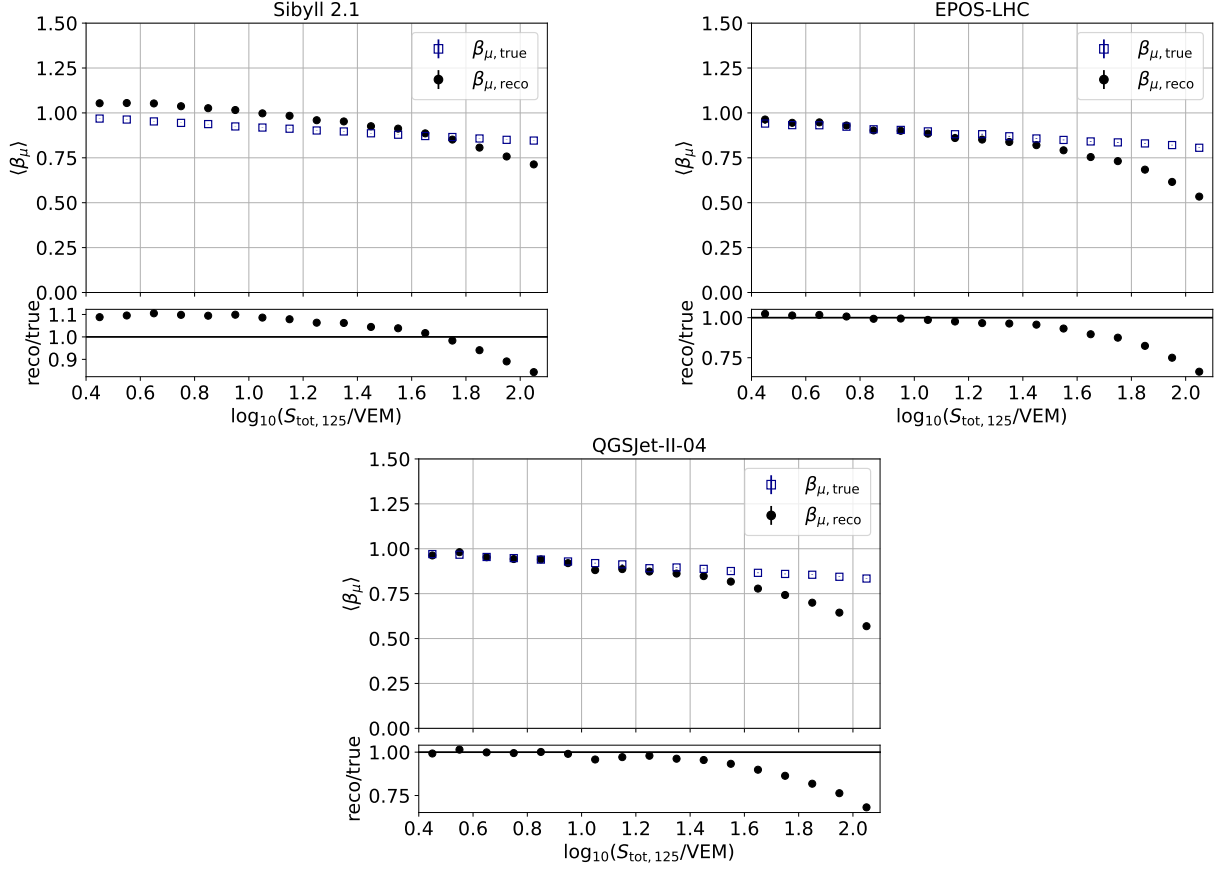


Figure 8.7.: Average values of the muon slope parameter β_μ as a function of $S_{125,\text{em}}$ for different hadronic interaction models and weighted to the H4a flux model. Reconstructed values are obtained from the two-component reconstruction, true values are derived from fits to the corresponding true muon lateral distributions extracted from CORSIKA.

hits discussed in section 8.1 is based on the muon density analysis presented in [199], both methods use the same procedure. A more detailed discussion about the systematic uncertainties included for the two-component reconstruction can be found in section 9.4.

8.3.4. Muon LDF

The ability of the reconstructed muon LDF to describe the true muon lateral distribution can be examined directly using the true CORSIKA muon density distributions. This is the case only under the assumption that the muon signal response is purely a function of their track length and that the muon energy is large enough to cross the entire detector while producing Cherenkov radiation along the entire track. It is shown in section 5.4, that a muon energy threshold of 420 MeV is sufficient to fulfill these assumptions in a satisfactory way for the snow heights observed in the year 2012. The muon number reconstruction with the two-component model is therefore based on muons above this

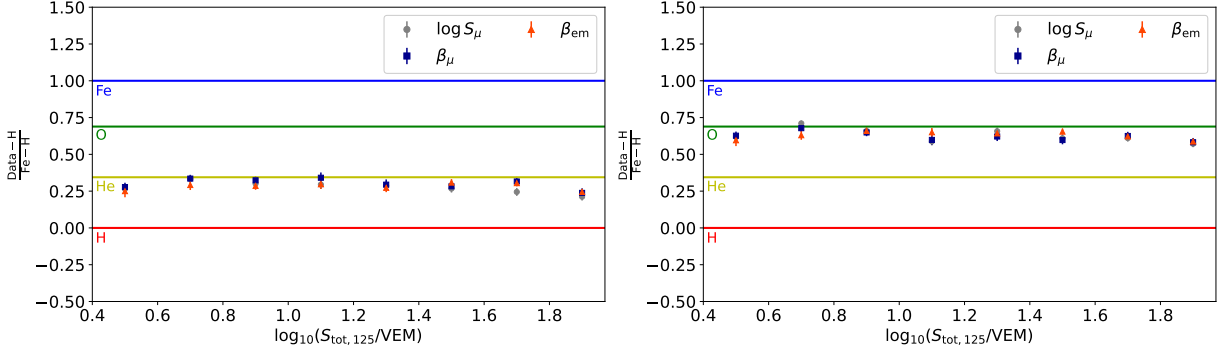


Figure 8.8.: Two-component LDF parameter values normalized to the proton-iron difference (Eq. (8.1) for simulations of helium (left) and oxygen (right) produced with Sibyll 2.1.

energy threshold (see section 7.2). Similarly, the true muon density distributions with $E_\mu \geq 420$ MeV can be used to derive the expected true muon LDF slope. For this purpose, for each reconstructed shower, the true muon lateral distribution is derived from CORSIKA. The muon LDF is then fit to the true distributions on a single-event basis and using the same values for $\gamma(\log_{10} S_{125})$ as in the two-component reconstruction. The fit is performed using a simple χ^2 minimization in the lateral distance range of 35 – 1000 m. This procedure was first applied in [242] and can be used to extract the true muon slope parameters, $\beta_{\mu,\text{true}}$. A comparison of the reconstructed average muon slope parameter, $\beta_{\mu,\text{reco}}$, obtained from the two-component reconstruction and the true average muon slope as a function of $S_{\text{tot},125}$ for the different hadronic interaction models and weighted to H4a is shown in Fig. 8.7. The evolution of the muon slope as a function of $S_{\text{tot},125}$ agrees fairly well with the expectation across all models for $\log_{10} S_{\text{tot},125} \lesssim 1.7$. For Sibyll 2.1, however, the reconstructed muon LDF is slightly more steep than the true muon LDF by a few percent. For QGSJet-II-04, the average slope agrees best with the true points. In the case of EPOS-LHC, a slight underestimation of the true muon slope on the few percent level is visible. At the highest energies, the reconstructed values consistently undershoot the expectation. This is likely due to the influence of saturated detectors on the two-component reconstruction and needs to be investigated in more detail in the future. Overall, the two-component reconstruction performs well in the reconstruction of the shape of the true muon LDF, in particular, in resolving the relative ordering of the magnitude of the average muon LDF slope across the different models. Combined with the good Data-MC agreement, this provides a good proof of the reliability of β_μ .

8.3.5. Internal consistency

The different composition-sensitive parameters can be tested for consistency in the prediction of the average composition. This is done without dependence on hadronic interaction models. This means that no conversion functions are used that are based on model assumptions, i.e., the raw (detector) observables⁶ are compared as functions of the energy proxies S_{125} and $S_{\text{tot},125}$ for the standard and the two-component reconstruction, respectively. To compare the different composition-dependent parameters, a similar normalization of the measured parameters to the difference between proton and iron primaries as introduced as the z-value in [199] is used [41]:

$$\frac{p_{\text{Data}} - p_{\text{H}}}{p_{\text{Fe}} - p_{\text{H}}}. \quad (8.1)$$

Here, the normalized values of the observables $p \in [\beta, \log \rho_{\mu}^{600}, \log \rho_{\mu}^{800}, \log dE/dX_{1500}]$ are calculated in bins of $\log_{10} S_{125}$ using the standard reconstruction, while the values for $p \in [\beta_{\text{em}}, \beta_{\mu}, \log S_{\mu,550}]$ are binned in $\log_{10} S_{\text{tot},125}$ obtained from the two-component reconstruction. The comparison of different composition-sensitive parameters requires a similar scaling with mass. By construction, Eq. (8.1) normalization can be expressed as $\log A_{\text{Data}} / \log 56$ for observables that scale linearly with the logarithm of the mass, $\log A$. For this reason, some observables are taken in logarithmic scale, while others are used in linear scale. Corresponding values for proton and iron, p_{H} and p_{Fe} , for each observable p are obtained by considering only the respective pure compositions for a specific hadronic model. Similar to the z-value, a pure proton and iron composition lines up at 0 and 1, respectively. To test the mass scaling of the different observables, a small simulation study based on [241] is performed by studying the behavior of the different parameters for intermediate masses. For this purpose, the parameter values normalized to the proton-iron difference are derived for helium and oxygen simulations. The resulting values for the parameters of the two-component reconstruction are visualized in Fig. 8.8 as a function of $S_{\text{tot},125}$ for near-vertical showers produced with Sibyll 2.1⁷. To guide the eye, the corresponding horizontal lines for helium and oxygen primaries are included at values of $\log 4 / \log 56$ and $\log 16 / \log 56$, respectively. The values agree well with the indicated pure composition lines, suggesting a similar scaling with the primary mass for all included parameters⁸.

The comparison of all mass-sensitive parameters is shown in Fig. 8.9 for Sibyll 2.1, EPOS-

⁶Note that the muon densities, ρ_{μ}^{600} and ρ_{μ}^{800} , are not detector observables but rather properties of the air shower itself [41].

⁷At the time of writing, no simulations of intermediate primaries masses are available for the post-LHC models for the considered data set. This study can therefore only be performed for simulations produced with Sibyll 2.1.

⁸An overview of a similar simulation study for all other parameters can be found in [241].

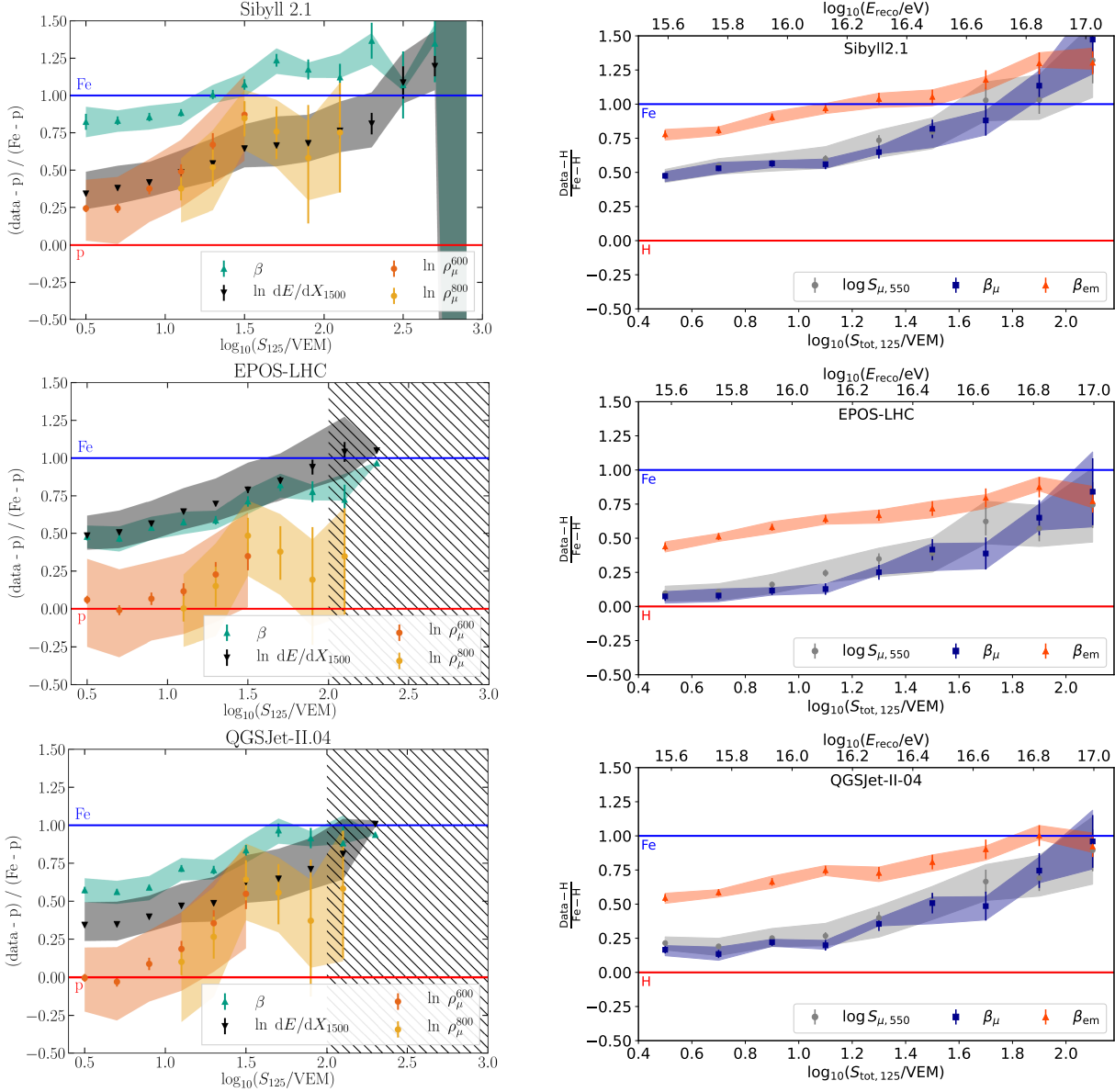


Figure 8.9.: Comparison of different mass-sensitive parameters obtained from previous analyses (left column) and for the two-component reconstruction (right column). Statistical and systematic uncertainties are shown as error bars and error bands, respectively. For reference, the approximate values for the reconstructed primary energies based on $\log_{10}(S_{\text{tot},125}/\text{VEM})$ are given as secondary x-axis in the right column. Figures on the left-hand side are taken from [41].

LHC, and QGSJet-II-04. Before discussing the results, important differences between the parameters studied in previous analyses and the parameters included for the two-component reconstruction should be noted. Firstly, for β , ρ_{μ}^{600} , ρ_{μ}^{800} , and dE/dX_{1500} , 10% of the data of the year 2012 is used, while for the parameters of the two-component

Table 8.1.: Number of events in measured data in each $\log_{10}(S_{\text{tot},125}/\text{VEM})$ bin.

$\log_{10}(S_{\text{tot},125}/\text{VEM})$	
bin center	$\#_{\text{evts}}$
0.5	$1.8495 \cdot 10^4$
0.7	$8.3760 \cdot 10^3$
0.9	$3.5700 \cdot 10^3$
1.1	$1.4820 \cdot 10^3$
1.3	$6.1200 \cdot 10^2$
1.5	$2.8000 \cdot 10^2$
1.7	$1.1100 \cdot 10^2$
1.9	660
2.1	22

LDF, only 1% is included⁹. Nevertheless, already with this limited statistics, the systematic uncertainty dominates for $\log_{10} S_{\text{tot},125} \lesssim 1.5$, depending on the specific parameter. The respective number of measured data events in each $\log_{10} S_{\text{tot},125}$ bin is listed in Tab. 8.1. Secondly, for the two-component reconstruction, only air showers below 100 PeV are included. This is similar to the energy range studied in the muon density analysis. Additionally, for the post-LHC models, no simulations above 100 PeV are available at the time of writing. For β and dE/dX_{1500} , simulations up to 1 EeV are included for Sibyll 2.1. Lastly, since the previous analyses use the standard IceTop reconstruction with S_{125} as energy proxy, the energy scale is slightly different for the two-component parameters. Due to the influence of SLCs on the reconstruction, $S_{\text{tot},125}$ is $\lesssim 10\%$ smaller compared to S_{125} around the full efficiency threshold. For increasing energy, the relative difference between both proxy parameters decreases and eventually reaches sub-percent level around 100 PeV (see Fig. C.4).

For all hadronic interaction models, the average values transition toward a heavier composition for increasing energy, qualitatively consistent with the expectations between the knee and the second knee. However, clear inconsistencies are visible in the composition prediction between different parameters and models. Only for Sibyll 2.1, the measurements of the low-energy muon parameters, ρ_{μ}^{600} , ρ_{μ}^{800} , $S_{\mu,550}$, and β_{μ} , and the high-energy muon parameter dE/dX_{1500} are consistent within the systematic uncertainties. For the post-LHC models, the low-energy muon parameters predict a significantly lighter mass composition which is expected due to the higher muon content. In the case of EPOS-LHC,

⁹This is related to a change in the IceCube collaboration guidelines for data usage in preliminary analyses that was introduced after the previous analyses were performed.

the predicted composition of $S_{\mu,550}$ is close to a pure proton flux for values of $\log_{10} S_{\text{tot},125}$ below ~ 0.9 . For the muon density, the composition is consistent with a pure proton assumption for $\log_{10} S_{125} \lesssim 1.2$. Note that the systematic uncertainty for the muon density measurement is significantly larger due to the involvement of model-dependent correction factors. For QGSJet-II-04, the predicted muon density at 600 m is also consistent with a pure proton flux, which is not the case for $S_{\mu,550}$. However, within the systematic uncertainties, the results for the low-energy muon parameters are in agreement across all models. The shift in the nominal values of the average composition for $S_{\mu,550}$ and β_{μ} compared to the muon density could be explained by remaining EM contribution. This is accounted for in the reconstruction of the average muon number presented in chapter 9 by means of a correction factor. Although Sibyll 2.1 produces the most consistent interpretation among the pure muon-based parameters, the average composition predicted by β and β_{em} exhibits values that are consistent with a heavier composition than iron at high energies, which is beyond physical expectations. The evolution of β and β_{em} is qualitatively similar, suggesting that also β is dominated by the electromagnetic component. The shift toward lighter compositions in β and β_{em} for the post-LHC models is in line with the observation of a steeper electromagnetic distribution in the pre-LHC model. Overall, the results qualitatively agree between the previous analysis and the new composition-sensitive parameters of the two-component LDF within uncertainties. However, none of the considered hadronic interaction models produces a self-consistent interpretation of the measured data. While for the pre-LHC model Sibyll 2.1, the muon-based parameters show a consistent composition prediction within the uncertainties, the observed values for β and β_{em} are inconsistent with these predictions and even transition beyond the physical expectation for high energies. This is also observed for β_{μ} and $S_{\mu,550}$ at the highest considered energies, however, this is likely because of the very limited statistics. In contrast to that, for the post-LHC models, β and β_{em} shift toward a lighter composition, which results in a better agreement with the measurement of high-energy muons. However, at the same time the low-energy muon parameters become inconsistent with dE/dX_{1500} . Generally, therefore, no considered model leads to a self-consistent interpretation of the EM and muon component. Moreover, the different models lead to a shift in the absolute composition for all considered parameters, where the post-LHC model Sibyll 2.1 predicts a heavier average composition compared to the post-LHC models.

8.4. Discussion

Using the composition-sensitive parameters of the two-component LDF reconstruction, the internal consistency in terms of average composition estimation is tested in the section 8.3. Since the underlying mass composition is the same for all parameters, this

method is used to test the ability of hadronic interaction models to consistently predict the mass composition. It can be applied in a straight-forward way to other models if corresponding simulations are produced. A similar study has been performed using established parameters from previous analyses, namely, the low-energy muon densities at large distances from the shower axis, ρ_μ^{600} and ρ_μ^{800} , the slope of the LDF used in the standard reconstruction, and the energy loss parameter of the high-energy muon bundle, dE/dX_{1500} . From the previous study it is clear, that the composition prediction of the different mass-sensitive parameters differs significantly, leading to large uncertainties in composition studies depending on which parameters are utilized. This is particularly problematic when comparing composition results between different experiments. Overall, it is obvious, that none of the considered hadronic interaction models produce a consistent description of the entirety of high-energy hadronic interactions during the shower development.

However, it is not trivial to draw conclusions for the tuning of hadronic interaction models from the detector observables like β and dE/dX_{1500} , since they do not simply correspond to one specific property of air showers. For example, the LDF slope β is both influenced by the EM component and by low-energy muons. Therefore, the inconsistency in the interpretation of measured data compared to other observables could, among others, stem from an unsatisfactory description of the EM component or the muon LDF. The addition of parameters of the two-component model which attempts to disentangle the EM from the muon component adds additional information to this problem. Since the composition prediction obtained for β_{em} qualitatively shows a similar behavior as for β , an issue in the description of the EM component is suggested. It should be noted, however, that the EM LDF and muon LDF in the two-component reconstruction are intrinsically linked, and therefore further studies are necessary to draw further conclusions.

dE/dX_{1500} as an estimate of the high-energy muon multiplicity has a limited resolution, therefore this analysis should be repeated with the deep-learning based TeV muon number reconstruction discussed in section 4.3.2. Similarly, a reduction of the systematic uncertainties, in particular with an updated ice model as the main source of uncertainty for high-energy muons reconstructions, is desirable for a stronger indication of the inconsistencies between different models. This is also true for the low-energy muon density parameters, which feature the largest systematic uncertainty. In this context, the normalization $S_{\mu,550}$ of the muon LDF within the two-component model as exhibits a significantly smaller systematic uncertainty. The prediction of the average composition in terms of $S_{\mu,550}$ for different hadronic interaction models qualitatively shows the same behavior compared to the low-energy muon density within the systematic and statistical uncertainties. This suggests, that the muon LDF measured at 550 m, 600 m, and 800 m from the shower axis results in a consistent description of the average composition within the statistical and systematic uncertainties. In fact, also the slope of the muon LDF at

550 m leads to a composition interpretation that is consistent with the low-energy muon density and $S_{\mu,550}$.

For improving such model tests, the inclusion of new mass-sensitive parameters obtained from reconstructions with the IceTop-enhancement/IceCube-Gen2 surface detectors is of great interest. While scintillation detectors feature a different response to different particle species compared to the IceTop-tanks, radio antennas can provide an estimate of the energy contained in the EM component and are sensitive to X_{max} . Such additional information can be crucial for an improved understanding of the shortcomings of different hadronic interaction models. Additionally, in particular for IceCube-Gen2, the zenith and energy range accessible for coincident events is significantly increased. This would allow for an extension of the phase space for tests of hadronic interaction models.

Muon number studies

As discussed in section 3.6.2, various experiments have reported discrepancies in the number of muons expected from simulations compared to measured data [199]. The predictions of the muon content of air showers as well as their energy distribution differs significantly between different hadronic interaction models. With the combination of a surface array and a deep in-ice detector, IceCube offers the unique possibility to study muons at two vastly different energy regimes. While IceTop measured low-energy muons in the GeV region, high-energy muons ($\gtrsim 400$ GeV) can be observed with the deep in-ice array. The latter is a direct result of the thick ice sheet between the surface and IceCube, which results in an increased energy threshold for muons in the range of several hundred GeV. As discussed in section 8.3, an internal comparison of multiple muon-based observables indicates a discrepancy between the low- and high-energy muons measured with IceCube and interpreted with different hadronic interaction models [241]. This suggests a disagreement of the muon energy spectrum or of the muon lateral distribution between the measured data and simulations.

