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INCREASE: An updated model suite to study the INfluence of Cosmic Rays on Exoplanetary AtmoSpherEs

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Abstract

Exoplanets are as diverse as they are fascinating. They vary from ultrahot Jupiter-like low-density planets to presumed gas-ice-rock mixture worlds such as GJ 1214b or worlds as LHS 1140b, which features twice the Earth's bulk density. Regarding the great diversity of exoplanetary atmospheres, much remains to be explored. For a few selected objects such as GJ1214b, Proxima Centauri b, and the TRAPPIST-1 planets, the first observations of their atmospheres have already been achieved or are expected in the near future with the launch of the James Webb Space Telescope envisaged in October 2021. However, in order to interpret these observations, model studies of planetary atmospheres that account for various processes—such as atmospheric escape, outgassing, climate, photochemistry, as well as the physics of air showers and the transport of stellar energetic particles and galactic cosmic rays through the stellar astrospheres and planetary magnetic fields—are necessary. Here, we present our model suite INCREASE, a planned extension of the model suite discussed in Herbst, Grenfell, et al. (2019).

KEYWORDS

atmospheres, biosignatures, cosmic rays, habitability

1 | INTRODUCTION

Exoplanetary diversity is as fascinating as it is wide-ranging. Bulk properties range from low-density ultrahot Jupiters (Gaudi et al. 2017) up to worlds such as LHS 1140b with over twice Earth's density (Dittmann et al. 2017). The mass-radius relation (see, e.g., Zeng et al. 2016) suggests that the planetary mass can vary widely for a given radius, and vice-versa covering sizes from sub-Earth up to several Jupiter radii. Thereby of particular interest is the proposed *Neptunian desert* (Mazeh et al. 2016) a region close to a star missing Neptune-sized (>0.1 M_{Earth}) exoplanets, and a radius gap between the population of terrestrial Super-Earths and Mini Gas Planets known as the *Fulton gap* (Fulton et al. 2017). However, interpreting this newly emerging, breathtaking phenomena requires knowledge of diverse processes such as planetary formation, migration, atmospheric escape, outgassing, climate, and photochemistry. A central task is to apply numerical models to understand the interplay of these processes and how they influence the observed planetary diversity. Regarding atmospheric diversity, Leconte et al. (2015) and Grenfell et al. (2020) reviewed the possible range of atmospheric compositions and masses.

Hu & Seager (2014) applied a chemical column model to study hydrogen-dominated atmospheres (based on primordial accretion models and mini gas planets, carbon dioxide atmospheres (based on rocky planets in the Solar System), and steam atmospheres (based on early Hadean Earth). Their study, however, used a fixed temperature profile without interactive climate calculations. Several model studies such as, for example, von Paris et al. (2013) and Kitzmann et al. (2015) investigated radiative effects of CO_2 in the context of habitability. Further, numerous coupled climate-chemistry column models have been applied to investigate Earth-like N_2—O_2-dominated atmospheres (see, e.g., Herbst et al. 2019a; Kozakis & Kaltenegger 2019; Rugheimer et al. 2015; Segura et al. 2010). Some model studies also investigate coupled interior-atmospheric processes (Godolt et al. 2019; Noack et al. 2014).

A key emerging concept is the importance of the incoming radiation field for shaping exoplanetary diversity. This field consists of, for example, stellar X-rays and UV photons, and energetic particles essentially consisting of two types: Galactic cosmic rays (GCRs) from supernova remnants (see, e.g., Büsching et al. 2005) and stellar energetic particles (SEPs) carried into the interplanetary field by the stellar wind or accelerated to high energies by coronal mass ejections (CMEs) and stellar flares (e.g., Buccino et al. 2007; France et al. 2013). Since the stellar magnetic field is frozen into the stellar wind, a region around a star that is filled by plasma of stellar origin is being built up (see, e.g., Wood et al. 2005). Like the heliosphere, such astrospheres protect the stellar environment and, thus, (exo-)planets against the isotropically distributed GCR flux. The extension of the astrosphere, and thus the amount of protection, is determined by the stellar magnetic field strength, the stellar wind, and the interstellar medium. Knowing the stellar characteristics and the radiation environment and, thus, modeling the radiation exposure on the planetary surface is crucial to assess its habitability. In addition to the stellar magnetic field, (exo)planetary magnetic fields, if present, also may protect against SEPs and the stellar wind.

The following text discusses briefly the modulation of cosmic rays by stellar astrospheres, planetary magnetic fields, and planetary atmospheres. We include a general overview and discuss recent studies.

1.1 | Cool star astrospheres and cosmic rays within

As discussed in Herbst et al. (2020b) not all cool stars may have massive astrospheres: Based on 3D magnetohydrodynamic (MHD) modeling utilizing the CRONOS code (e.g., Kissmann et al. 2018) the astrosphere of Proxima Centauri was suggested to be comparable in size to the heliosphere. At the same time, LHS 1140 may only drive an astrosphere which may fit well within the orbit of Neptune.

Further, the transport of GCRs through an astrosphere depends on its volume, structure, and turbulent state, which are governed by, for example, the stellar type, rotation rate, the stellar wind dynamics, the stellar activity, the magnetic field as inner boundary conditions, and the local interstellar spectrum as an outer boundary condition. Based on 1D Stochastic Differential Equation (SDE, e.g., Strauss & Effenberger 2017) modeling, Herbst et al. (2020b) further showed that GCRs in the astrospheres of both M-stars most likely significantly impact the exoplanetary atmospheres and thus their habitability.

In addition, previous studies suggested that strong solar (magnetic) activity can cause particle acceleration, particularly for protons and for electrons and heavier ions in the solar corona to energies ranging from tenths to several GeV (Marsch 2006). Such high energetic particles can have a significant impact on the composition of the terrestrial middle atmosphere (the region between tropopause and mesopause), and particularly hard spectral events can even be measured on the Earth's surface (see, e.g., Shea & Smart 2000). Such events, also known as *Ground Level Enhancements* GLEs, are also anticipated to occur in exoplanetary atmospheres. However, the SEP flux close to the exoplanet is currently not observable in contrast to that near the Earth. Therefore, Herbst et al. (2019c) updated the well-known solar relation between the solar X-ray flux and the solar peak proton flux to the cool star regime, providing, for the first time, best- and worst-case scenarios of the expected stellar proton fluxes around rocky planets orbiting (active) G-, K-, and M-stars. In addition, in INCREASE we will update the SDE-based model by Strauss & Fichtner (2015) to also compute stellar particle spectra numerically.

1.2 | Planetary magnetospheric and atmospheric shielding

Planetary magnetic fields may also act as rigidity (momentum per charge) filters for CRs: Low-rigidity particles are scattered back to interplanetary space so that the CR flux at the top of the atmosphere depends on the magnitude and geometry of the planetary magnetic field (see, e.g., Herbst et al. 2013). We note that rocky exoplanets may be tidally locked, which may lead to weaker magnetic fields (Grießmeier et al. 2009). Cohen et al. (2014) suggested that the magnetospheric structure of habitable planets orbiting

M-dwarf stars could be widely different from that of the Earth since potentially strong Joule heating due to strong stellar winds can impinge on the upper planetary atmosphere (the region above the mesopause).

Energetically charged particles