The first measurement of the low-energy muon content with the IceCube Neutrino Observatory was performed in [199]¹. This approach is based on a statistical analysis with charge distributions of HLCs and SLCs binned in lateral distance, using a large set of observed shower events for each bin. However, for the study of correlations between low- and high-energy muons, the muon content is required to be estimated on a single-event basis. For the high-energy muons measured with the in-ice detector, an event-by-event based reconstruction of the average number of muons is possible with a machine learning based method presented in [41] and further discussed in section 4.3.2. The two-component LDF reconstruction developed in this work offers the possibility of an event-by-event based estimation of the low-energy muon number², which can be combined with an estimation of the high-energy muon content to derive constraints on hadronic interaction models based on the muon-energy spectrum.

¹A detailed discussion can be found in section 4.3.2

²In principle, the two-component LDF is tuned to reconstruct the total number of muons above 420 MeV and with lateral distances below 1000 m. However, this number is dominated by low-energy muons in the $\sim$ GeV region (see Fig. 5.1).

The event selection applied for the reconstruction of the muon content with the two-component model is described in detail in section 6.3. Most importantly, the applied quality cuts ensure that the core position of measured shower events is contained within IceTop. Additionally, only showers up with $\cos\theta > 0.9$ ($\theta \lesssim 26^\circ$) are considered. Such near-vertical events can potentially produce high-energy muons that propagate through the in-ice array and can therefore be used in a future study for a combined analysis using surface and in-ice measurements. For IceTop alone analyses, the zenith angle range can be extended to make use of the higher relative muon content of more inclined air-shower events.

In this chapter, the average muon number as a function of primary energy derived on a single-event basis using the reconstruction developed in chapter 6 is analyzed. Firstly, in section 9.1, the differences in the prediction of the muon content in air showers between the considered hadronic interaction models is discussed. To correct for the remaining biases of the two-component reconstruction, a correction factor is introduced in section 9.2 based on MC simulations, which is used to correct the average muon number obtained in measured data. To ensure a proper performance of the correction procedure, several tests are conducted in section 9.3. Furthermore, in section 9.4, the correction is applied to the measured data and connected systematic uncertainties of the reconstruction are quantified. The resulting average muon number as a function of primary energy and including systematic uncertainties is shown in section 9.5. A discussion of the results in the context of previous analyses is given in section 9.6. Finally, an outlook to following applications of the two-component reconstruction is presented in section 9.7.

9.1. MC expectation

Within this analysis, the reconstructed energy and muon number is compared to the expectation obtained from simulations for different hadronic interaction models. Fig. 9.1 shows linear fits to the true average muon number as a function of true primary energy for proton- and iron-initiated air showers produced with the hadronic interaction models Sibyll 2.1, EPOS-LHC and QGSJet-II-04. The corresponding values of the fit parameters are listed in Tab. 9.1. It can be noted, that the increase of the total muon number with primary energy has a slope of $p_1 \sim 0.9$, which is in agreement with the expectation from the Heitler-Matthews model (Eq. (3.14)). Additionally, the muon number observed for Sibyll 2.1 is more than 20% smaller than for the post-LHC models. The average muon number also increases slightly faster compared to Sibyll 2.1. For the following, the derived linear fit can be used to various purposes, such as the derivation of z-scale plots for the muon number reconstruction. Over the next sections, the reconstruction bias of the two-component model as well as systematic uncertainties are studied in order to draw data

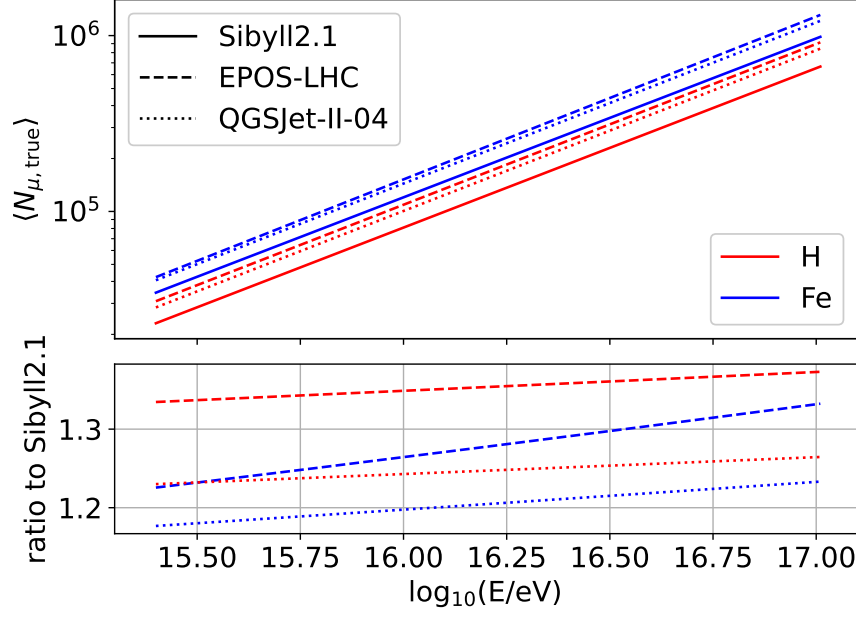


Figure 9.1.: **Top panel:** Linear fits to the true average muon number in proton and iron initiated air-showers simulated with Sibyll 2.1, EPOS-LHC and QGSJet-II-04. **Bottom panel:** Ratio of the linear fits of the post-LHC models EPOS-LHC and QGSJet-II-04 with Sibyll 2.1.

points derived from real measurements into Fig. 9.1.

9.2. Correction factor

The two-component LDF developed in this work can be used to reconstruct the primary energy and muon number for the same air-shower events. The reconstructed muon number can therefore be studied as a function of the reconstructed primary energy. The corresponding reconstruction performance is discussed in detail in chapter 7. Fig. 9.2

Table 9.1.: Parameters values for linear fit to the true average muon number as a function of the true primary energy.

Hadronic model	Proton		Iron	
	p_1	p_2	p_1	p_2
Sibyll 2.1	0.907	-9.596	0.904	-9.376
EPOS-LHC	0.914	-9.589	0.926	-9.635
QGSJet-II-04	0.914	-9.621	0.916	-9.500

shows the average reconstructed muon number ($E_\mu \geq 420$ MeV, $r_\mu \leq 1000$ m) binned in primary energy with a bin size of 0.1 in $\log_{10} E$ for the hadronic interaction models Sibyll 2.1, EPOS-LHC and QGSJet-II-04. Additionally, lines show the MC expectations for the average true muon number as a function of the true primary energy. In the case of Sibyll 2.1, the four primary masses proton, helium, oxygen, and iron are available. For the post-LHC models, only proton and iron primaries are shown. Both, the standard error of the mean for the average reconstructed muon number for all primaries as well as the standard deviation for proton and iron are shown as error bars and error bands, respectively. Generally, the trend of the reconstructed average muon number agrees well with the true one. In particular, a clear splitting between the different primary masses for the same primary energy are visible as is expected from the superposition model. However, a reconstruction bias can be observed when comparing the reconstructed points with the MC truth. Especially for low primary energies, the two-component reconstruction is overestimating the average muon number for heavier primaries and, in the case of Sibyll 2.1, even for proton-initiated showers. In order to better understand the systematic bias, the ratio of the reconstructed average muon number to the MC expectation is shown as a function of primary energy in Fig. 9.3. An important feature is the mass dependence in the bias as a function of primary energy. This bias is a direct result of the remaining mass dependence of the two-component reconstruction. While the bias in the muon number estimation influences the calculation of the average directly, a bias in the energy reconstruction enters by means of bin migration. For heavier primaries, the average muon number tends to be overestimated by the reconstruction for the range below ~ 10 PeV. For the lowest energies included and depending on the hadronic interaction model, this overestimation can be of the order of 20% and decreases to a few percent level around 10 PeV. At higher energies, the reconstruction starts to be underestimated the average muon number by a few percent for heavy primaries. As opposed to heavy primaries, the muon content in proton-initiated showers tends to be underestimated for energies below ~ 10 PeV and overestimated for higher energies for the post-LHC models. In the case of Sibyll 2.1, the average muon number is overestimated almost for the entire energy range for proton primaries, with a maximum bias of $\sim 10\%$. It can be noted, that the shift in the systematic bias from over- to underestimation is produced by the energy reconstruction bias, in which a similar behavior is observed.

To account for the two-component reconstruction bias, a correction factor is derived to describe the resulting systematic shift for this analysis, which is necessary for the inclusion and subsequent interpretation of measured data. The behavior of the systematic bias for different primaries can be modeled via fits to Fig. 9.3. The evolution of the mass-dependent bias is found to be well described by third-order polynomials of form

$$c(\log_{10} E) = p_0 + p_1(\log_{10}(E/\text{eV}) - c_E) + p_2(\log_{10}(E/\text{eV}) - c_E)^2 + p_3(\log_{10}(E/\text{eV}) - c_E)^3, \quad (9.1)$$

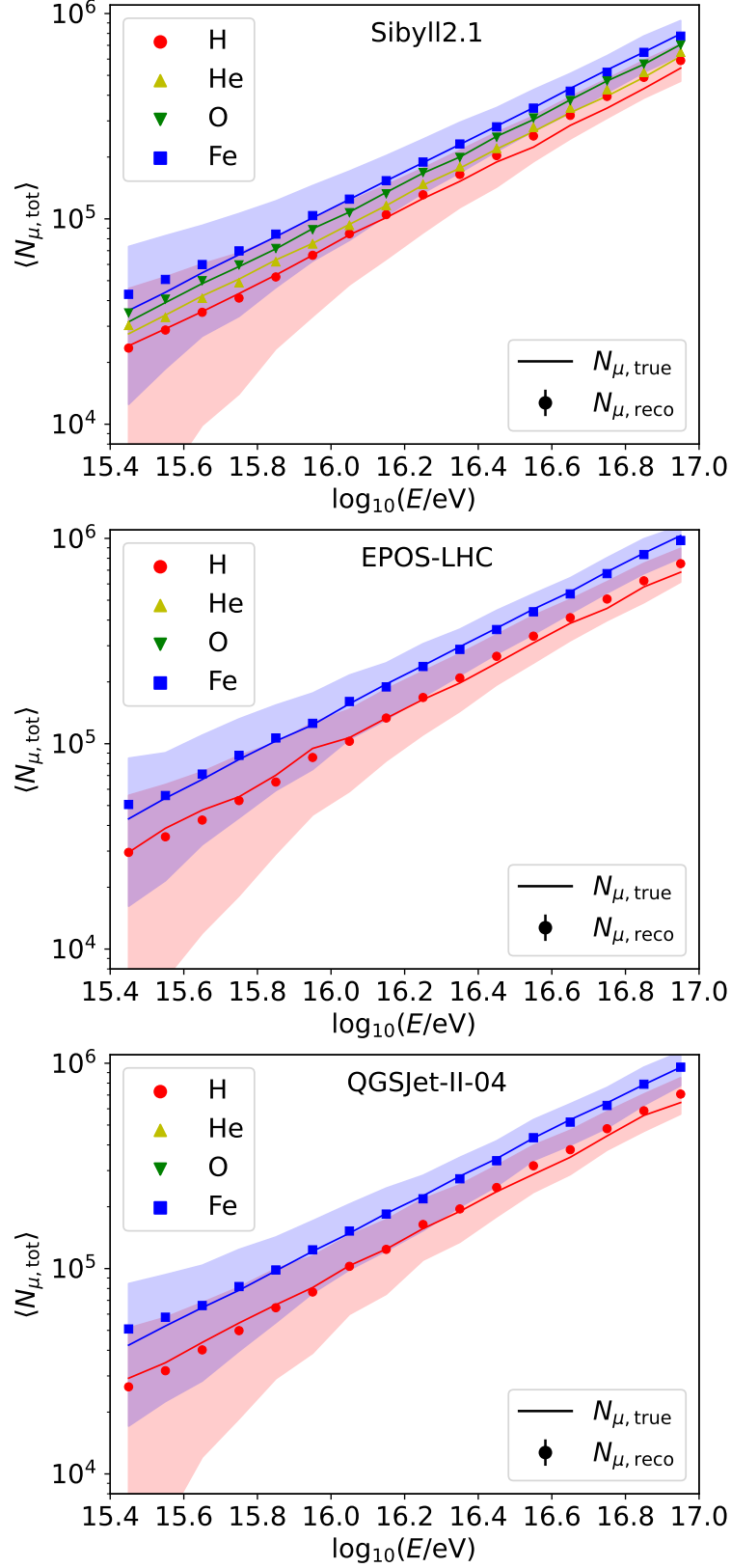


Figure 9.2.: Raw reconstructed average muon number as a function of reconstructed primary energy are shown as points for the three hadronic models Sibyll 2.1, EPOS-LHC and QGSJet-II-04. Lines show the true average muon number as a function of true primary energy. Error bars indicated the standard error of the mean, while the blue and red shaded regions illustrate the standard deviation for proton and iron primaries.

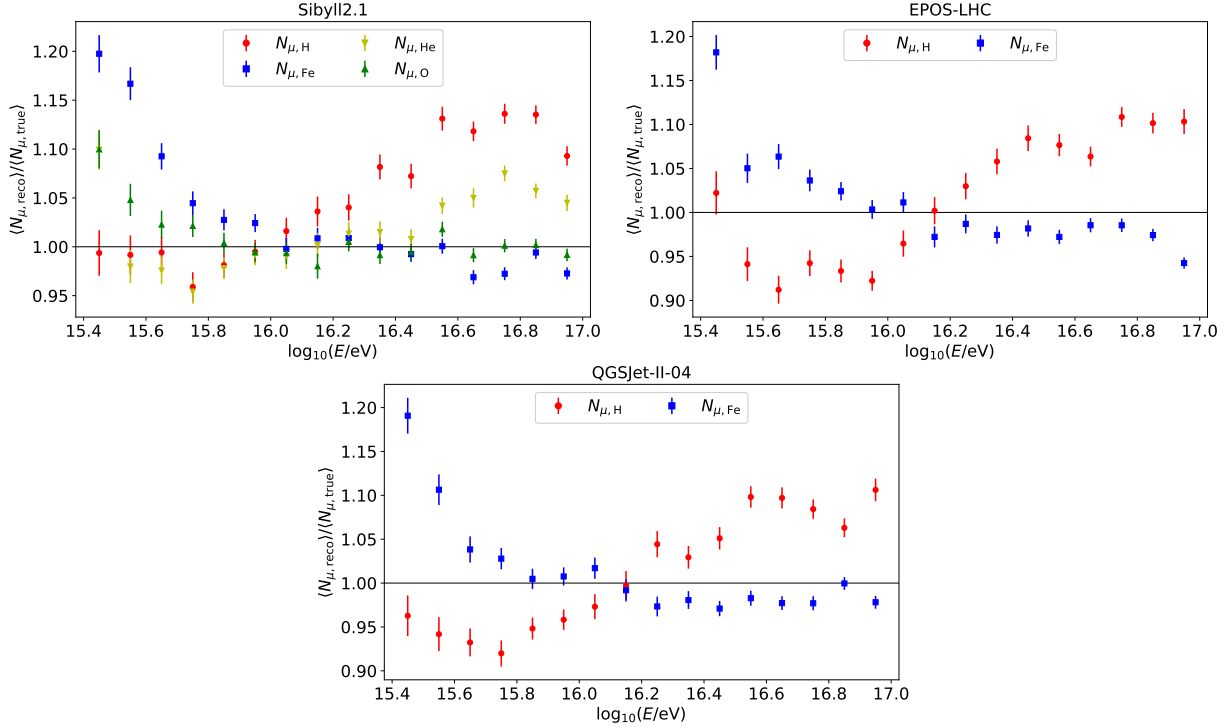


Figure 9.3.: Ratio of the average reconstructed muon number to the MC expectation obtained from CORSIKA for events simulated with the hadronic interaction models Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 as illustrated in Fig. 9.2.

where the constant $c_E = 16.0$. Fig. 9.4 shows the resulting fits for the different hadronic interaction models along with the corresponding 1σ uncertainty band. An interesting observation is the smaller statistical uncertainty in the systematic bias for heavy primaries compared to proton. This is due to the larger shower-to-shower fluctuations for light primaries for the same energy, resulting in a larger statistical uncertainty of the average muon content. Additionally, the systematic bias for light primaries exhibits an s-shaped form as a function of energy, while heavy primaries, in first order, produce monotonically decreasing bias. This behavior could be caused by the fact that $X_{\max}$ can be below the IceTop level for light primaries with sufficient primary energy. For IceTop, which is located at an atmospheric depth of $\sim 690 \text{ g/cm}^2$ [199], this can happen already above $\sim 10 \text{ PeV}$ for proton primaries (see Fig. 3.9). An average value of $X_{\max}$ that changes from above to below the observation level could influence the energy calibration, potentially modulating the evolution of the reconstruction bias as a function of primary energy.

Since the modeling of the systematic bias clearly depends on the choice of the hadronic model, a later interpretation of the data has to be carried out in the context of each hadronic interaction model separately. Since the mass composition in the data is unknown, a correction factor should take into account the entire range of the systematic uncertainty introduced by the reconstruction bias. In a previous analysis discussed in [199], an average

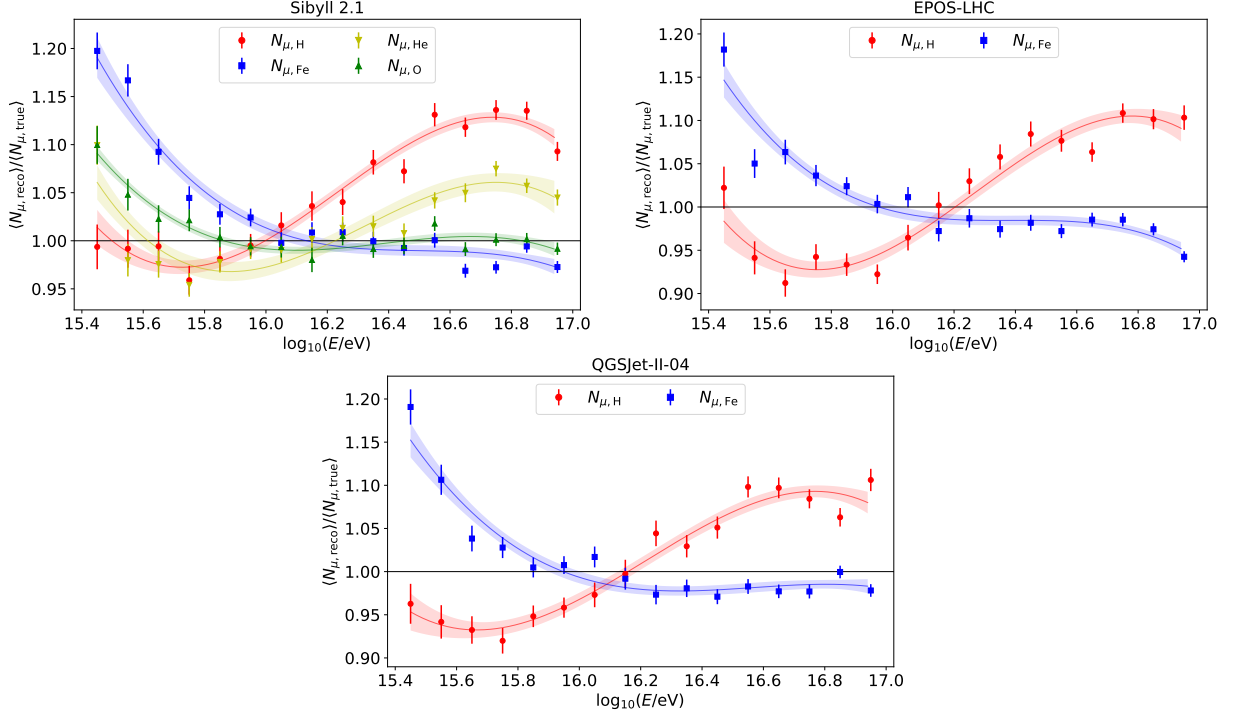


Figure 9.4.: Polynomial fits to the ratio of the average reconstructed muon number to the MC truth shown in Fig. 9.2 for Sibyll 2.1, EPOS-LHC and QGSJet-II-04.

uncertainty band defined by the correction factors for proton and iron is used to quantify the systematics. However, this intrinsically assumes a scaling of the correction factors for individual intermediate masses that is within the proton and iron lines. From the correction factors derived for Sibyll 2.1, it is clear that this assumption is not necessarily true. In principal, a correction factor can be obtained by assuming a specific cosmic-ray composition determined by a given flux model. However, the knowledge about the true composition is very limited and therefore might lead to an underestimation of the systematic uncertainty in the derivation of a correction factor. Therefore, two different approaches are tested to define a more conservative systematic uncertainty that brackets all primary types available in the simulations.

Envelope of fits

In a first approach following the correction factors obtained within the GeV muon density analysis [199], a correction factor with a corresponding uncertainty band can be obtained based on the average of the extrema of the combination of all correction factors for a corresponding hadronic interaction model. The average effective correction factor, $c_{\text{eff,avg}}$,

and its corresponding systematic uncertainty, $\sigma_{\text{tot},c_{\text{eff}}}$, can then be written as

$$\begin{aligned}
c_{\text{eff,avg}} &= \frac{\max(c_{\text{H}}, \dots, c_{\text{Fe}}) + \min(c_{\text{H}}, \dots, c_{\text{Fe}})}{2}, \\
\sigma_{\text{tot},c_{\text{eff}}} &= \sqrt{\sigma_{\text{dev},c_{\text{eff}}}^2 + \sigma_{\text{sta},c_{\text{eff}}}^2}, \\
\sigma_{\text{dev},c_{\text{eff}}} &= \frac{\max(|c_{\text{eff,avg}} - c_{\text{H}}|, \dots, |c_{\text{eff,avg}} - c_{\text{Fe}}|) + \min(|c_{\text{eff,avg}} - c_{\text{H}}|, \dots, |c_{\text{eff,avg}} - c_{\text{Fe}}|)}{2}, \\
\sigma_{\text{sta},c_{\text{eff}}} &= \sqrt{\sigma(\max(c_{\text{H}}, \dots, c_{\text{Fe}}))^2 + \sigma(\min(c_{\text{H}}, \dots, c_{\text{Fe}}))^2}.
\end{aligned} \tag{9.2}$$

The correction factor therefore describes the average of the upper and lower limits of the individual correction factors for each primary mass. The total uncertainty includes the statistical uncertainty, $\sigma_{\text{sta},c_{\text{eff}}}$, of the combination of the individual correction factors as well as the average deviation, $\sigma_{\text{dev},c_{\text{eff}}}$, of the individual correction factors to the effective correction factor. The latter can be understood as the uncertainty introduced by the unknown composition in measured data. Both contributions are added in quadrature to obtain $\sigma_{\text{tot},c_{\text{eff}}}$. Since the cosmic-ray composition is better known than an equal-fraction flux, the effective correction factor used for the correction is weighted to H4a as a more realistic flux model to obtain $c_{\text{eff,H4a}}$. Note that the choice of the effective correction factor in between the systematic boundaries is arbitrary and does not change the result as the systematic uncertainty is unchanged and only the nominal values are shifted. Fig. 9.5 shows the resulting correction factors $c_{\text{eff,H4a}}$ for Sibyll 2.1, EPOS-LHC and QGSJet-II-04, where $\sigma_{\text{tot},c_{\text{eff}}}$ is indicated as a gray band. The general form of the correction factors is similar for all three hadronic interaction models. Nevertheless, a difference in the magnitude of the error band can be observed at lower energies for the post-LHC models. This is the result of differences in the statistical uncertainties, the reconstruction bias, and the energy scale for the different models.

Envelope of points

Instead of the correction factors obtained for individual primary types, out of all primary masses, the minimum and maximum ratio of the average reconstructed muon number to the MC truth shown in Fig. 9.3 can be modeled via Eq. (9.1). The resulting fit functions for both extrema are shown in Fig. 9.6 for Sibyll 2.1, EPOS-LHC and QGSJet-II-04. Similarly to the previous procedure, the average effective correction factor, $c_{\text{eff,avg}}$, and

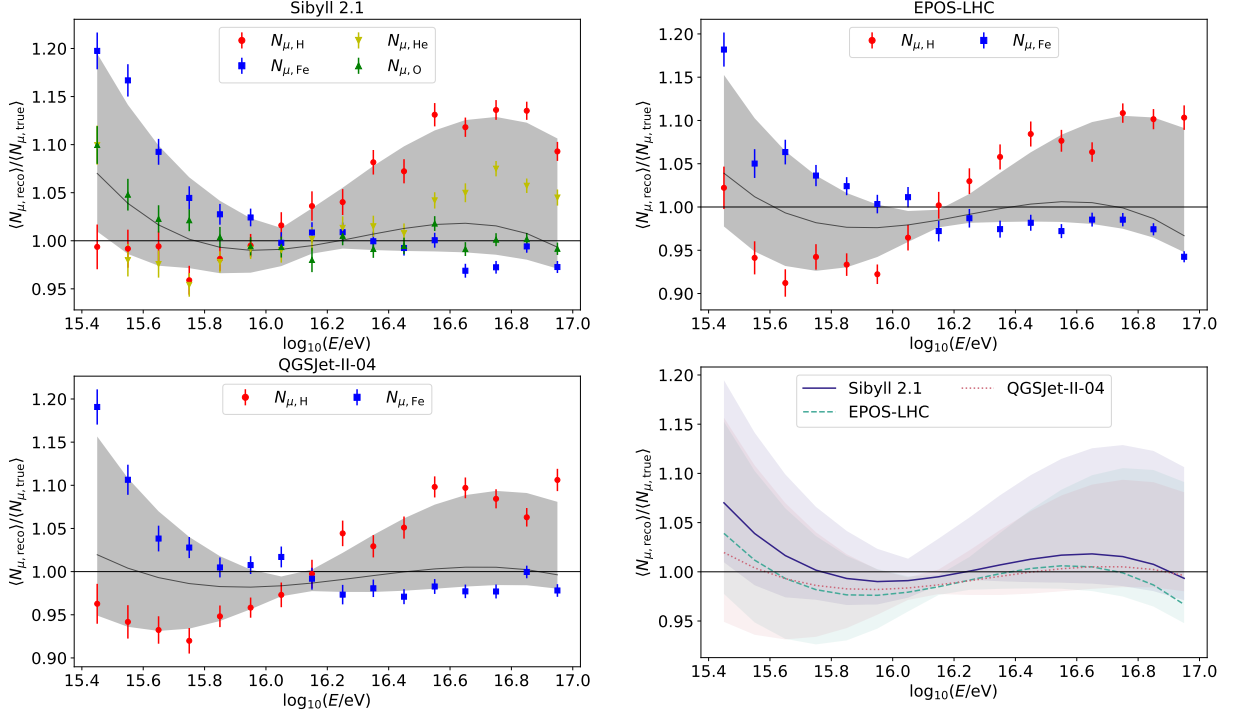


Figure 9.5.: Average correction factors for Sibyll 2.1, EPOS-LHC and QGSJet-II-04. The black lines describe the effective correction factors obtained from a combination of the extrema of the individual correction factor fits for different primary masses shown as colored lines. The gray bands indicate the systematic uncertainty band including the statistical and composition uncertainties for the given models. A comparison of the derived average correction factors is shown in the bottom right figure.

its systematic uncertainty, $\sigma_{\text{tot}, c_{\text{eff}}}$, can then be defined as

$$\begin{aligned}
 c_{\text{eff}, \text{avg}} &= \frac{c_{\text{max}} + c_{\text{min}}}{2}, \\
 \sigma_{\text{tot}, c_{\text{eff}}} &= \sqrt{\sigma_{\text{dev}, c_{\text{eff}}}^2 + \sigma_{\text{sta}, c_{\text{eff}}}^2}, \\
 \sigma_{\text{dev}, c_{\text{eff}}} &= \frac{\max(|c_{\text{eff}, \text{avg}} - c_{\text{max}}|) + \min(|c_{\text{eff}, \text{avg}} - c_{\text{min}}|)}{2}, \\
 \sigma_{\text{sta}, c_{\text{eff}}} &= \sqrt{\sigma_{c_{\text{max}}}^2 + \sigma_{c_{\text{min}}}^2},
 \end{aligned} \tag{9.3}$$

with the statistical uncertainties of the upper and lower bounds in Fig. 9.6, $\sigma_{c_{\text{max}}}$, and $\sigma_{c_{\text{min}}}$, respectively. The average effective correction factor is given by the average of both bounds, with a systematic uncertainty accounting for the statistical and composition uncertainties. Similar to the previous procedure, the effective correction factor used for the correction of the nominal results is weighted to the H4a flux assumption. $c_{\text{eff}, \text{H4a}}$ and the corresponding systematic uncertainty is illustrated in Fig. 9.7 as black lines and gray bands, respectively. Again, the general shape is similar for all three hadronic interaction models. The magnitude of the systematic uncertainty is on the order of 10% for energies

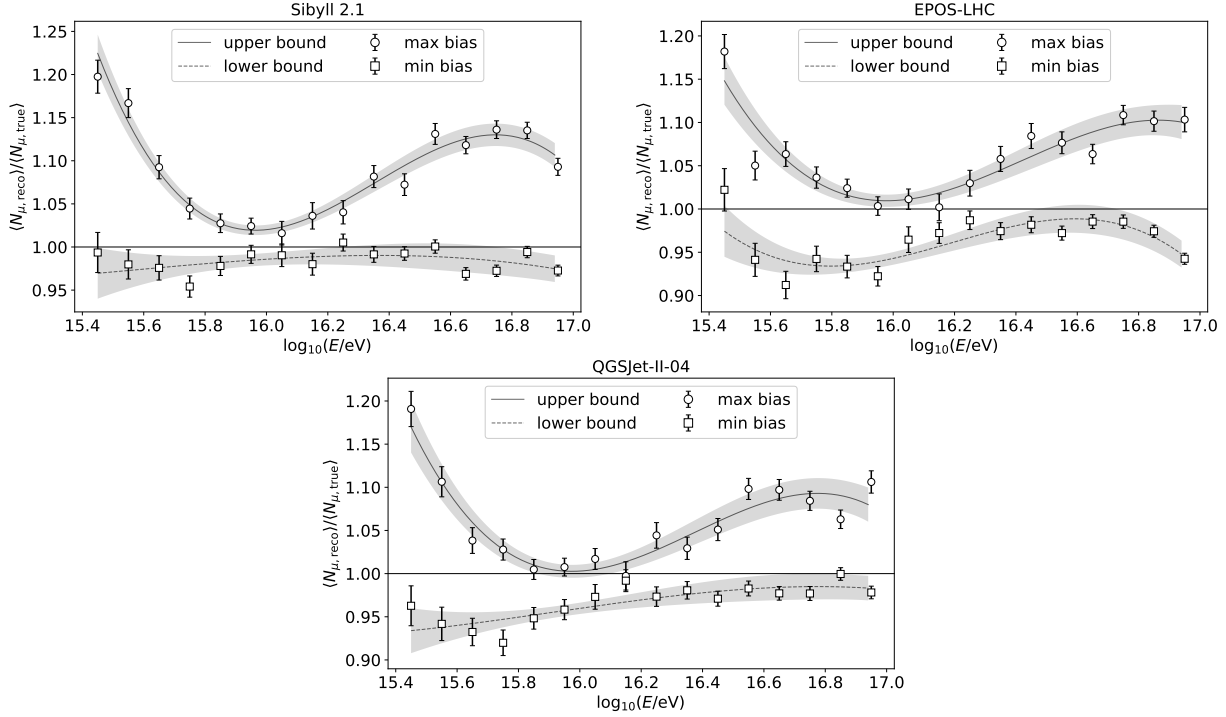


Figure 9.6.: Maximum and minimum of the reconstruction bias and corresponding polynomial fits (black solid and dashed lines) for Sibyll 2.1, EPOS-LHC and QGSJet-II-04.

above ~ 10 PeV and can increase to values of $> 20\%$ depending on the model. In order to compare the relative performance of the different correction factors, a set of MC tests is carried out and discussed in the next section.

9.3. Validation of the correction factor

Both methods of obtaining a correction factor to utilize in the interpretation of measured data lead to very similar shapes and magnitudes of the systematic uncertainty. In contrast to the previous analysis of GeV muon reconstruction [199], the correction factors for proton and iron primaries exhibit significant differences for the low- and high-energy region of this analysis. Additionally, with the two-component reconstruction, the systematic uncertainty is larger for low energies, while at energies above ~ 10 PeV, the bias is at maximum of the order of 10% for all three hadronic interaction models. A third difference to the previous analysis is given by the small magnitude of the systematic bias around ~ 10 PeV, where the differences between different primary types are smallest. To study the performance of the correction factors, the ability of the two-component model to reconstruct a given MC input flux is tested. Fig. 9.8 shows the true average muon number for Sibyll 2.1 weighted with the H4a flux model and converted to the z-scale using the

9.3. Validation of the correction factor

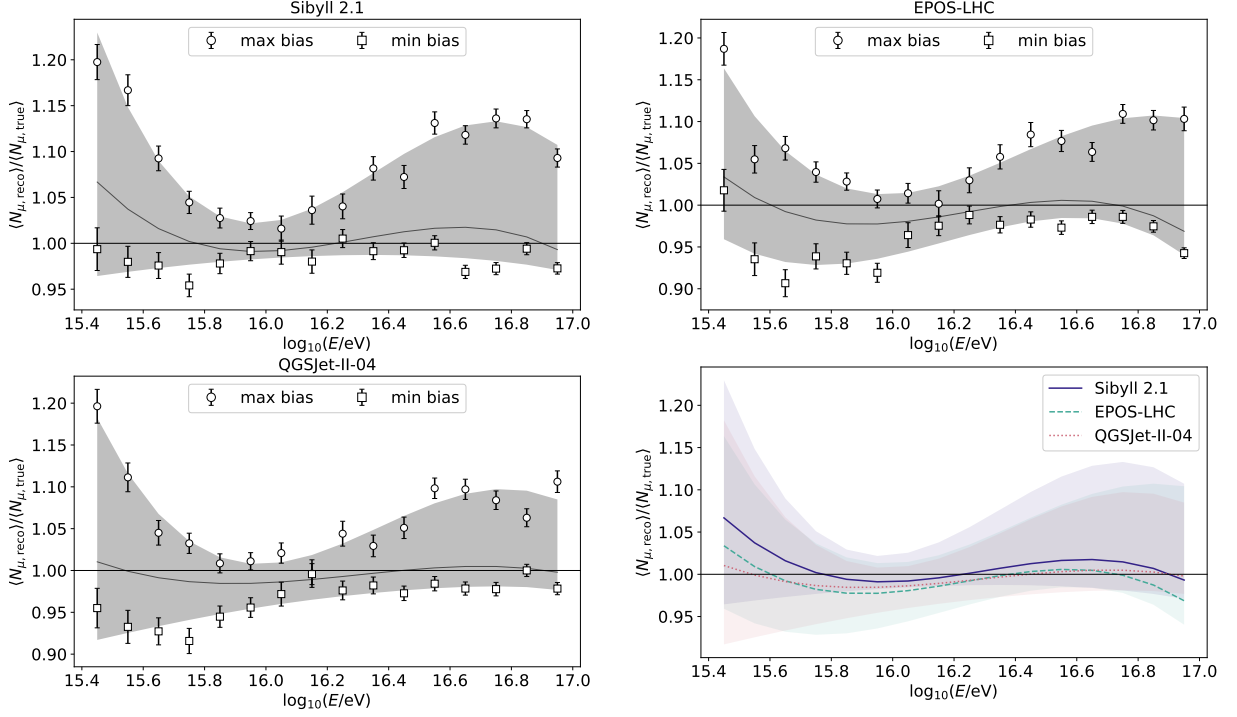


Figure 9.7.: Average correction factors for Sibyll 2.1, EPOS-LHC and QGSJet-II-04. Black lines describe the effective correction factors obtained from the upper and lower bounds in Fig. 9.6. Gray bands indicate the corresponding systematic uncertainties. A comparison between the different hadronic models is shown in the bottom right figure.

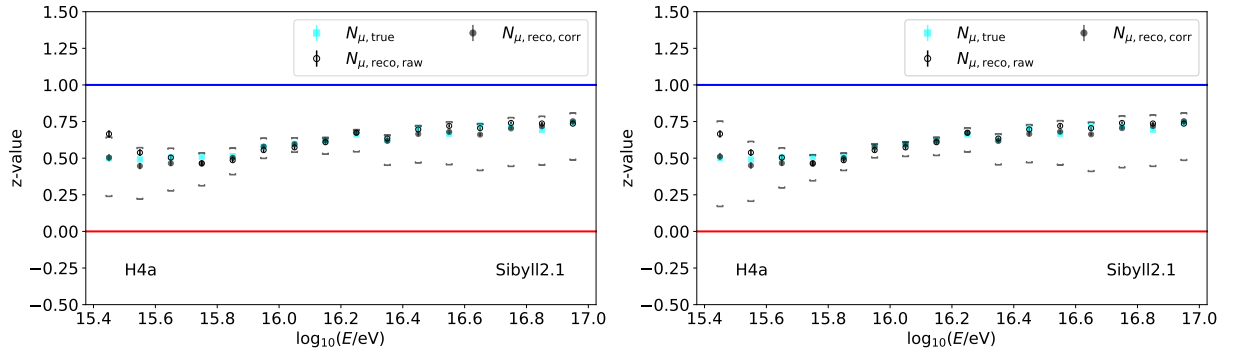


Figure 9.8.: Average muon number weighted to H4a and expressed as z-values for the correction factor based on the envelope of fits (left) and the envelope of points (right). True values are shown in cyan, the raw reconstructed muon number and the muon number after correction are shown as unfilled and filled black points, respectively. The uncertainty band connected to the correction is illustrated with brackets.

fits to the average muon number for proton and iron primaries as a function of energy (see Fig. 9.2). The corresponding raw reconstruction output is drawn as black unfilled points, while the black filled points and the brackets indicate the reconstruction output that is corrected with a correction factor and its systematic uncertainty, respectively.

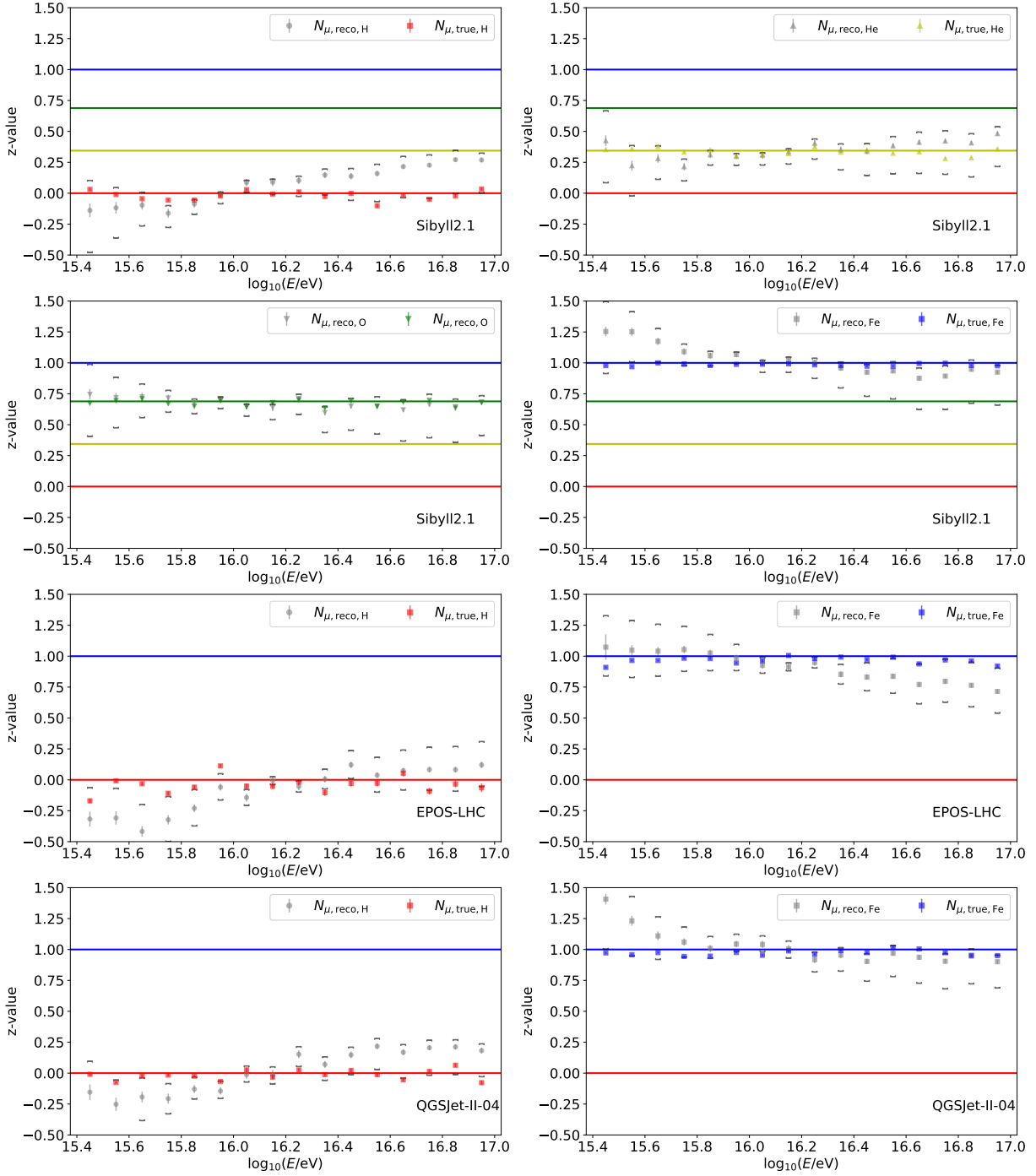


Figure 9.9.: z-values obtained from the average muon number reconstructed with the two-component model for pure proton and iron composition assumptions and for different hadronic interaction models. In the case of Sibyll 2.1, also the pure helium and oxygen scenarios are shown. True values are drawn in color, black points and brackets indicate the corrected reconstructed points and the corresponding systematic uncertainty.

While the raw reconstruction points are close to the true values particularly at energies above ~ 10 PeV, at lower energies a systematic pull toward heavier compositions is visi-

ble. This bias is corrected successfully with both correction factors and the input flux is well reproduced within the systematic uncertainties that are assigned to the correction procedure. The main differences between the two different correction factors are visible at energies below $\log_{10} E \lesssim 15.6$, where the correction factor based on the envelope of points features a larger systematic uncertainty. However, the reconstruction bias does not scale perfectly with mass around the crossing point of proton and iron for Sibyll 2.1 (see Fig. 9.4) and a similar behavior is expected for the post-LHC models. Therefore, the correction factor based on the envelope of the individual fits likely underestimates the systematic uncertainty for the latter due to the missing contribution of intermediate primaries. Ideally, respective simulations need to be produced to study the behavior for the post-LHC models in more detail for future analyses. For the purpose of this work, however, the correction factors based on the envelope of points is used, as they feature a more conservative estimate of the systematic uncertainty in this energy region. Therefore, for further investigation, only the correction factor determined with the second method is considered. To benchmark the performance of the correction factor, the ability to reconstruct pure composition scenarios is tested. Fig. 9.9 shows z-value plots for a pure proton, helium, oxygen, and iron scenario for Sibyll 2.1. For this purpose, simulations for only the respective primary mass are considered and weighted to the H4a all-particle spectrum, assuming a pure cosmic-ray composition consisting only of one primary type. Again, the reconstructed points are corrected and include the corresponding systematic uncertainty. Also for the pure composition scenario, true average muon number can be reconstructed within the systematic uncertainties of the correction procedure. To validate the applicability of the correction procedure to other hadronic interaction models, Fig. 9.9 additionally shows the pure composition tests for EPOS-LHC and QGSJet-II-04. For both post-LHC models, the input flux is recovered within statistical and systematic uncertainties. Along with the application on realistic flux scenarios, the pure composition tests illustrate that the two-component reconstruction along with the correction procedure is able to recover the average muon number independent of the true composition.

9.4. Systematic uncertainty

The effect of the application of the correction factors dependent on the hadronic interaction model on measured data is shown in Fig. 9.10. In addition to the comparison of the average muon number reconstructed for data before and after the application of the correction factor, the results are compared to the MC expectation for proton and iron primaries as derived in section 9.1. Since the shifts of the data points introduced by the correction are hardly visible in some energy bins, a conversion of the data to z-values is shown for better visibility. The shift in each energy bin can be well understood when

considering Fig. 9.5 (bottom right). For example, around intermediate energies in the studied energy range, the applied correction is comparably small. This is because in this region the mass dependence of the two-component reconstruction is the smallest. For all hadronic models, the measured data is contained within the pure proton and iron expectations within the systematic uncertainties of the correction factor.

In Fig. 9.10, the error bars indicate the error of the mean of the measured data. The better visualize the limited statistics of the data set used for this analysis especially at high energies, the respective number of events in each energy bin is shown in Fig. 9.11. As indicated, in the three highest energy bins, on average, less than ~ 50 events are present. Around 100 PeV, less than 20 events are included in the analysis.

Aside from the hadronic model dependent correction factor, additional sources of systematic uncertainties have to be considered for the interpretation of measured data. While the systematics band assigned to the correction factor includes the uncertainties due to the unknown composition, statistical uncertainties, and accounts for effects of bin migrations caused by the finite energy resolution, systematics inherent to the detector need to be considered as well. For reconstructions using the IceTop array, two uncertainties need to be accounted for, namely, the uncertainty in the snow attenuation factor, λ_{snow} , and the uncertainty in the VEM calibration procedure. An uncertainty in the snow attenuation factor affects the electromagnetic signal expectation value in the reconstruction by means of signal attenuation (see Eq. (4.12)) and consequently the entire two-component fit. This can produce a systematic shift in the reconstructed values of $S_{\text{em},125}$ and $S_{\mu,550}$ and therefore influence the energy and muon number reconstruction as well as the reconstruction of the shower axis. The uncertainty of the snow attenuation factor is estimated to be ± 0.2 m based on studies of S_{125} spectra for different parts of IceTop that feature different snow heights [186]. As detailed in section 4.3.1, the calibration of IceTop charges to units of VEM is performed regularly for measured data using atmospheric muons. To set the energy scale of IceTop, the VEM calibration procedure is repeated in a similar manner using low-energy air shower simulations, where the simulated charges are calibrated such that the location of the observed muon peak matches the one in measured data. It was shown in the context of a detailed simulation study, testing for the influence of differences in the snow accumulation, atmospheric variations, energy spectra, hadronic interaction models, and differences between the high-gain DOMs as well as other factors, that the total uncertainty on the VEM definition is around 2–3% [273]. A systematic uncertainty of 3% is therefore assumed for the VEM unit.

To determine the influence of these systematic detector uncertainties, the two-component reconstruction is re-applied on experimental data successively with modified values of $\lambda_{\text{snow}} \pm 0.2$ m and VEM values that are shifted by $\pm 3\%$. The results for the three hadronic interaction models compared to the nominal values obtained from the recon-

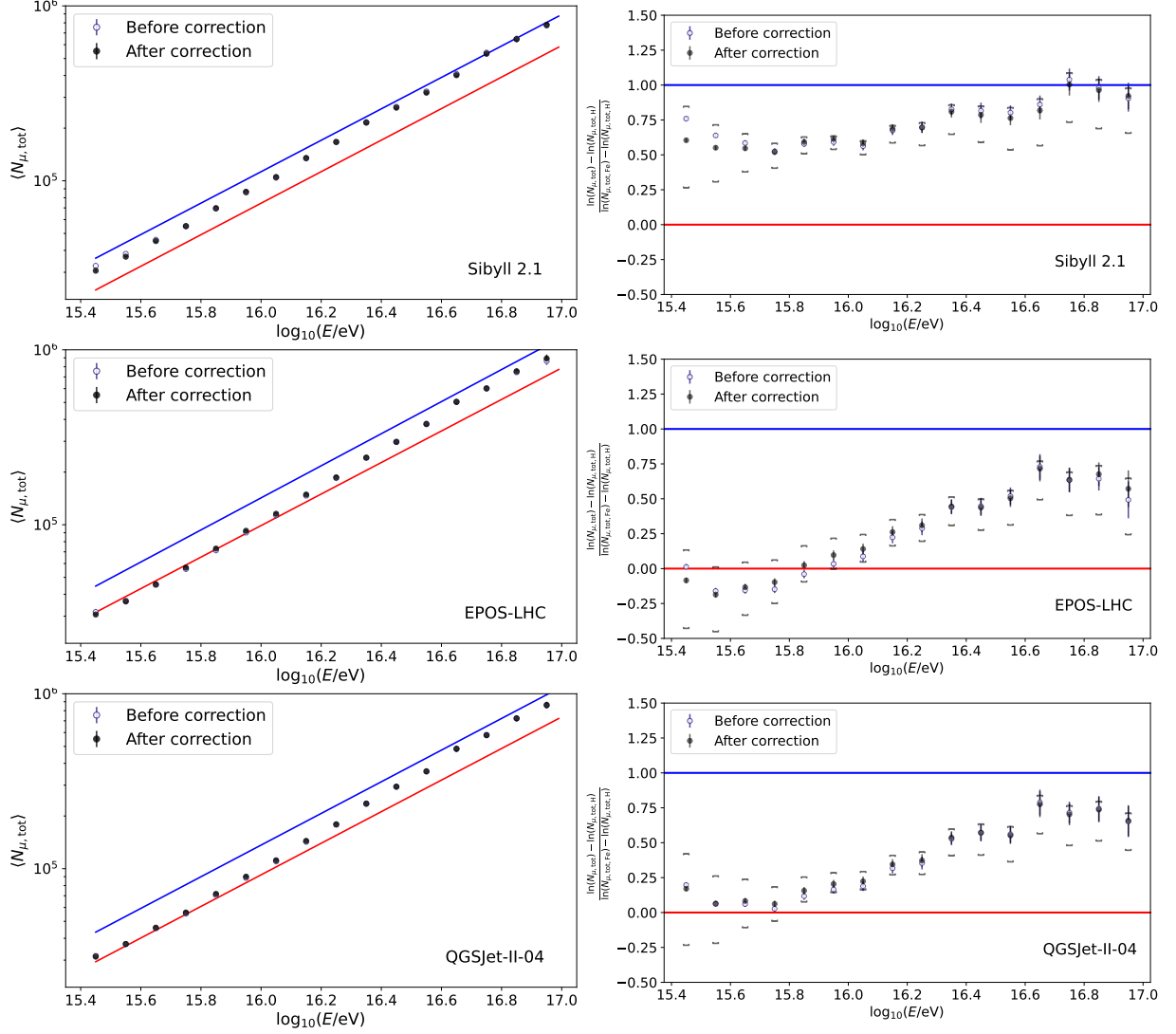


Figure 9.10.: Average muon number reconstructed from measured data before and after correction with the hadronic interaction model dependent correction factor compared to the MC expectation for proton and iron initiated air-showers (left column) and corresponding distributions converted to z-values including the systematic uncertainty band assigned for each correction factor (right column).

struction run without modified values are shown in Fig. 9.12. Shown are both the reconstructed average muon number and the corresponding z-values compared to the pure proton and iron expectations. It is noticeable, that the systematic uncertainty introduced by the model dependent correction factor has the largest influence on the result for low ($\log_{10}(E_{\text{reco}}/\text{eV}) \lesssim 15.8$) and high ($\log_{10}(E_{\text{reco}}/\text{eV}) \gtrsim 16.5$) energies, with differences of up to $\sim 14.6\%$ with respect to the nominal values. In the case of the uncertainty of the snow attenuation factor, average differences of approximately $\pm 2.9\%$ for $\lambda_{\text{snow}} \pm 0.2 \text{ m}$ are observed. Finally, shifts of $\pm 3\%$ of the VEM values result in shifts of $\pm 1.5\%$ on average with respect to the nominal values.

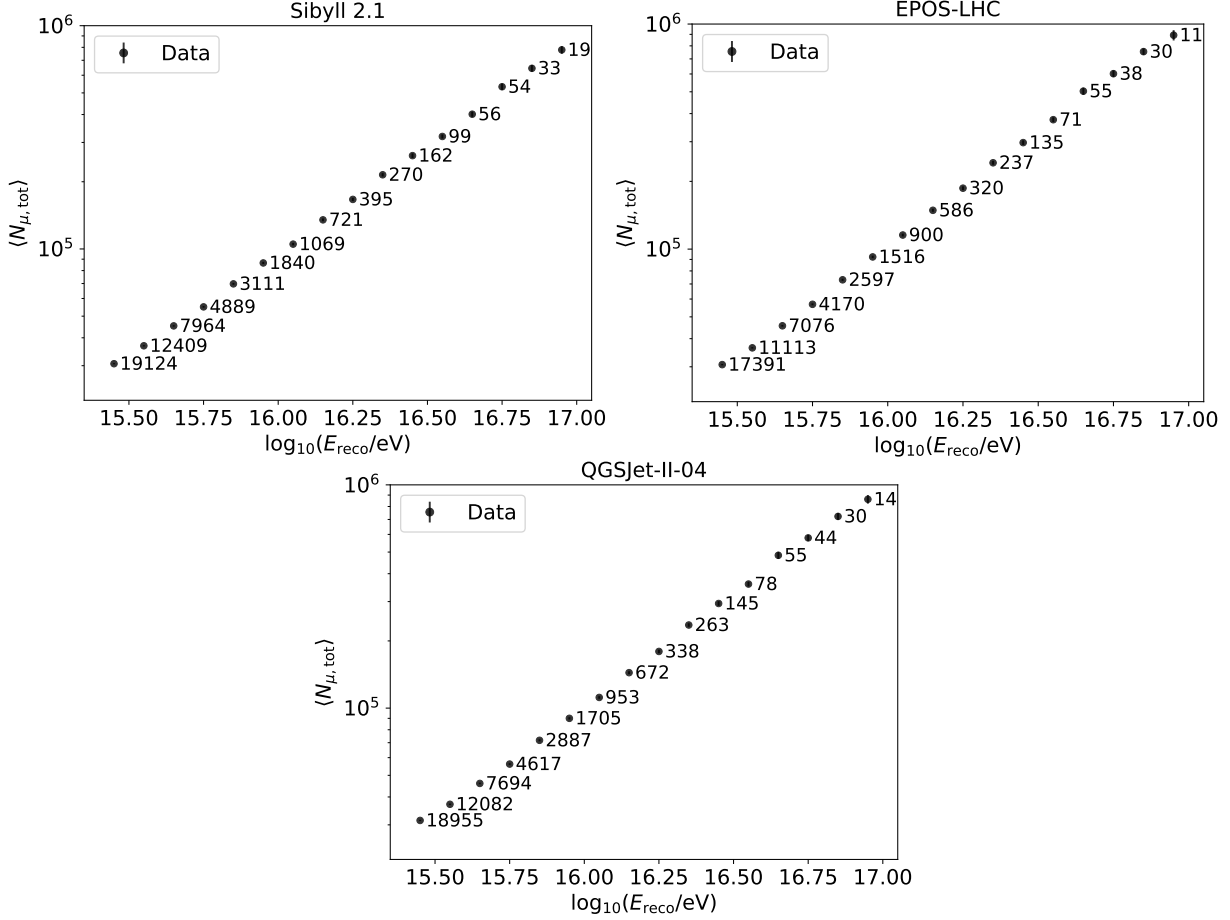


Figure 9.11.: Average muon number reconstructed from measured data after correction with the hadronic interaction model dependent correction factor. Numbers indicate the amount of events in each energy bin.

In addition to the detector effects, also the composition assumption in the calibration of the proxy parameters to the reconstructed energy and muon number introduces a systematic uncertainty. For this reason, the reconstruction of the average muon number as a function of energy is repeated for different realistic flux assumptions used for the derivation of the calibration functions and the impact on the final result is studied in Fig. C.5. It is shown that a conservative estimate of the systematic uncertainty due to the composition assumption is of the order $+3\%$ & -6% , $+5\%$ & -6% , and $+6\%$ & -6% for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04, respectively, with respect to the nominal calibration with H4a and applied over the entire energy range.

The differences to the nominal values are added in quadrature as individual contributions to determine the total systematic uncertainty. It should be noted, that the systematic detector uncertainties assumed for this work are based on previous studies. In particular, the uncertainty on λ_{snow} is obtained from studies with a more extended zenith angle range and could therefore likely be reduced by a dedicated study tailored specifically

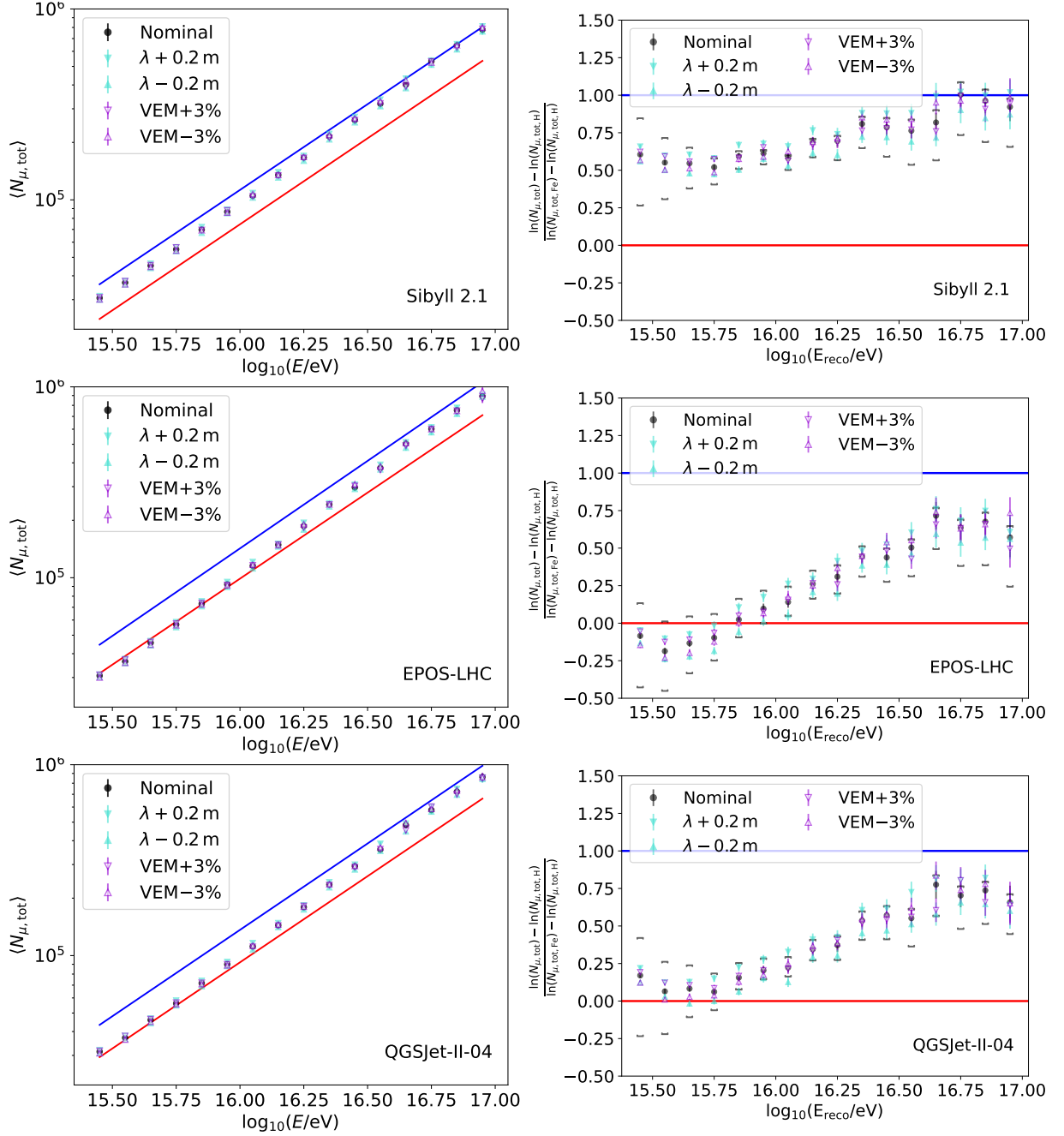


Figure 9.12.: Average muon number reconstructed from measured data including systematic uncertainties for different hadronic interaction models compared to the MC expectation for proton and iron initiated air-showers (left column) and corresponding z-values (right column).

for this work. Additionally, more sophisticated methods to account for effects of snow attenuation are currently under development [41]. A new *Radius-Dependent* (RADE) snow model [188], that uses a lateral distance and shower size dependent snow attenuation factor rather than a constant one could significantly improve the treatment of the snow attenuation. This is done to account for the dependence of the snow attenuation

on the energy spectrum of arriving particles and could therefore lead, particularly, to a different impact of the systematic uncertainty in λ_{snow} on the muon number estimation. For future studies, the IceTop enhancement scintillators can be used for cross calibration and therefore to improve the understanding of the snow attenuation.

9.5. Results

The final results of the measured average muon number between $\sim 3 - 100$ PeV compared to the expectations of Sibyll 2.1, EPOS-LHC, and QGSJet-II-04 are shown in Fig. 9.13. They gray band indicates the total systematic uncertainty, including the contributions of the correction factors, the snow attenuation factor, and the VEM calibration. In addition to the single-model distributions, the reconstructed muon number averaged over the three hadronic models is shown compared to their expectations. In this case, gray band includes the entire range of systematic uncertainties for the three models. The statistical uncertainties for each model are combined but are small compared to the systematic uncertainties over the entire energy range. Generally, the evolution of $\langle N_\mu \rangle$ as a function of primary energy qualitatively agrees with the expectation of an increasingly heavy composition between the knee and the second knee. The ratio of each model to the average result is shown in the bottom figure of Fig. 9.13. The average muon number is generally larger for the post-LHC models as expected from their increased amount of low-energy muons compared to Sibyll 2.1. The fact that at low energies the ratio to the average muon number is very similar for EPOS-LHC and Sibyll 2.1 is likely caused by the systematics of the correction factors. Overall, deviations of up to $\gtrsim 10\%$ from the average are visible for Sibyll 2.1. For QGSJet-II-04 and EPOS-LHC, the maximum deviations are below the $\sim 5\%$ level and below 10% , respectively. It should be noted, however, that the statistics used for this analysis is very limited, as indicated by the comparably large statistical uncertainties, and should therefore be repeated using a larger data set.

For an improved visibility of the reconstructed average muon number compared to the MC expectations, the corresponding z-values are shown in Fig. 9.14. Additionally, the evolutions of the average muon number as a function of energy for realistic cosmic-ray composition models, H4a, GST, and GSF, are indicated as lines³. For the derivation of their evolution, the *crflux* python module⁴ is used, which provides the flux fraction f_i of a given mass group i with respect to the all-particle flux. Using these fractions, the expectations for the average muon number of different mass groups can be weighted according

³It should be noted, that the H4a and GST flux models do not feature uncertainties but only represent the best-fit values.

⁴<https://github.com/mceq-project/crflux>. See [274] for more details.

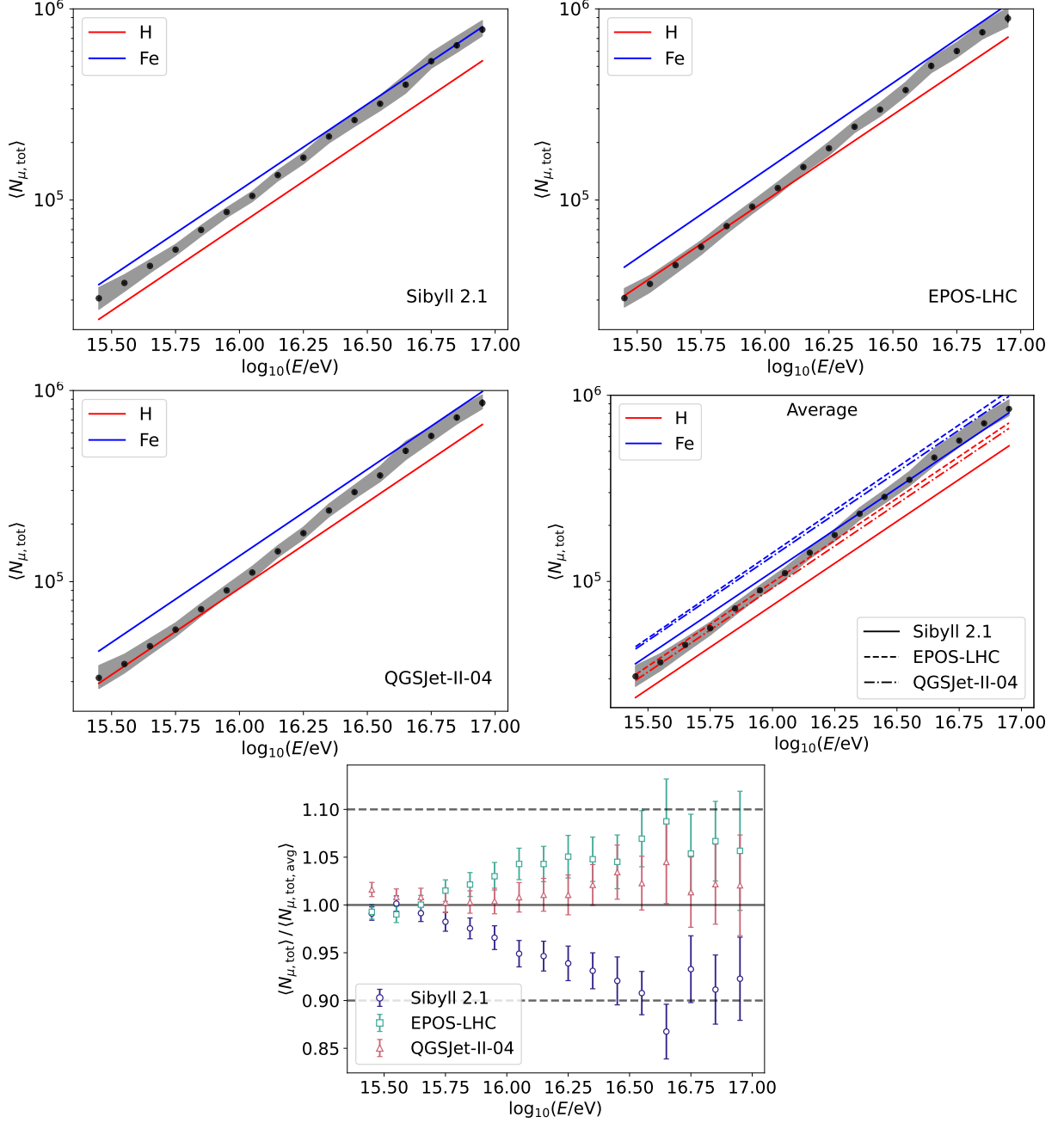


Figure 9.13.: Reconstructed average muon number in experimental data compared to MC expectations for proton and iron primaries produced with Sibyll 2.1 (top left), EPOS-LHC (top right), and QGSJet-II-04 (center left). The error band illustrates the total systematic uncertainty for each model. To combine all models, the average results for all models including the combined systematic uncertainty and all model expectations for proton and iron are shown in the center right figure. The ratio of the individual results to the average is shown in the bottom figure.

to a flux assumption:

$$\langle N_{\mu,\text{tot}} \rangle_{\text{flux}} = \sum_i f_i \cdot \langle N_{\mu,\text{tot}} \rangle_i, \quad (9.4)$$

where $i \in [\text{H}, \text{He}, \text{CNO}, \text{O}, \text{Fe}]$ for GST $i \in [\text{H}, \text{He}, \text{CNO}, \text{MgAlSi}, \text{Fe}]$ ⁵ for H4a, and $i \in [\text{H}, \text{He}, \text{CNO}, \text{Fe}]$ for GSF. For the calculation of the average expected muon number, the parametrization for $\langle N_\mu \rangle_{\text{H}}$ and $\langle N_\mu \rangle_{\text{Fe}}$ derived in section 9.1 for the different hadronic interaction models are used for proton and iron primaries, respectively, and to interpolate the intermediate mass groups via [41]

$$\langle N_\mu \rangle_A \approx \langle N_\mu \rangle_{\text{H}} \cdot A^{\frac{\log \langle N_\mu \rangle_{\text{Fe}} - \langle N_\mu \rangle_{\text{H}}}{\log 56}}, \quad (9.5)$$

motivated by the Heitler-Matthews model. The z-value representation allows for a simple visualization of the consistency of the measured average muon number interpreted with a given hadronic interaction model. Sibyll 2.1 and QGSJet-II-04 result in an average muon number that is bracketed within the pure proton and iron expectations. However, for the latter, the composition is compatible with a pure proton flux for energies below a few PeV. For EPOS-LHC, the results even suggest a composition slightly lighter than pure proton below ~ 8 PeV and are compatible with an almost pure proton flux within the systematic uncertainty. Compared to the expectations of the realistic flux models, significant differences in the scale of the average muon number are visible for the post-LHC models. Only for energies above ~ 30 PeV, the post-LHC models are compatible with the flux models within uncertainties. For Sibyll 2.1, the observed average muon number aligns well with the flux models within the systematic uncertainties. The average muon numbers ($E_\mu \geq 420$ MeV, $r_\mu \leq 1$ km) observed in near-vertical showers ($\theta \lesssim 26^\circ$) at the observation level of IceTop (~ 2835 m above sea level) obtained for the post-LHC models are therefore in tension with the given composition models.

It is noticeable that the shape of the average muon number as a function of energy differs between Sibyll 2.1 and the post-LHC models. For the latter, a steeper transition toward a heavier composition is visible. However, this is likely due to the differences in the average correction factor and, consequently in the mass dependence of the reconstruction bias present for Sibyll 2.1 compared to the post-LHC models caused by the different amounts of muons and the differences in X_{max} . This is also why, for QGSJet-II-04, the shape of the average muon number is less steep compared to EPOS-LHC. However, by construction, the systematic uncertainty assigned to each correction factor contains the differences in shape between the different models. It should also be noted that the transition of the nominal results for the post-LHC models is steeper compared to the muon density at large lateral distances discussed in section 4.3.2. This could be caused by the fact that for the reconstruction of the muon density, the energy scale is derived purely based on Sibyll 2.1, which is in contrast to the analysis presented in this work, where individual calibration functions are applied separately for each model.

⁵Here, CNO and MgAlSi are the carbon, nitrogen, and oxygen group and the magnesium, aluminum, and silicon group, respectively.

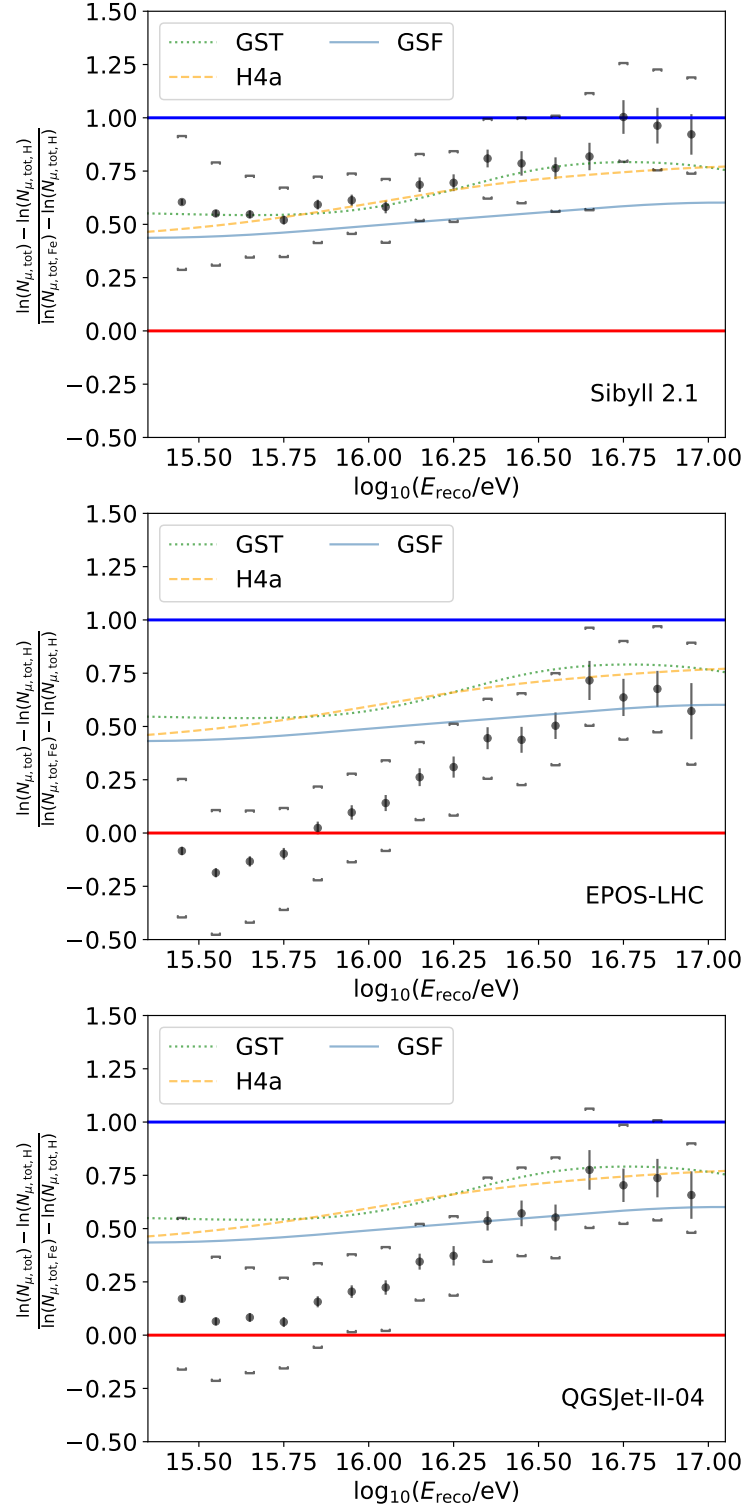


Figure 9.14.: Reconstructed average muon number as a function of primary energy for Sibyll 2.1 (top), EPOS-LHC (center), and QGSjet-II-04 (bottom) expressed as z-values. For comparison, the two realistic flux models H4a, GST, and GSF, are drawn as dashed and dotted lines, respectively.

9.6. Discussion

In this chapter, an event-by-event based reconstruction of the muon number in air showers is presented for energies between $\sim 2.5 - 100$ PeV. Due to the observed discrepancy in the muon multiplicity when comparing results from measured data with the MC expectations throughout different experiments, a more detailed study of the muon content measured with IceTop is motivated. This is in particular true since IceTop does not observe a muon deficit in the energy range of a few PeV to 100 PeV for the post-LHC models EPOS-LHC and QGSJet-II-04, which is the region before the reported muon excess begins (see section 3.6). Therefore, in the context of the muon puzzle, the results obtained for IceCube have a large impact on the significance [124] obtained for the meta-analysis presented in [2].

Qualitatively, the results obtained for the reconstruction of the average muon number are consistent with the density of GeV muons at 600 m and 800 m within the systematic and statistical uncertainties. For all studied hadronic interaction models, the evolution as a function of energy is consistent with the expectation of an increasingly heavy mass composition toward the second knee. However, for the post-LHC models, the composition prediction is very close or even slightly below a pure proton flux assumption below ~ 6 PeV, which is not consistent with recent composition measurements in this energy range [187] and modern flux models (see Fig. 9.14). While for Sibyll 2.1, the average muon number agrees well with the model expectations, the post-LHC models are in tension with the realistic flux models. This behavior is also observed for the measurement of the muon density at large lateral distances [199]. The muon content is therefore not described correctly in the post-LHC models for energies below 100 PeV. It also suggests that, in the included energy range, the muon density at large distances can be used to estimate the number of muons in air showers. The disagreement in the muon LDF at large lateral distances between the data and the MC is therefore disfavored as a possible explanation of the observed inconsistency between high- and low-energy muons⁶. Instead, a mismatch of the muon energy spectrum between the data and the MC could lead to the observed inconsistencies. A simple adjustment of the total muon content is therefore likely not sufficient for a potential tuning of hadronic interaction models, but rather the physical processes influencing the shape of the muon energy spectrum need to be considered.

At energies around 100 PeV, the composition prediction obtained from the reconstruction of the average muon number and from the muon density at large distances and from the average muon number generally results in a mixed composition. This is in agreement with measurements of > 10 GeV muons at distances up to 200 m from the shower axis with

⁶Note that more detailed tests of the muon lateral distribution are ongoing at the time of writing.

the EAS-MSU surface detector that are interpreted with QGSJet-II-04 [275]. It is also consistent with measurements of the energy loss of high-energy ($\gtrsim 300$ GeV) muons with IceCube for primary energies between 2.5 PeV and 1 EeV [187, 241] and with the reconstructed average muon multiplicity for $E_\mu > 500$ GeV with IceCube for primary energies between 2.5 PeV and 100 PeV [200] (see section 4.3.2).

It is important to mention, however, that a shift in the absolute energy scale can introduce a significant offset of the average reconstructed muon number. For example, a 20% of the energy scale translates to a shift in 0.5 in the z-values [199] shown in Fig. 9.14. For this reason, comparisons with other observatories and over a wide range of primary energy are of high importance [151] and should include the reconstruction of the average muon number presented in this work. Additionally, the event-by-event based two-component reconstruction enables the opportunity to study correlations of high- and low-energy muons measured with IceCube and IceTop for single air showers. These correlations are directly related to the muon energy spectrum and can therefore be used to derive strong constraints on hadronic interaction models as they probe the corresponding hadronic processes at two vastly different energy regimes. Since the study of the muon energy spectrum is of high interest for model tests, the various data from different observatories should be studied in a similar fashion as for the meta-analysis presented in section 3.6.2 but including a specific dependence on the muon energy thresholds and ranges obtained for each experiment. Furthermore, the two-component LDF allows for the reconstruction of the muon LDF and can therefore be used to probe the muon lateral distribution and study deviations between data and MC. This is already to some extent part of the preliminary study presented in section 8.3, but should be analyzed in more detail in the future as the muon lateral spread is related to the muon energy (see Eq. (5.1)). Preliminary analyses in this context are ongoing at the time of writing [242, 238, 192].

The main shortcoming of the presented reconstruction of the average muon number is the limited data set. For future studies, a larger portion of measured data should be included to increase the statistics particularly at high energies. Moreover, also intermediate primaries as well as primary energies up to EeV should be produced for the post-LHC models EPOS-LHC and QGSJet-II-04. Due to the larger mass overburden for inclined showers, the produced lateral distribution at the observation level is typically more muon rich. Therefore, the inclusion of further zenith angle bins is of high interest for the muon number reconstruction. At the same time, measurements of the muon attenuation using the constant intensity cut (CIC) method can be performed and compared with the results from KASCADE-Grande [153] located at sea level and LHAASO [276] situated at ~ 600 g/cm² which are not compatible with each other. With IceTop at an atmospheric depth of ~ 690 g/cm², the muon attenuation as a function of mass overburden can be studied in more detail.

Since the effective attenuation of the EM component in IceTop increases over the years

due to the increasing snow accumulation, the inclusion of data from different years is of particular interest, as the muon signal becomes less contaminated. Since also muons are not entirely unaffected by snow attenuation, the two-component reconstruction can employ snow dependent muon PDFs and an adjusted muon energy threshold for the reconstruction of the muon content in air showers. With the snow dependent spline fits developed in chapter 5, this work creates the opportunity for such analyses.

9.7. Further applications

The two-component LDF reconstruction holds the potential for a variety of related and follow-up analyses, which are being developed at the time of writing. One important application of the model are IceTop-uncontained events, i.e., EAS events with core position outside of the IceTop array. For these events, the in-ice track produced by a coincident high-energy muon bundle can be used to constrain the shower geometry, while the tail of the lateral distribution can be described mainly by the muon LDF. Because the shower tail is dominated by muon contribution, IceTop-uncontained events are of great interest, both, for analyses employing the muon number reconstruction and to increase the acceptance for cosmic-ray measurements with IceTop. In particular, combined IceTop and in-ice analyses that are typically limited to zenith angles $\lesssim 36^\circ$ [42] could be extended to higher inclinations. A preliminary analysis is presented in [184], which utilizes the two-component reconstruction in the context of IceTop-uncontained events of proton- and iron-initiated showers with coincident in-ice information in the energy range of PeV to EeV and $\theta \lesssim 36^\circ$, where the in-ice signal provides an anchor for the shower geometry. In this study, the EM signal at a distance of 400 m is used as an energy proxy, while the muon number is reconstructed using $S_{\mu,550}$. The resulting parameter distributions and reconstruction performance is shown in Fig. 9.15, where events filtered by a set of preliminary quality cuts are shown with lower opacity. Already for this first analysis including uncontained events and an extended zenith and energy range, the muon number reconstruction is as good as $\sim 20\%$ and is below of $\sim 30\%$ between ~ 10 PeV and $\sim$ EeV. This illustrates the capability of the two-component approach in the context of IceTop-uncontained events, where mainly the tail of the signal distribution is observed. However, in case of the energy reconstruction, further optimization is needed to stabilize the reconstruction close to the shower axis, where the signal distribution is not directly observed.

Moreover, due to the increasing snow accumulation on top of the IceTop tanks mostly attenuating the EM component, IceTop becomes a more effective muon detector. In this context, for the next generation observatory, IceCube-Gen2, which will feature a surface array with scintillation detectors and radio antennas around and within the IceTop ar-

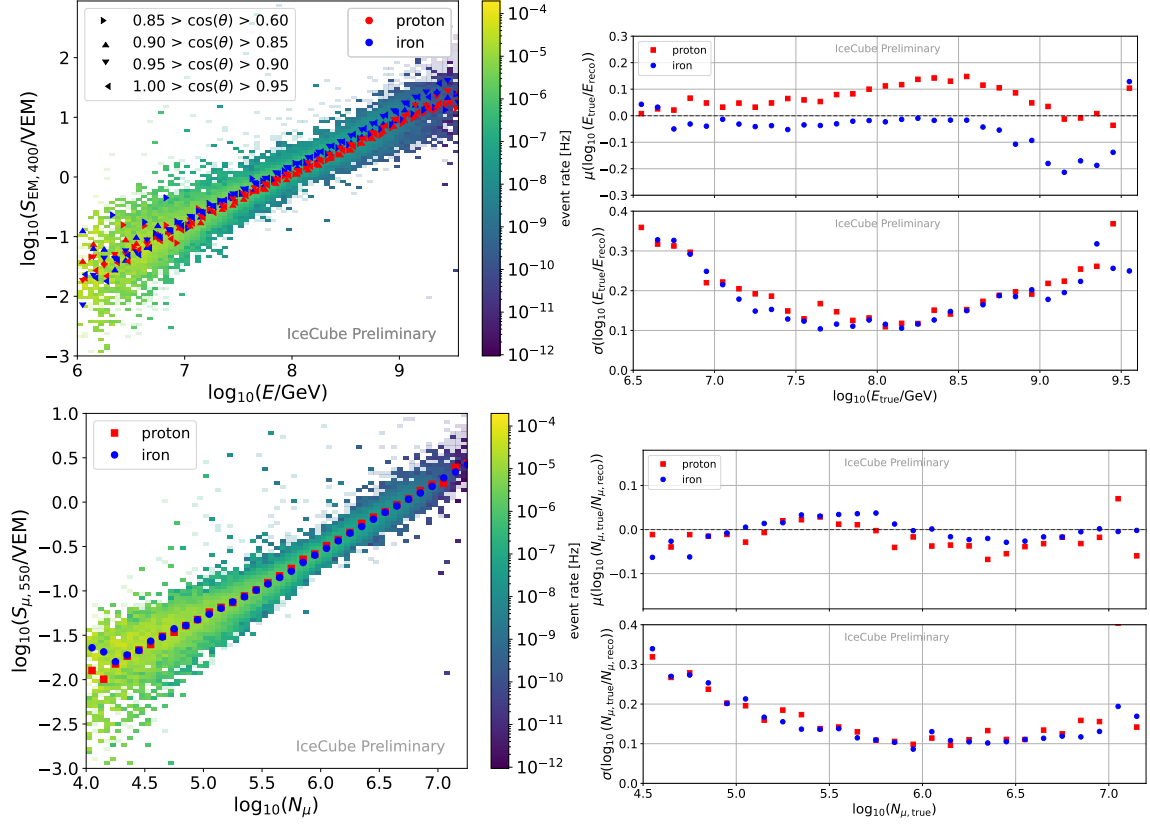


Figure 9.15.: Distribution of the energy proxy $S_{\text{em},400}$ (top left) and the muon number proxy $S_{\mu,550}$ (top right) as a function of true energy and muon number, respectively, for proton- and iron-induced showers produced with Sibyll 2.1 and weighted to the H4a flux model. Markers show average values of different zenith bins for the energy proxy and of the all zenith bins combined for the muon number proxy. The energy (bottom left) and muon number (bottom right) reconstruction bias and resolution for all zenith angles is shown in the upper and lower panels, respectively.

ray (see section 4.5), the two-component LDF can be of great benefit. This is especially true for the reconstruction of showers with core position outside of IceTop but within the IceCube-Gen2 surface array, for which the EM component can be reconstructed using the scintillation detectors, while the tail of the distribution observed with IceTop is a measure of the muon component. A preliminary study presented in [277] shows that with the snow level expected for 2035 (~ 5.2 m on average), which roughly corresponds to the planned time line for the IceCube-Gen2 operation, the tail observed with IceTop is effectively a pure muon measurement. In this study, the response of proton- and iron-induced showers of the IceCube-Gen2 scintillator array and IceTop is simulated. Fig. 9.16 shows the corresponding true contribution of muons and EM particles to the measured signal distributions with IceTop for near-vertical showers. At lateral distances $\gtrsim 400$ m relevant for the muon proxy, the observed signal has a negligible contribution of EM particles for,

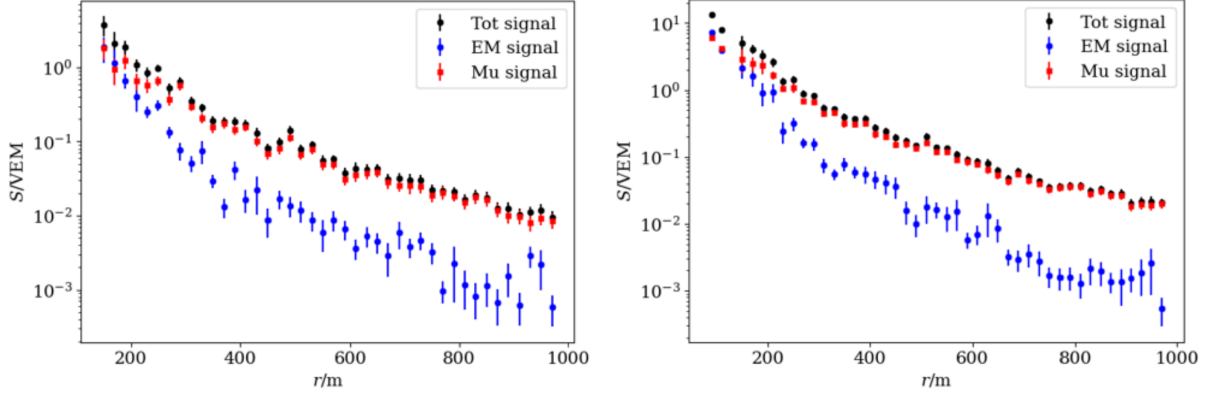


Figure 9.16.: Average true EM and muon lateral distributions of near-vertical ($\theta \leq 18^\circ$) proton (left) and iron (right) showers with energies $16.5 \leq \log_{10}(E/\text{eV}) \leq 16.6$. The total signal (sum of EM and muon components) is shown in black. Error bars indicate the standard deviation in each bin. Figures taken from [277].

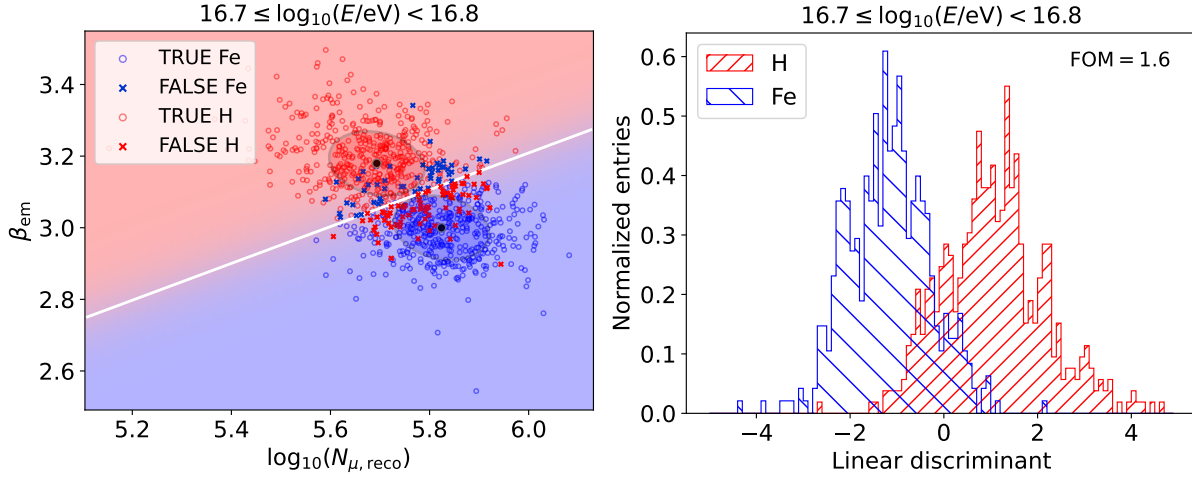


Figure 9.17.: Correlation between β_{em} and $N_{\mu, \text{reco}}$ for near-vertical showers ($\lesssim 26^\circ$) proton and iron showers with $16.7 \leq \log_{10}(E/\text{eV}) \leq 16.8$ (left). The 2σ regions around the mean are illustrated as ellipses. Corresponding distribution of the linear discriminant along the axis of maximum separation shown as white line is the left figure (right).

both, proton and iron primaries. In addition, due to the elevation of the scintillation detectors, cross-calibrations with the IceTop tanks will lead to an improved modeling of the snow attenuation.

Due to its relation to the primary mass, the reconstruction of the muon content can be of great benefit for cosmic-ray composition studies. The two-component reconstruction effectively generates three new composition-sensitive parameters. $S_{\mu, 550}$, or the reconstructed muon number $N_{\mu, \text{reco}}$, and the slopes of the EM and muon LDF, β_{em} and β_{μ} . To test the potential in mass separation using the two-component parameters, $N_{\mu, \text{reco}}$

and β_{em} are folded into a combined analysis⁷. For this purpose, a simple linear discriminant analysis (LDA) can be performed, constructing a one dimensional classifier based on the two input parameters to maximize separation between different classes, which in this case are proton and iron-induced showers (see [278] for more details). To quantify the separation between proton and iron, the *figure of merit* (FOM) is defined as

$$\text{FOM} = \frac{|\mu_{\text{H}} - \mu_{\text{Fe}}|}{\sqrt{\sigma_{\text{H}}^2 + \sigma_{\text{Fe}}^2}}, \quad (9.6)$$

where the mean, μ_{H} and μ_{Fe} , and the standard deviation, σ_{H} and σ_{Fe} , of proton and iron are calculated from the respective samples of the classifier. The correlation between both parameters and the resulting discriminant distribution are shown in Fig. 9.17⁸. For near-vertical showers with energies of $16.7 \leq \log_{10}(E/\text{eV}) \leq 16.8$, a FOM of 1.6 is observed, indicating that both parameters can be valuable additional input for composition analyses.

⁷Note, that β_{μ} is highly correlated with $S_{\mu,550}$, as it described the muon slope at a lateral distance of 550 m.

⁸The LDA is performed using the scikit-learn python package. See https://scikit-learn.org/stable/supervised_learning.html for more details.

Summary and outlook

Within this thesis, a novel approach for the single-event based reconstruction of cosmic-ray air shower events measured with the surface array of the IceCube Neutrino Observatory, IceTop, is developed. The *two-component LDF* is based on a likelihood model of the electromagnetic (EM) and muon component of air showers, with the aim of reconstructing both the energy of the shower and its muon content.

The number of muons is one main observable for the reconstruction of the cosmic-ray composition, which is crucial for an improved understanding of the nature of cosmic ray sources and propagation. As such, the possibility of a reconstruction of the muon content can significantly enhance the cosmic-ray mass discrimination with the IceCube Neutrino Observatory. However, due to its dependence on MC simulations, the indirect reconstruction of air showers is prone to large uncertainties. This is mainly caused by the requirement to extrapolate the description of high-energy hadronic interactions beyond the phase space reachable with accelerator experiments. These interactions are described by *hadronic interaction models* within air-shower simulations. It is established based on measurements from various air shower observatories, that these models lead to a discrepancy in the description of the muon content when compared to measured data, which become significant around primary energies of 40 PeV (~ 8 TeV cms energy) and is sometimes referred to as the *Muon Puzzle* in cosmic-ray air showers.

The IceCube Neutrino Observatory as EAS muon detector

The IceCube Neutrino Observatory consists of a cubic-kilometer in-ice array with 86 strings instrumented with photo-multipliers and deployed deep in the antarctic ice at a depth of ~ 1.5 km for the measurement of astrophysical neutrinos, and a surface array, IceTop, with ice-Cherenkov tanks following the footprint of the strings that acts as a veto detector. IceTop is also an independent air-shower detector which measures cosmic rays with energies between PeV and EeV. With the combination of a surface array and a deep in-ice detector, the IceCube Neutrino Observatory has the unique capability to measure the EM component and low-energy ($\sim$ GeV) muons with IceTop in coincidence

with the high-energy ($\gtrsim 400$ GeV) muons with the in-ice array. The threshold for high-energy muons is set naturally through the requirement of such muons to traverse 1.5 km of ice to produce a signal in the in-ice detector. The measurement of low- and high-energy muons is of particular interest for studies of hadronic interaction models, as it probes the corresponding hadronic physics at two vastly different energy regimes, and therefore at different stages of the air-shower development. In fact, the measurement of the low-energy ($\sim$ GeV muon density) at large lateral distances measured with IceTop based on a statistical analysis in the energy range of $\sim 2.5 - 100$ PeV does not show a significant excess. The two-component reconstruction grants access to the entire muon lateral distribution function and allows for the reconstruction of the total muon content, which is used to test the predictions of different hadronic interaction models compared to measured data with the improved reconstruction procedure and on a single-event basis.

Two-component EAS reconstruction

For the two-component reconstruction, two separate lateral distribution functions (LDFs) are employed for the description of the EM and muon contribution to the signal distribution measured with IceTop. It is shown, that parametrized versions of the *Double Logarithmic Parabola* (DLP) function (Eq. (6.2)), which is well known from the standard IceTop reconstruction, and of the modified *Nishimura-Kamata-Greisen* (NKG) function (Eq. (6.3)) are well suited for the description of the EM and muon lateral signal distribution, respectively. While the former can be modeled via a log-normal distribution, the underlying signal distribution for the muon component is described by means of dedicated IceTop tank response simulations. The resulting muon signal probability distributions as a function of muon inclination (muon PDFs) are modeled and saved for different muon multiplicities using cubic spline fits as that can be evaluated during the reconstruction procedure. The muon PDFs are produced using the injection of 1 GeV muons, which roughly corresponds to the peak of the muon energy spectrum observed with IceTop, and under the assumption of muon propagation in air showers that is coherent with the shower direction. To validate these approximations, alternative muon PDFs are produced using different underlying assumptions.

The two-component reconstruction using two LDFs simultaneously is implemented by means of a convoluted likelihood within a new multi-detector framework for the reconstruction of air-shower events, which allows for the combination of multiple likelihood functions in a global minimization procedure. The normalization $S_{\text{tot},125}$ and $S_{\mu,550}$ of the total and muon LDF at a distance of 125 m and 550 m, respectively, is used to estimate the cosmic-ray energy and the muon content of air shower events by means of a calibration function, where the total LDF is given as the sum of the EM and muon

contribution. Both distances are optimized for minimal dependence on the cosmic-ray mass, which reduces systematic biases due to the unknown composition. For the purpose of this work, a dedicated event sample containing near-vertical showers with zenith angles $\lesssim 26^\circ$ and primary energies above full efficiency but high statistics is chosen. It should be mentioned that despite the simpler standard IceTop reconstruction utilizing a single LDF fit, the full efficiency threshold is compatible for the two-component LDF. For the chosen event sample, the primary energy and muon number can be reconstructed with minimal dependence on the cosmic-ray mass and with a resolution of $< 10\%$ and $< 20\%$, respectively, at a few tens of PeV. Note, that a muon number resolution of $\sim 20\%$ is adequate to, on average, differentiate between proton and iron showers, for which the muon content differs by $\sim 40\%$. The energy resolution using the two-component LDF is improved by $> 12\%$ compared to the standard IceTop reconstruction. At the same time, the accuracy in the estimation of the shower core position on the ground is improved by around 20% compared to the standard reconstruction.

The reconstruction of the muon content of air showers is of special interest for cosmic-ray analyses, as it directly relates to the hadronic shower development and contains information about the mass of the cosmic ray. The cosmic-ray mass composition is a probe of cosmic-ray sources but requires a detailed understanding of the EAS development. Since hadronic interaction models introduce large systematic uncertainties in the interpretation of air-shower data, indirect studies of hadronic shower physics using the muon production in air showers are of great importance.

Hadronic interaction models

Using the novel two-component reconstruction, new parameters sensitive to the cosmic-ray mass are studied to test the validity of hadronic interaction models. For this purpose, the muon number proxy $S_{\mu,550}$, and the slope of the EM and muon LDF, β_{em} and β_{μ} , respectively, are tested for internal consistency in the prediction of the average composition as a function of the energy proxy $S_{\text{tot},125}$ compared to the extreme cases of a pure proton and iron flux. In a previous analysis using the LDF slope of the standard reconstruction, β , an estimate of the high-energy muon multiplicity, dE/dX_{1500} , observed with the in-ice detector, as well as the density of GeV muons ρ_{μ}^{600} and ρ_{μ}^{800} at lateral distances of 600 m and 800 m, the hadronic interaction models Sibyll 2.1, EPOS-LHC, and QGSJet-II-04, lead to an inconsistent description of different EAS components (see Fig. 8.9). In particular, for Sibyll 2.1, the low- and high-energy muon parameters are found to be consistent within uncertainties, while β suggests a significantly heavier average mass composition even beyond iron above a few tens of PeV. Conversely, for the state-of-the-art models EPOS-LHC and QGSJet-II-04, especially at energies below 10 PeV, the high-energy muon content and

the GeV muon density at large lateral distances are incompatible in their composition prediction. At the same time, β and dE/dX_{1500} are consistent within uncertainties for EPOS-LHC, while dE/dX_{1500} and ρ_{μ}^{600} & ρ_{μ}^{800} become increasingly consistent with increasing primary energy. The inclusion of the two-component LDF parameters shows a similar trend toward a heavier average composition as a function of energy in the energy range of a few PeV to 100 PeV, which is expected from the transition between Galactic and extragalactic cosmic rays. The muon proxy $S_{\mu,550}$ and the muon slope β_{μ} at a lateral distance of 550 m are compatible within uncertainties with the muon density at 600 m and 800 m from the shower axis. However, a shift of the nominal values towards a slightly heavier composition is visible, which could be due to remaining EM contribution to the raw reconstructed $S_{\mu,550}$ and β_{μ} . Interestingly, β_{em} leads to an interpretation of the average composition qualitatively similar to β . Since the latter was believed to be influenced by EM particles and low-energy muons, this suggests a potential mis-modeling of the EM component rather than an issue with the muon contribution at 125 m. It should be noted, however, that, except for $\rho_{\mu}^{600}/\rho_{\mu}^{800}$, all studied parameters are detector observables which cannot be interpreted in a straight-forward way. Nevertheless, the internal inconsistencies for all three models illustrate the challenges connected to the interpretation of the cosmic-ray composition.

The internal consistency using the two-component LDF parameters is studied without the application of any model dependent calibration functions. In a further study, the muon number for near-vertical air showers measured with IceTop is reconstructed with the two-component model as a function of primary energy. The single-event based reconstruction of the muon content is crucial for studies of correlations of low- and high-energy muons, which are well motivated through the differences in the muon-energy spectrum between different hadronic interaction models. Additionally, an estimate of the muon content can be of great benefit for studies of the cosmic-ray composition. For the reconstruction of the average muon number in bins of the primary energy, remaining biases are taken into account by means of a correction factor that includes a systematic uncertainty mainly introduced by small mass dependencies and finite resolution of the two-component reconstruction. Additional systematic detector uncertainties as well as an energy scale uncertainty are included for the interpretation of the results. The reconstructed average muon number is consistent with modern cosmic-ray flux models for Sibyll 2.1. However, for EPOS-LHC and QGSJet-II-04, the composition prediction by the average muon number is compatible with pure proton and even lighter compositions for energies below a few PeV, which is in tension with recent composition measurements and flux models (see Fig. 9.14). However, these results are consistent with a previous measurement of the muon density at large lateral distances with IceTop presented in [199]. This suggests that the low-energy muon yield predicted by EPOS-LHC and QGSJet-II-04 is too high in the PeV to 100 PeV energy range for near-vertical showers and at the observation level of IceTop.

In contrast to that, too few muons are observed for ultra-high energy cosmic-rays [148, 2]. At the same time, the measurement of the high-energy muon multiplicity with IceCube for near-vertical showers in the PeV to 100 PeV regime shows no discrepancies between the studied hadronic interaction models (see [201, 200]). Sibyll 2.1 is the only model that leads to a consistent prediction of the composition for the low- and high-energy muons, but shows deficiencies in the description of the EM component. This points toward a discrepancy of the muon-energy spectrum between data and simulations and strongly motivates a correlation study of low- and high-energy muons using the two-component reconstruction for events with coincident in-ice information.

Muons in EASs

The first application of the two-component LDF reconstruction developed within this work is successful in the reconstruction of the EM and muon components in EASs and enhances the reconstruction performance of IceTop. It holds potential for a variety of different follow-up analyses as well as an extension toward a wider phase space. In future analyses, a refinement and improvement of the presented method can be achieved, e.g., by tests of a variety of different model functions for a potential improvement in the description of the EM and muon lateral distribution, which could further enhance the reconstruction performance. A preliminary study using the NKG function ([233]) for the description of the EM lateral distribution is presented in [277]. Additionally, a larger range of zenith angles and primary energies up to EeV should be included. For this purpose, a parametrization of the LDFs as a function of zenith angle in addition to the shower-size dependence can be beneficial. This is of particular interest since more inclined air showers feature a higher relative muon content because of the stronger attenuation of the EM component with mass overburden. The inclusion of more inclined events would also allow for measurements of the muon attenuation, which can be compared to the results of KASCADE-Grande [153] and LHAASO [276]. This is of special interest in the context of the Muon Puzzle, since modern hadronic interaction models show deficiencies that might be caused by the description of the muon attenuation in the measured data [2].

In addition, with an event-by-event based two-component reconstruction, studies of fluctuations of the muon number can be conducted with IceTop and compared to hadronic model predictions, further constraining potential contributions to the Muon Puzzle. At the same time, the two-component reconstruction allows insights into the entire muon lateral distribution. This allows to further test hadronic interaction models and a potential mis-modeling of the muon content at different distances from the showers axis. Preliminary studies of the reconstruction of the muon LDF have been investigated (see Fig. 8.7). The muon lateral distribution is of great interest as it indirectly relates to the

muon energy spectrum.

Furthermore, the two-component LDF is well suited for the application on air-showers with core position outside of the IceTop array that feature a coincident in-ice signal. In such IceTop-uncontained events, the in-ice track from the high-energy muon bundle can be used to constrain the shower geometry, while the tail of the lateral distribution measured with IceTop can be reconstructed using the combination of an EM and muon LDF. Because the tail of the lateral distribution is dominated by the muon component, the reconstruction of IceTop-uncontained events is both of interest for the muon number reconstruction and to increase the general acceptance of IceTop for cosmic-ray analyses. This is especially important for combined IceTop and in-ice analyses, as coincident events that require IceTop containment are limited to zenith angles $\lesssim 36^\circ$ [42]. A preliminary analysis using the two-component LDF for the reconstruction of IceTop-uncontained events of proton and iron in the energy range of PeV to EeV and zenith angles $\lesssim 36^\circ$ with coincident in-ice information, providing an anchor for the shower geometry, is presented in [184]. This follow-up study based on the two-component model developed in this thesis illustrates its capability of the reconstruction of EAS events for which mainly the tail of the lateral distribution is observed with IceTop.

In addition, due to the increasing snow accumulation on top of the IceTop tanks, IceTop becomes a more effective muon detector over the years, as mainly the EM component is attenuated. This strongly motivates the study of more recent years of IceTop data. In this context, the more sophisticated treatment of the snow attenuation presented in [188, 184] becomes increasingly important and is well suited for application within the two-component reconstruction, as it attempts to differentiate the EM and muon contributions. A more sophisticated attenuation model becomes crucial for the next generation observatory, IceCube-Gen2, which will feature average snow heights above ~ 5 m. IceCube-Gen2 will feature a surface array with scintillation detectors and radio antennas around and within the IceTop array. For IceCube-Gen2, the two-component model can be of great benefit for the reconstruction of EASs with core position outside of IceTop but within the IceCube-Gen2 surface array. For these events, the EM component can be reconstructed using the scintillation detectors, while the tail of the distribution observed with IceTop is a measure of the muon component. A preliminary study presented in [277] illustrates, that the tail observed with IceTop is effectively a pure muon measurement. In addition, the description of the snow attenuation used in the two-component model will greatly benefit from cross-calibrations of the elevated scintillation detectors with the IceTop tanks.

Naturally, because of its relation to the cosmic-ray mass, the separation of the EM and muon components is of great interest for composition analyses. A preliminary study shows that, with the EM slope β_{em} and the muon number, the two-component model constitutes

two observables that can be used as valuable additional input for composition studies.

Summary

Overall, the two-component reconstruction improves on various aspects of the standard reconstruction and is therefore foreseen as the future IceCube standard reconstruction. In addition, it offers opportunity for a variety of follow-up studies and can be of benefit for all cosmic-ray analyses. Most importantly, it provides an event-by-event estimation of the muon content in air showers measured with IceTop, which can be combined with in-ice information to derive strong tests of hadronic interaction models in the energy range in which the discrepancy between data and simulations in the muon content becomes significant and enhance cosmic-ray composition analyses in the transition region of Galactic to extragalactic cosmic rays.



Muon response

The knot settings used for the production of muon spline fits (see section 5.2) are shown in Tab. A.1. The custom knot sampling is optimized to provide the highest accuracy of the B -splines in the main part of the muon PDFs. For this reason, the signal knots are placed with a finer grid in the signal region in which the shape of the PDF changes most rapidly. Since the width of the PDFs changes with the muon multiplicity, this signal region is adapted accordingly. In case of the second fit dimension, the zenith angle, the location of the knots can be held constant for all muon multiplicities while still maintaining sufficient fit accuracy. It should be noted, that the signal and zenith ranges feature knots beyond the defined signal and zenith ranges. This additional padding is added for improved fit stability through additional support at the boundary¹.

¹see <https://github.com/icecube/icetray/tree/main/topsimulator> for reference.

Appendix A. Muon response

The spline fit settings for different muon multiplicities for the production of 1 GeV muon and spectrum-weighted splines are shown in Tab. 5.2. However, the fit settings for snow-dependent splines slightly differ and are shown in Tab. A.2, where the smoothing parameters and number of knots for each dimension are listed.

Table A.1.: Custom knot settings for the spline fits of the muon tank response distributions as a function of signal strength and zenith angle.

n	knots (min,max,step)	
	signal / VEM	zenith / rad
1	$[(-2,2.0,0.1),(2.0,40,0.2)]$	$(-0.349,1.396,0.087)$
2	$[(-2,1.0,0.2),(1,2.5,0.1),(2.5,40,0.2)]$	$(-0.349,1.396,0.087)$
3	$[(-2,1.5,0.2),(1.5,4.5,0.1),(4.5,40,0.2)]$	$(-0.349,1.396,0.087)$
4	$[(-2,1.5,0.2),(2.0,6.5,0.1),(6.5,40,0.2)]$	$(-0.349,1.396,0.087)$
5	$[(-2,2.2,0.2),(2.2,7.0,0.1),(7.0,40,0.2)]$	$(-0.349,1.396,0.087)$
6	$[(-2,2.5,0.2),(2.5,8.5,0.1),(8.5,40,0.2)]$	$(-0.349,1.396,0.087)$
7	$[(-2,3.0,0.2),(3.0,9.0,0.1),(9.0,40,0.2)]$	$(-0.349,1.396,0.087)$
8	$[(-2,3.5,0.2),(3.5,10.5,0.1),(10.5,40,0.2)]$	$(-0.349,1.396,0.087)$
9	$[(-2,4.0,0.2),(4.0,12,0.1),(12,40,0.2)]$	$(-0.349,1.396,0.087)$
10	$[(-2,4.5,0.2),(4.5,13.5,0.1),(13.5,40,0.2)]$	$(-0.349,1.396,0.087)$
11	$[(-2,5.0,0.2),(5.0,15,0.1),(15,40,0.2)]$	$(-0.349,1.396,0.087)$
12	$[(-2,5.5,0.2),(5.5,16.5,0.1),(16.5,40,0.2)]$	$(-0.349,1.396,0.087)$
13	$[(-2,6.0,0.2),(6.0,18,0.1),(18,40,0.2)]$	$(-0.349,1.396,0.087)$
14	$[(-2,6.5,0.2),(6.5,19.5,0.1),(19.5,40,0.2)]$	$(-0.349,1.396,0.087)$
15	$[(-2,7.0,0.2),(7.0,21,0.1),(21,40,0.2)]$	$(-0.349,1.396,0.087)$

Table A.2.: Spline fit settings for the application on muon tank response distributions as a function of signal strength and zenith angle.

n	signal bin step size / VEM	number of knots			smoothing factor		
		signal	zenith	snow	signal ($\cdot 10^{-5}$)	zenith ($\cdot 10^{-7}$)	snow ($\cdot 10^{-12}$)
1	0.10	258	19	19	1.0	100.0	5
2	0.12	258	19	19	1.0	50.0	5
3	0.14	266	19	19	10.0	50.0	5
4	0.16	273	19	19	10.0	50.0	5
5	0.18	274	19	19	10.0	50.0	5
6	0.20	281	19	19	100.0	50.0	5
7	0.20	280	19	19	100.0	50.0	5
8	0.20	286	19	19	100.0	10.0	5
9	0.20	290	19	19	100.0	10.0	5
10	0.20	296	19	19	100.0	5.0	5
11	0.20	300	19	19	100.0	5.0	5
12	0.20	306	19	19	100.0	5.0	5
13	0.20	310	19	19	100.0	5.0	5
14	0.20	316	19	19	100.0	5.0	5
15	0.20	320	19	19	100.0	5.0	5

In the following, the zenith-dependent muon spline fits derived from the injection of 1 GeV muons for muon multiplicities up to $n = 15$ are shown.

Appendix A. Muon response

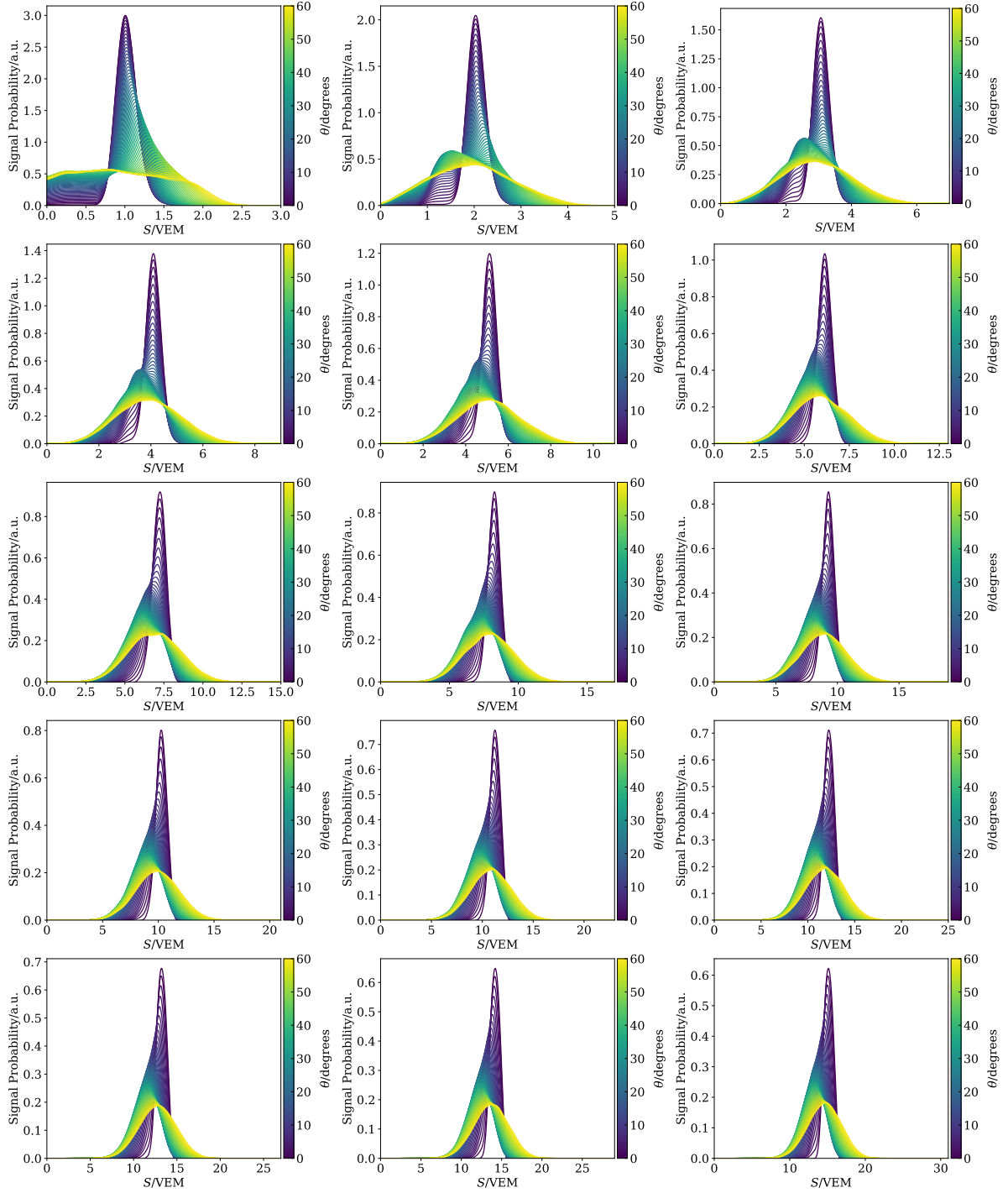


Figure A.1.: Muon spline fits for injection of 1 GeV muons at different multiplicities as a function of muon inclination.

Two-component model

LDF parametrization

The LDFs used for the description of the EM and muon contribution to the measured signal distributions within the two-component model (see chapter 6) are the DLP function Eq. (6.2) and the modified NKG function Eq. (6.3). Both functions are parametrized as a function of the energy proxy S_{125} of the standard IceTop reconstruction to provide an accurate description of the respective contribution. For this purpose, the average true EM and muon lateral distributions are fit with the respective LDF. While the slope parameters κ and γ of the DLP function and the modified NKG function, respectively, are fully parametrized during reconstruction, the parametrization of the slope parameters β_{em} and β_{μ} is only used to initialize both LDFs. The parametrization is performed individually for Sibyll 2.1, EPOS-LHC, and QGSJet-II-04. The final selected parametrizations are based on the average between the three models. The resulting average LDF fits for the three models are shown in the following.

Appendix B. Two-component model

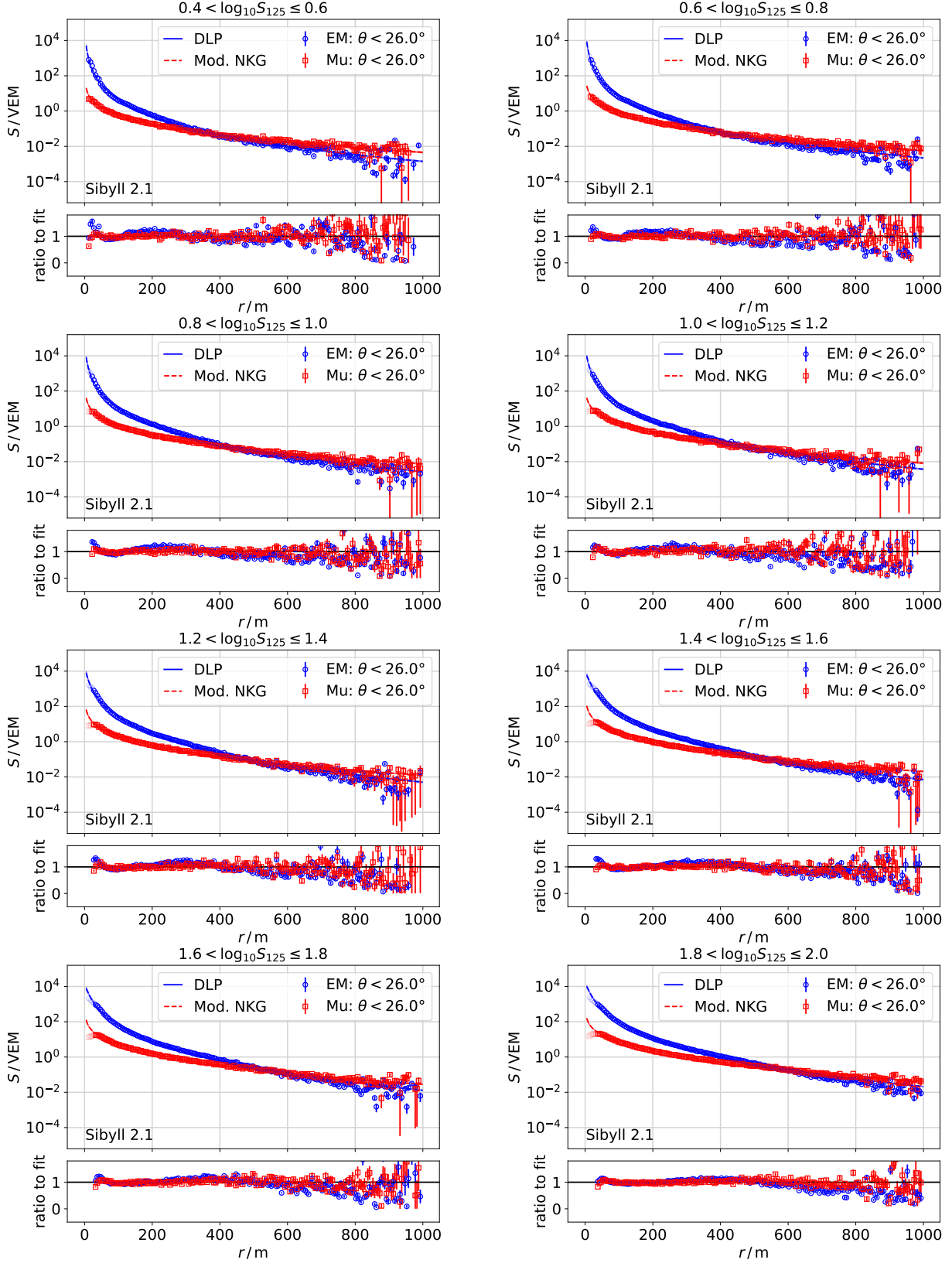


Figure B.1.: Average lateral distributions from electromagnetic particles and muons produced in proton and iron induced near-vertical air-showers (weighted to the H4a flux assumption) produced with Sibyll 2.1 for two different bins in the energy proxy S_{125} . Fits for two different LDFs are shown as lines. Residuals for the LDF fits to the average electromagnetic and muon lateral distributions are shown in the lower panels.

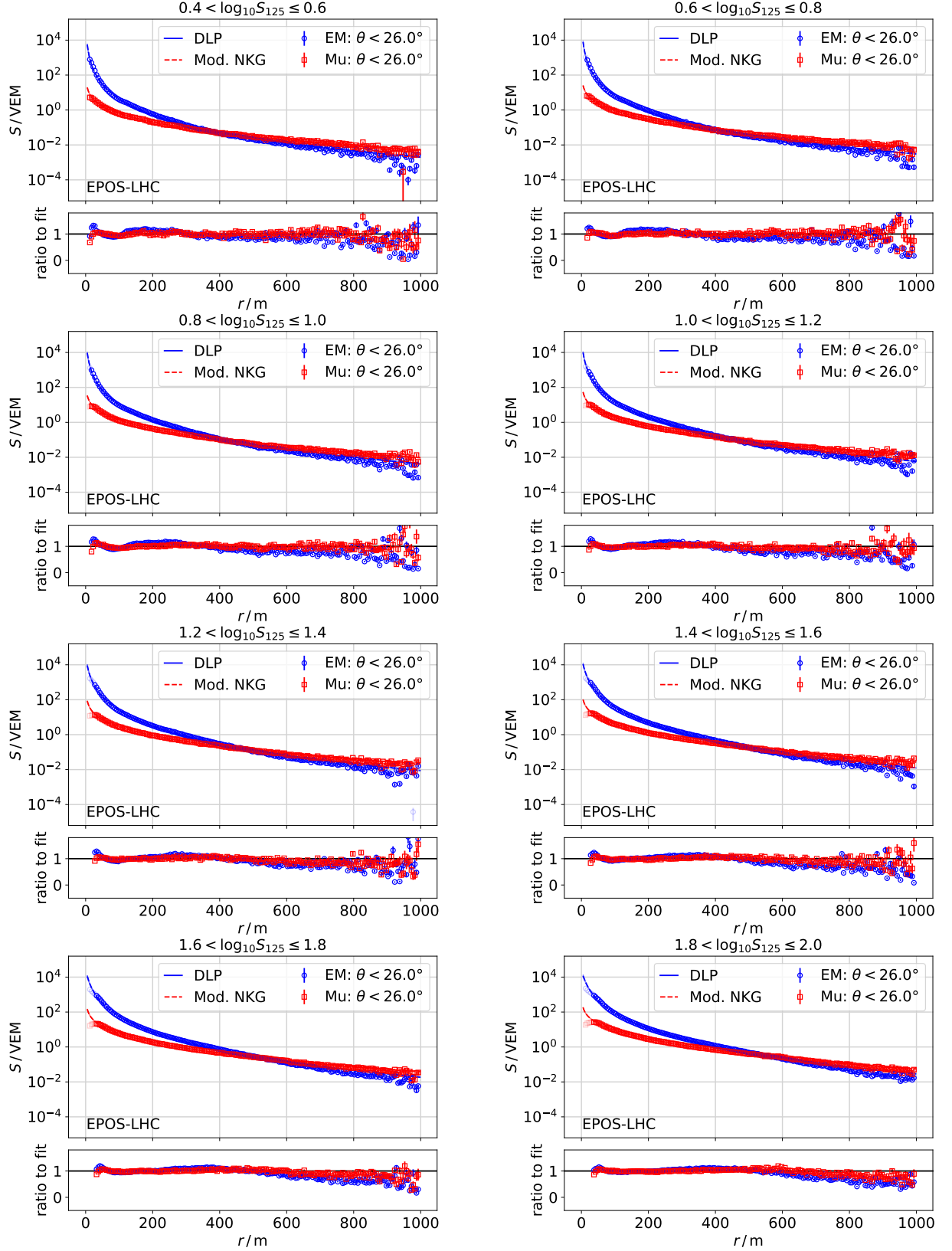


Figure B.2.: Average lateral distributions from electromagnetic particles and muons produced in proton and iron induced near-vertical air-showers (weighted to the H4a flux assumption) produced with EPOS-LHC for two different bins in the energy proxy S_{125} . Fits for two different LDFs are shown as lines. Residuals for the LDF fits to the average electromagnetic and muon lateral distributions are shown in the lower panels.

Appendix B. Two-component model

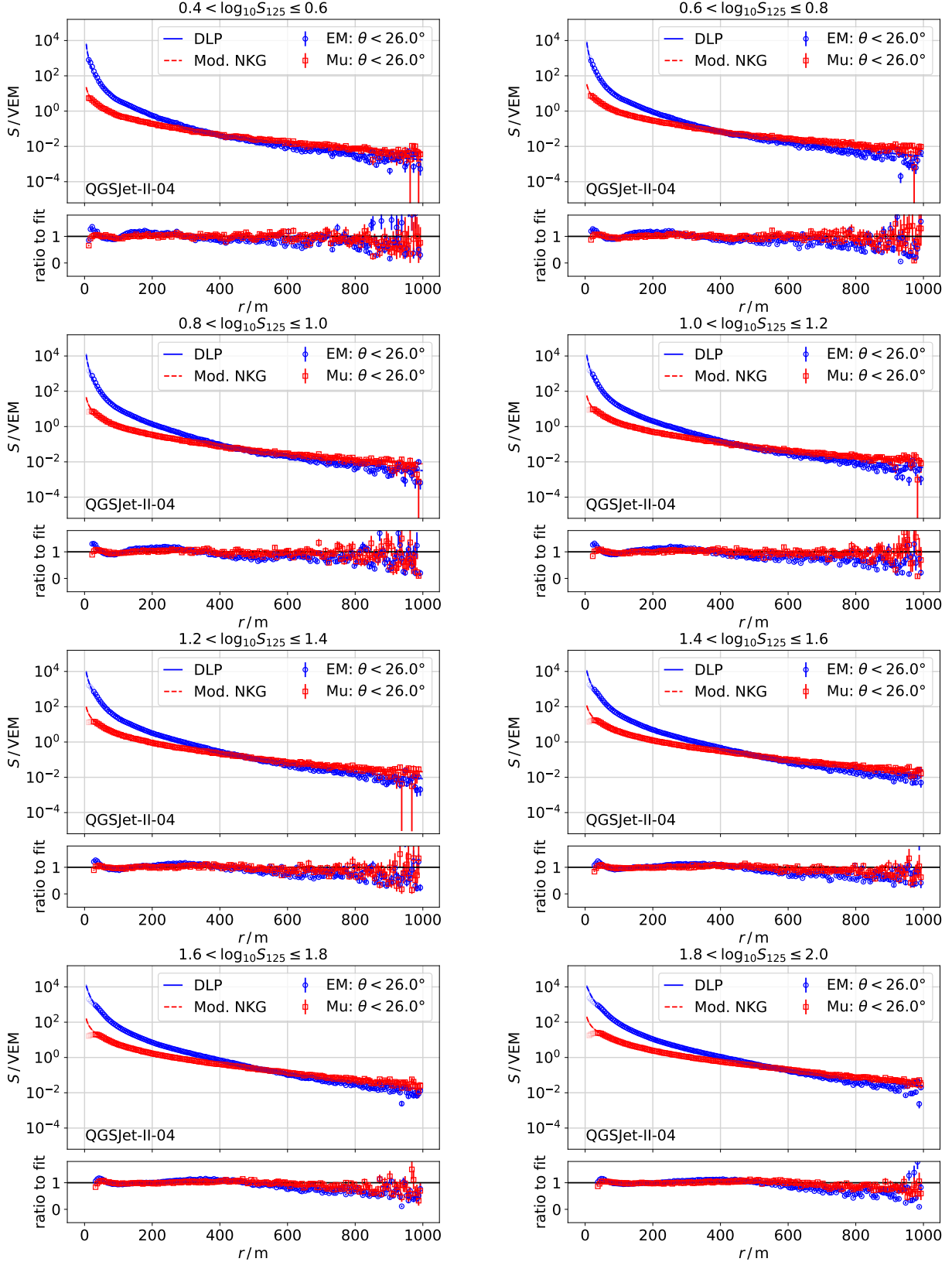


Figure B.3.: Average lateral distributions from electromagnetic particles and muons produced in proton and iron induced near-vertical air-showers (weighted to the H4a flux assumption) produced with QGSJet-II-04 for two different bins in the energy proxy S_{125} . Fits for two different LDFs are shown as lines. Residuals for the LDF fits to the average electromagnetic and muon lateral distributions are shown in the lower panels.

HLC signal model

In the small signal regime of the HLC signal model within the two-component LDF, a threshold is defined in the average HLC signal below which the underlying signal distribution for HLCs can be approximated to be log-normal. Below this threshold, therefore, the average signal expectation can be approximated as EM dominated. The log-signal difference distributions of neighboring HLC tanks in bins of the average HLC signal are shown in Fig. B.4. It can be observed that below $\sim 10^{-0.25}$ VEM and above $\sim 10^{-0.35}$ VEM in the average HLC signal, the difference distribution can be approximated with a Gaussian fit in logarithmic space. In between this average signal range, the muon contribution is significant and leads to a clear deviation from a log-normal distribution. For the purpose of the two-component reconstruction, a threshold of $\log_{10}\langle S/\text{VEM} \rangle = -0.2$ is chosen to define the small signal regime. This threshold acts as a constraint for the muon contribution, leading to a good performance in the reconstruction of the average EM and muon lateral distribution.

Appendix B. Two-component model

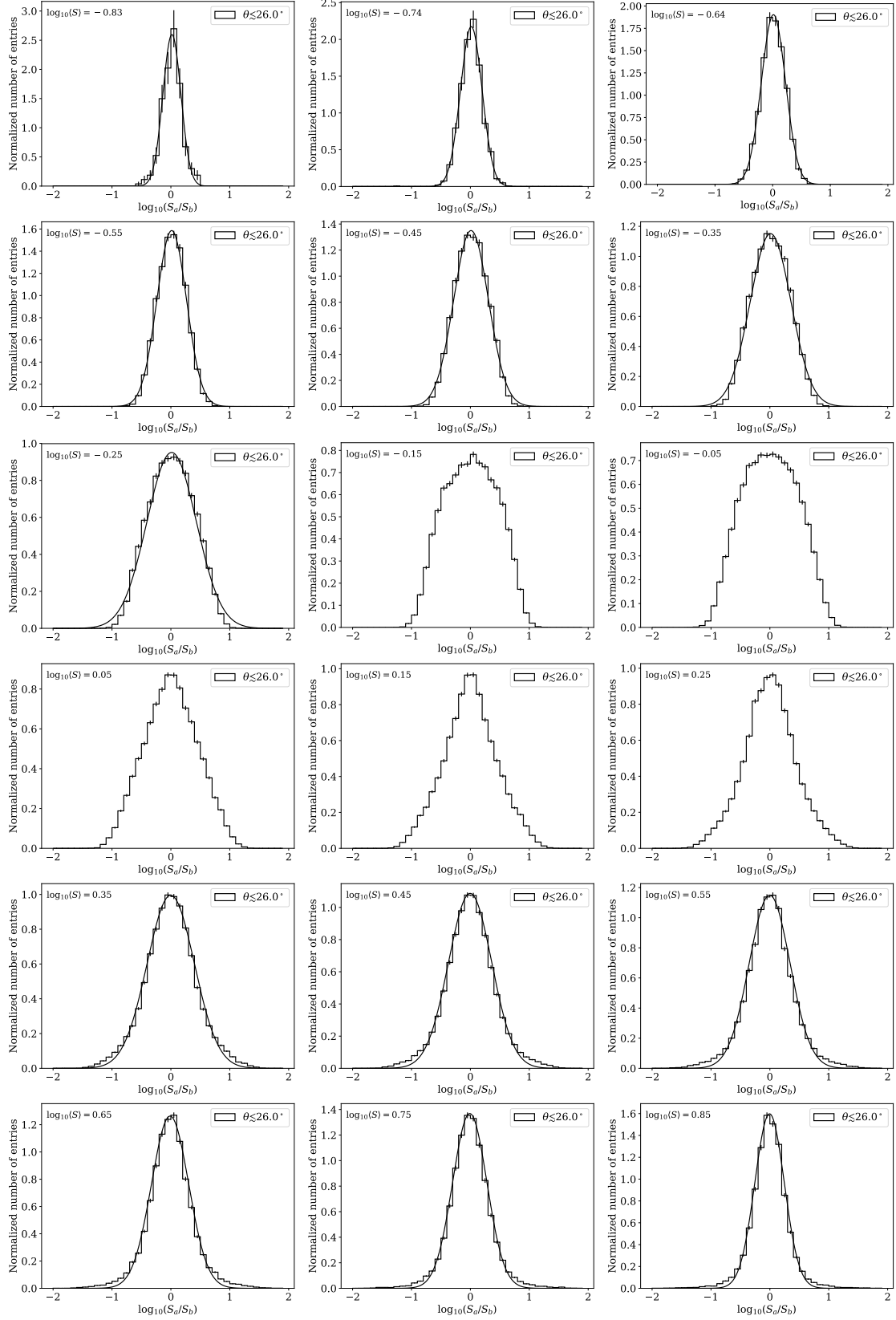


Figure B.4.: Distributions of the differences of the signals in logarithmic space for neighboring HLC tanks in bins of the average signal. A Gaussian fit is included for bins that are approximately normally distributed.

Validity tests

Muon spread parametrization

The construction of the two-component model presented in this thesis is based on various approximations that are tested for validity in section 7.3. One approximation is the coherence of the primary and muon direction in air showers. It is found that for near-vertical showers ($\theta \lesssim 26^\circ$) this assumption is well justified since no significant systematic effect is found in a preliminary study including a model for muon angular separation with respect to the primary axis. However, for more inclined events, the dependence of the muon spread on the zenith angle could be important. This effect is illustrated in Fig. B.5. As expected, since lower-energy muons are attenuated more strongly with increasing shower inclination, the muon spread decreases (see Eq. (7.6)) as a function of the zenith angle. A parametrization as shown in Fig. B.6 can be used for future studies that extend the considered zenith range.

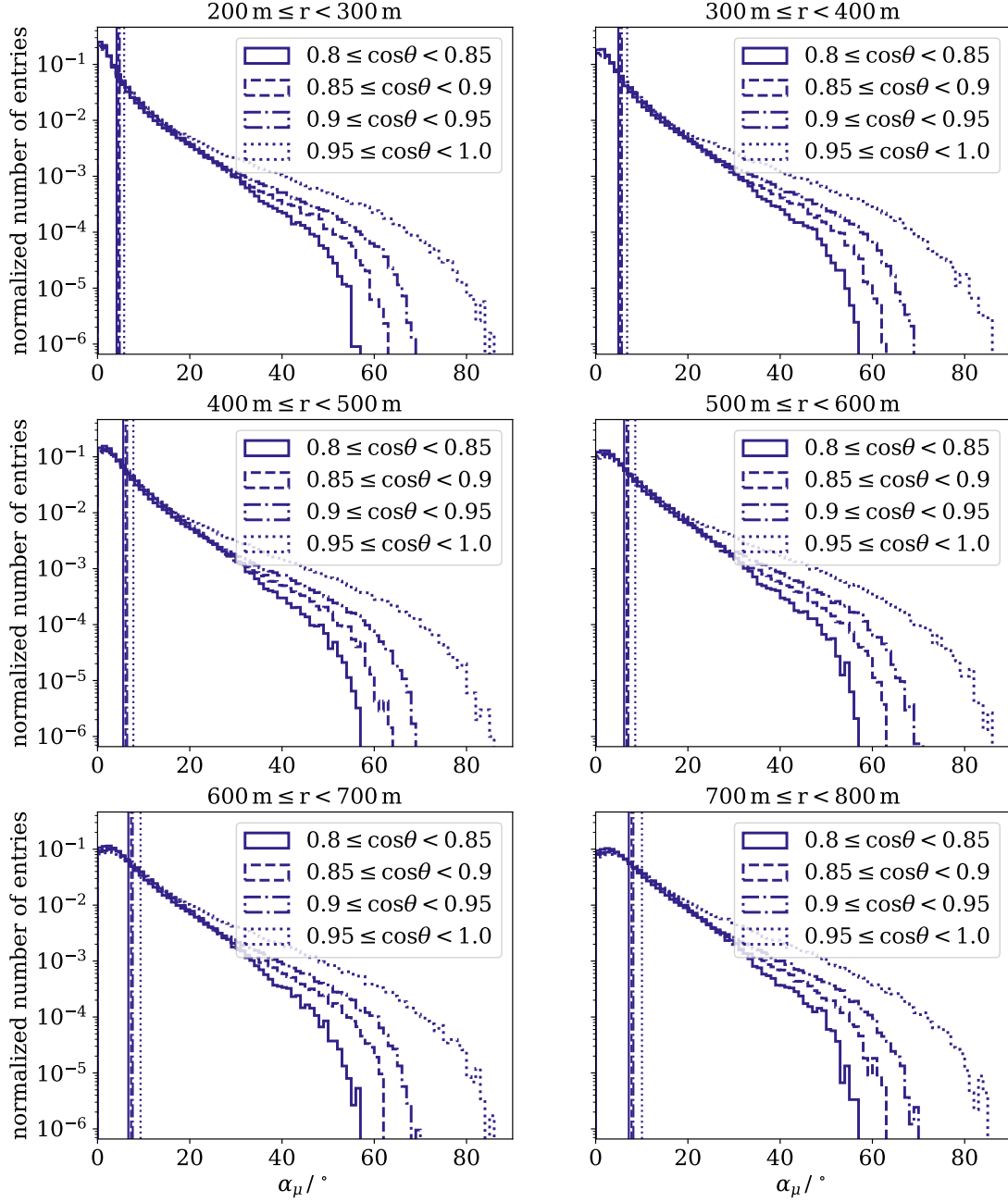


Figure B.5.: Muon angular separation with respect to the primary direction in bins of lateral distance for four primary zenith bins. Included are CORSIKA showers for proton and iron primaries produced with Sibyll 2.1. Vertical lines indicate the average value of each histogram.

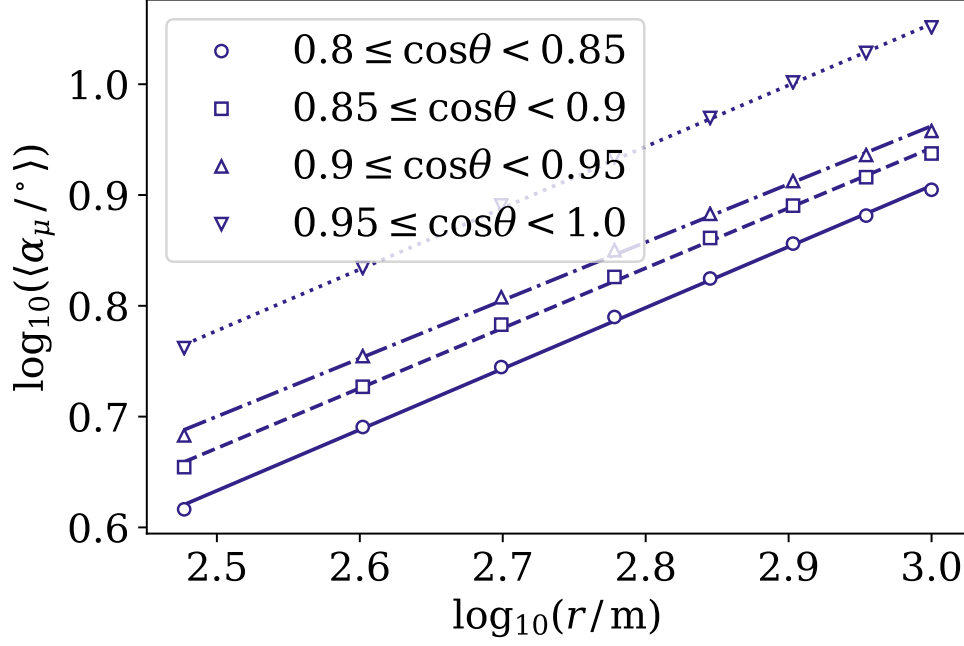


Figure B.6.: Average muon angular spread as a function of lateral distance for four different bins in the primary zenith angle derived from Fig. B.5.

EM sigma parametrization

To estimate the radius dependence of the electromagnetic signal uncertainty derived in section 7.3, a preliminary study based on [189] is performed assuming a factorization of the signal strength and the lateral distance dependence, i.e.:

$$\sigma_{\text{em}}(\langle S_{\text{em}} \rangle, r) = \sigma_{\text{em}}(\langle S_{\text{em}} \rangle) \sigma_{\text{em}}(r). \quad (\text{B.1})$$

The lateral distance dependence is then given as the standard deviation of the distribution of signal differences divided by the signal strength dependence and by a factor of $\sqrt{2}$:

$$\sigma_{\text{em}}(r) = \frac{\log_{10} S_{\text{em},a} - \log_{10} S_{\text{em},b}}{\sqrt{2} \sigma_{\text{em}}(\langle S_{\text{em}} \rangle)} \quad (\text{B.2})$$

Fig. B.7 shows the resulting distribution of the lateral distance dependence of the electromagnetic signal uncertainty for proton and iron initiated air-showers weighted for the H4a flux model. The distributions can be well described by an error function fit of form

$$\sigma_{\text{em}}(r) = p_{r,1} \operatorname{erf}\left(\frac{r - p_{r,2}}{200 \text{ m}}\right) + p_{r,3}. \quad (\text{B.3})$$

The resulting parameter values are listed in Tab. B.1. For both primaries, the electromagnetic signal uncertainty is overestimated close to the shower axis and underestimated at large distances to the shower axis. This is because the intrinsic shower fluctuations increase with increasing lateral distance, leading to increasingly unequal signal expectation

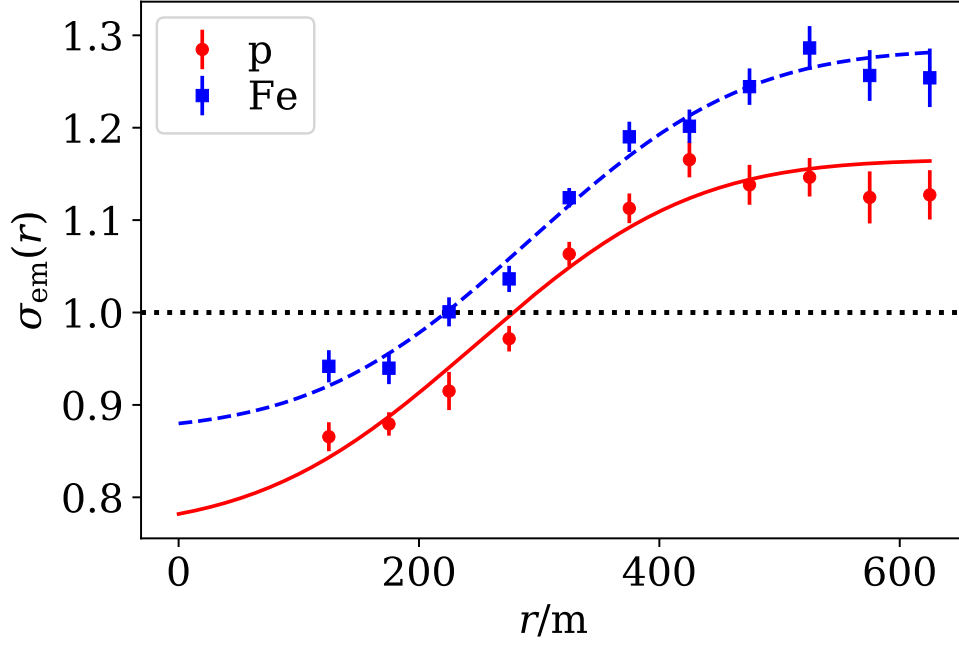


Figure B.7.: Lateral distance dependence of the electromagnetic signal uncertainty for proton and iron showers weighted to H4a.

Table B.1.: Parameters values for the error function fit to the lateral distance dependence of the electromagnetic signal uncertainty.

primary	$p_{r,1}$	$p_{r,2}$	$p_{r,3}$	$\sigma(p_{r,1})$	$\sigma(p_{r,2})$	$\sigma(p_{r,3})$
proton	$1.997 \cdot 10^{-1}$	$2.476 \cdot 10^2$	$9.657 \cdot 10^{-1}$	$1.971 \cdot 10^{-2}$	$3.171 \cdot 10^1$	$2.907 \cdot 10^{-2}$
iron	$2.067 \cdot 10^{-1}$	$2.926 \cdot 10^2$	1.079	$1.138 \cdot 10^{-2}$	$1.921 \cdot 10^1$	$1.807 \cdot 10^{-2}$

values for neighboring tanks. Closer (but not too close) to the shower axis, the approximation of similar signal expectation value for neighboring tanks becomes more valid, leading to a more accurate estimation of the signal uncertainty. In principle, this lateral distance dependence could be implemented as correction factor for the signal uncertainty derived in section 7.3. However, due to the significant difference in the parametrization for proton and iron primaries, the lateral dependence is not used for the two-component reconstruction as to not introduce a dependence on a cosmic-ray flux model used to derive the parametrization.

C

Analysis

Coincidence background

The estimation of the muon content from signals at large lateral distances can lead to a bias through the contribution of accidental background hits coincident to physical event. This is because such coincident background is not part of the standard simulation chain (see section 4.3.1) and its description is not trivial. To include the influence of accidental coincidences on the interpretation of measured data, an approximate simulation is performed in section 8.1 and added at the end of the standard processing, before the two-component reconstruction is applied. The impact of the inclusion of accidental background in simulations produced with Sibyll 2.1 is shown in Fig. C.1. Because of the tight time-cleaning window for SLCs, the influence is fairly small, with a shift of $\lesssim 2\%$ of the data points with respect to interpretation with MC without background simulations. The difference decreases to $\sim 0.1\%$ for increasing primary energy (except for the last bin, which, however, can be explained by fluctuations), as the relative influence of background coincidences on the reconstruction also decreases.

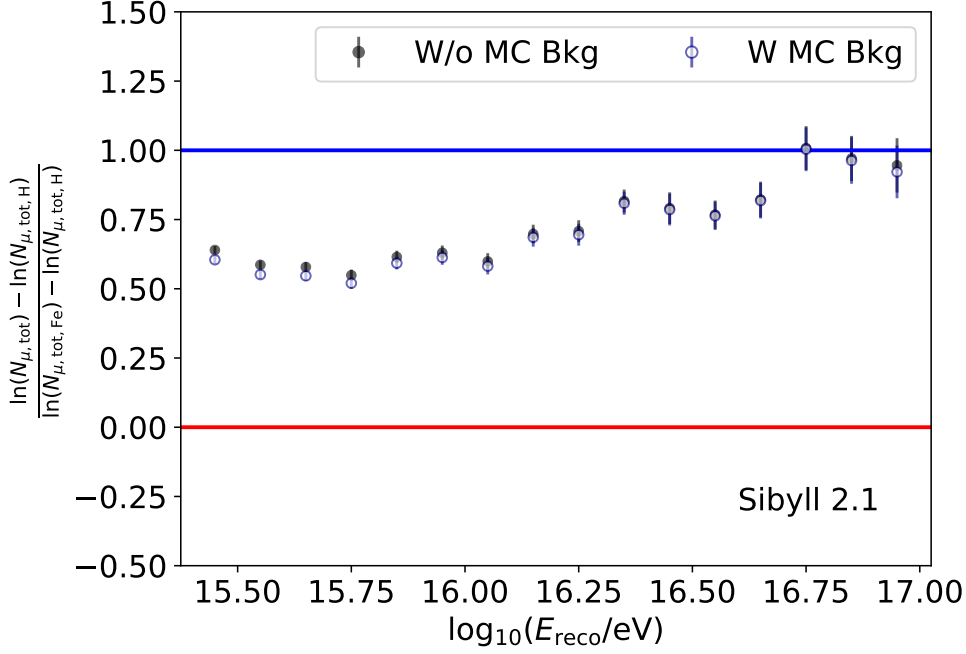


Figure C.1.: z-values obtained from the reconstructed and corrected average muon number in measured data as a function of the reconstructed energy interpreted with simulations produced with Sibyll 2.1 without (filled circles) and including (empty circles) background.

Data-MC comparison

Before the analysis of measured data using the two-component reconstruction, it is important to test the consistency of the reconstruction output when applied to data and MC. To ensure reasonable behavior of the reconstruction procedure, the prediction for measured data should be within the physical expected range, i.e., within the extreme cases of cosmic-ray flux assumptions, pure proton and iron. Clearly, the interpretation of measured data depends on the hadronic interaction models used for the production of MC simulations, which is also visible in data-MC comparisons. In Figs. C.2 and C.3, high-level parameter distributions derived from the two-component reconstruction and, for comparison, of the standard reconstruction (see section 4.3.1, are shown for EPOS-LHC and QGSJet-II-04.

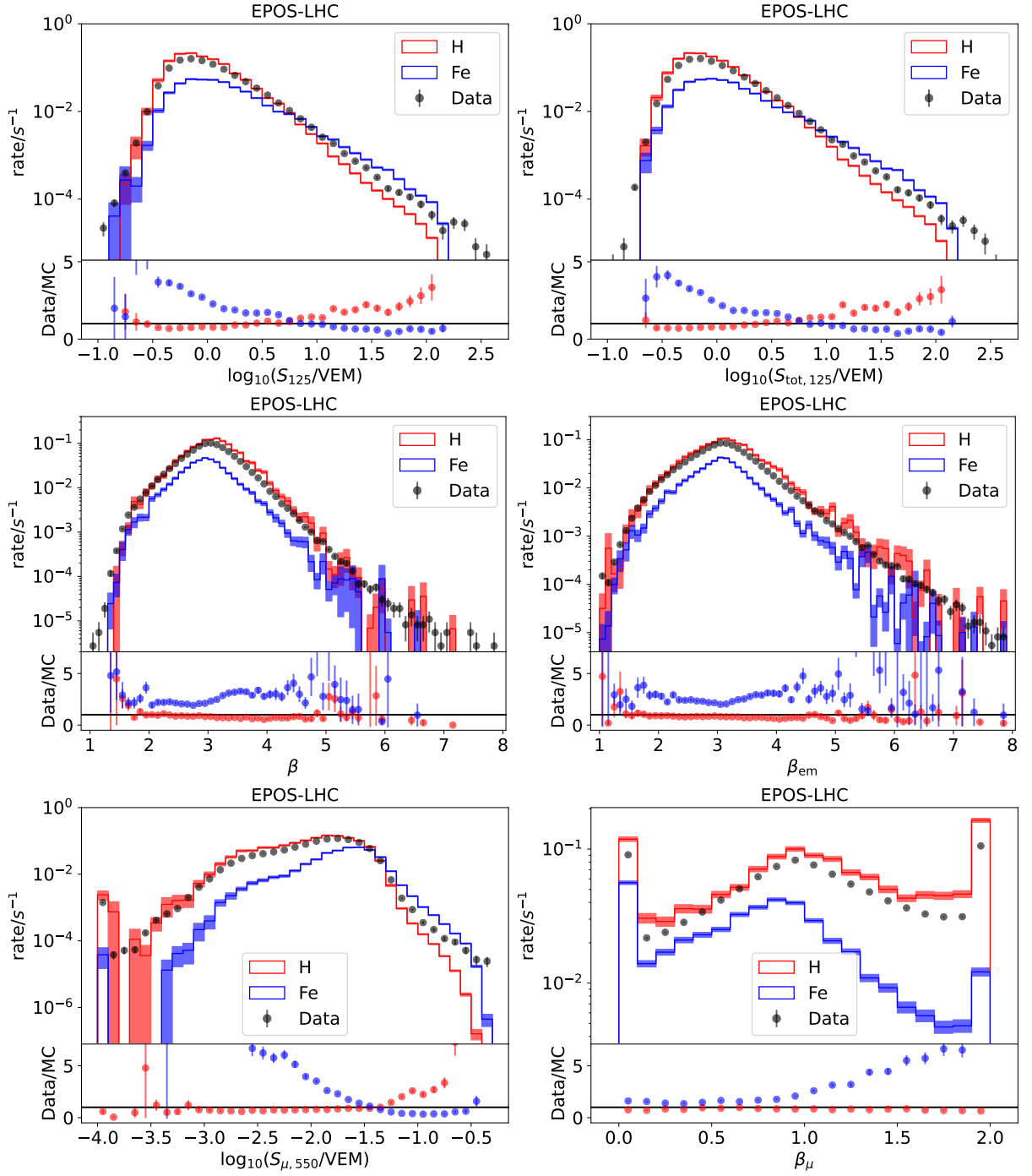


Figure C.2.: Parameter distributions of $S_{\text{tot},125}$, β_{em} , β_{μ} , and $S_{\mu,550}$ obtained for the application of the two-component reconstruction on experimental data and simulations for EPOS-LHC. For comparison, also the parameter distributions for S_{125} and β derived from the standard reconstruction are shown. For all distributions, the quality cuts listed in Tab. 6.4 are applied.

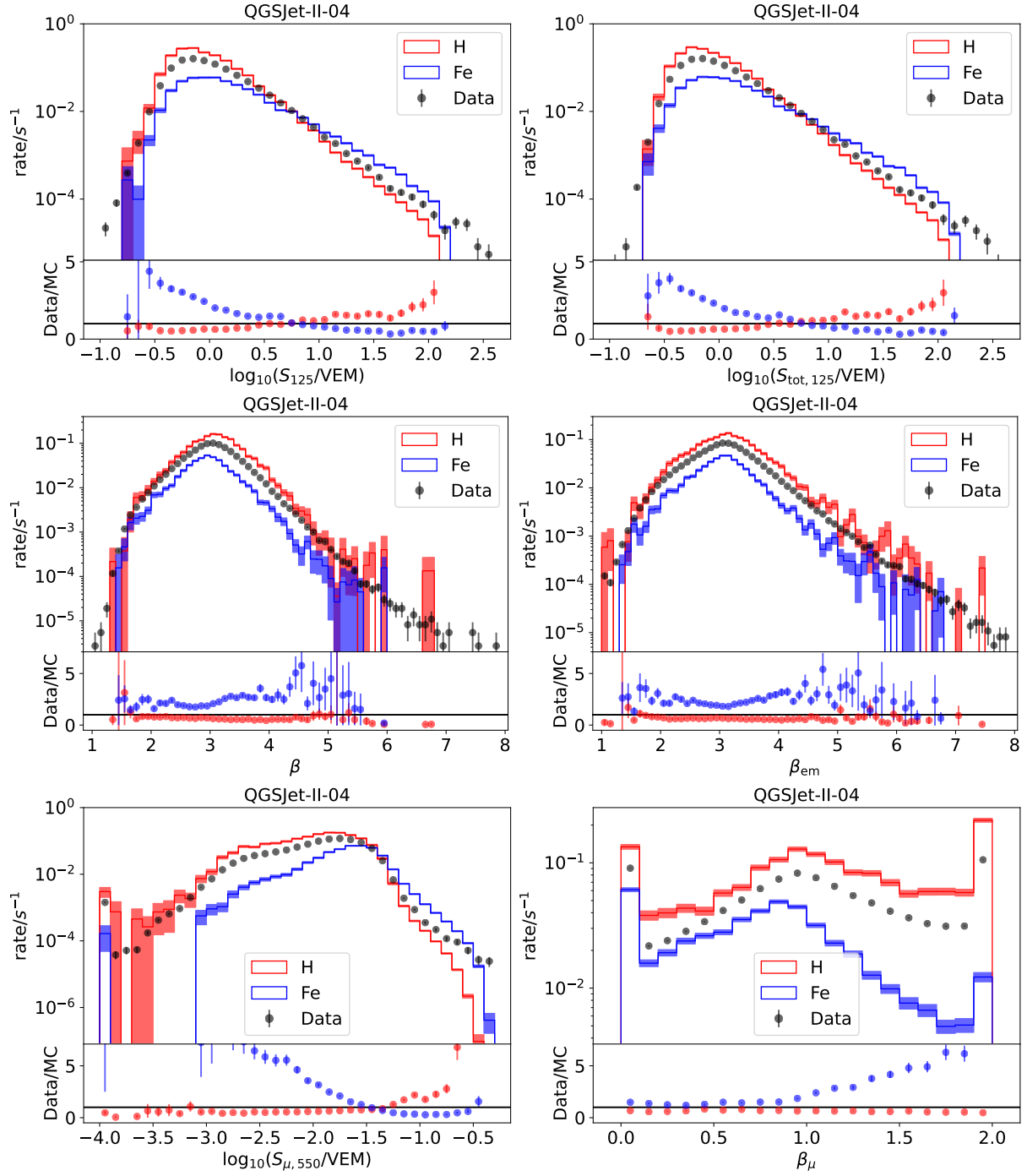


Figure C.3.: Parameter distributions of $S_{\text{tot},125}$, β_{em} , β_{μ} , and $S_{\mu,550}$ obtained for the application of the two-component reconstruction on experimental data and simulations for QGSJet-II-04. For comparison, also the parameter distributions for S_{125} and β derived from the standard reconstruction are shown. For all distributions, the quality cuts listed in Tab. 6.4 are applied.

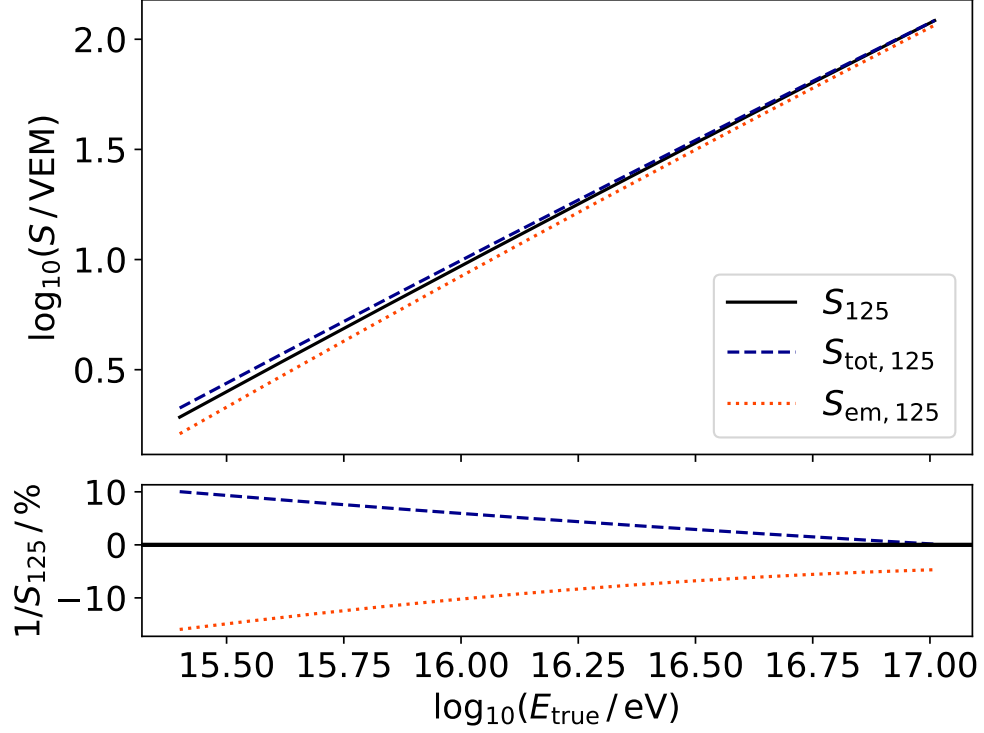


Figure C.4.: Comparison of the energy proxy parameters of the two-component reconstruction, $S_{\text{tot},125}$ and $S_{\text{em},125}$, with the energy proxy of the standard reconstruction, S_{125} , as a function of true primary energy for MC produced with Sibyll 2.1 and weighted to H4a.

Internal consistency

In chapter 8, the internal consistency in the prediction of the average composition of different hadronic interaction models is tested. The analysis includes new composition-sensitive parameters obtained from the two-component model (see chapter 6) and previous parameters obtained on the basis of the standard IceTop reconstruction. Since the two-component reconstruction employs a different energy proxy ($S_{\text{tot},125}$) compared to the standard reconstruction (S_{125}), the respective energy scale differs slightly. To gauge the difference between the energy proxies, their evolution as a function of the true energy is shown in Fig. C.4. For the lowest energies considered, $S_{\text{tot},125}$ is about 10% larger compared to S_{125} . This difference reduces to the sub-percent level toward 100 PeV.

Systematic uncertainty

For the estimation of the systematic uncertainty introduced due to the composition assumption used in the reconstruction of the primary energy and muon number via a calibration fit (see sections 7.1 and 7.2), different realistic cosmic-ray flux assumptions are compared. Since the simulation set produced with Sibyll 2.1 is the only one containing also the intermediate primaries, first, the influence of the presence of helium and oxygen on the calibration fit is quantified. Fig. C.5 shows the reconstructed average muon number as a function of energy after application of the correction introduced in section 9.2 for different flux assumptions. Generally, for Sibyll 2.1, the fluctuations with respect to H4a are at maximum of the order of $+2\% / -5\%$. When excluding intermediate primaries, the fluctuations can increase slightly. Therefore, a more conservative relative uncertainty of $+3\% / -6\%$ is assigned. For a conservative estimation of the systematic uncertainty connected to the composition assumption, therefore, a similar margin is applied for the post-LHC models. The corresponding systematic uncertainty for EPOS-LHC and QGSJet-II-04 therefore amounts to $+5\% / -6\%$ and $+6\% / -6\%$, respectively.

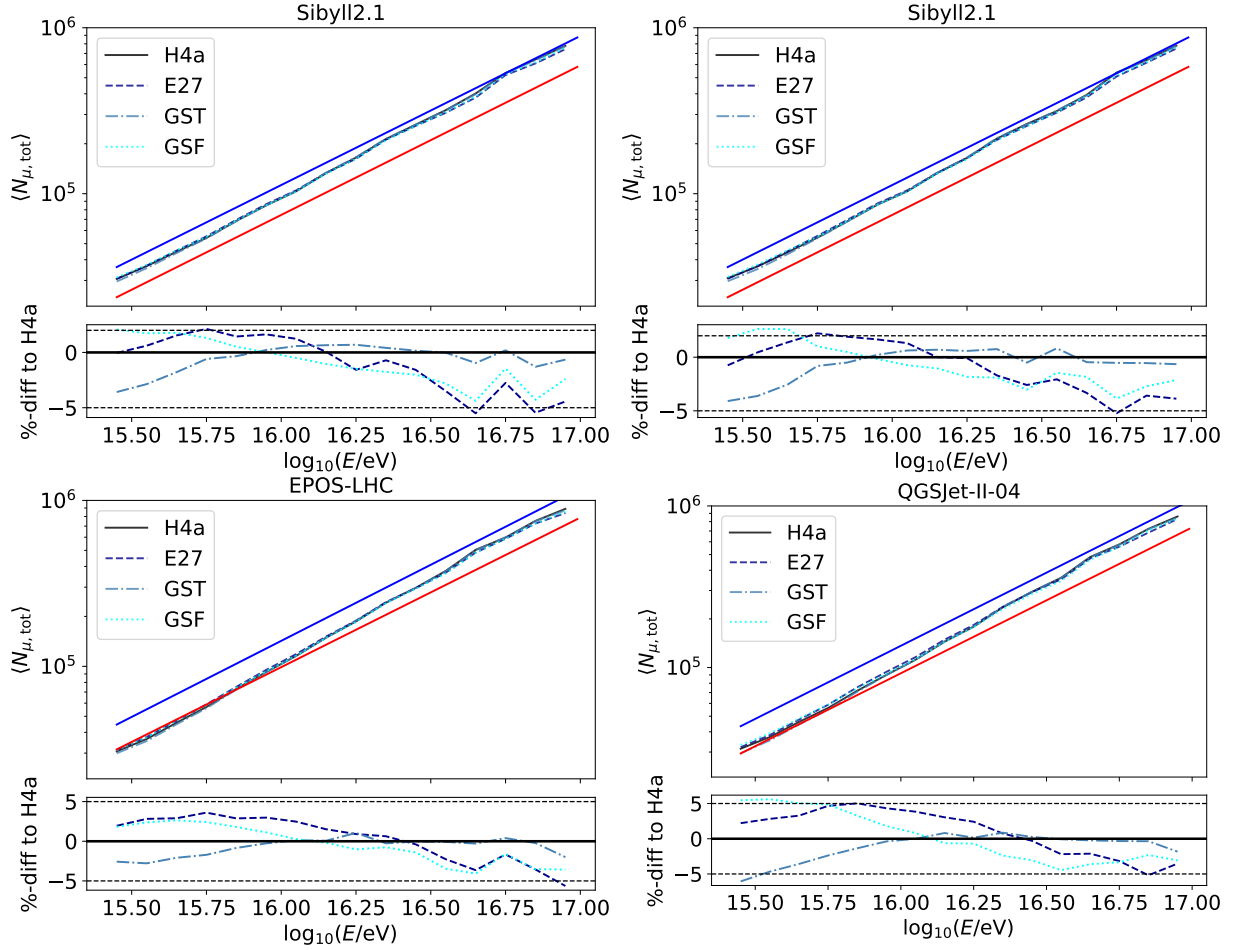


Figure C.5.: Influence of the composition assumption on the reconstruction of the average muon number as a function of energy. Included are the modern flux model assumptions H4a, GST, and GSF as well as a weighting with a spectral index of 2.7. The results for Sibyll 2.1 are shown with (top left) and without (top right) the inclusion of the intermediate primaries helium and oxygen. The post-LHC models EPOS-LHC and QGSJet-II-04 are shown in the bottom row. To guide the eye, additional horizontal lines are drawn in the lower panels at +2% & -5% for Sibyll 2.1 and $\pm 5\%$ for the post-LHC models.

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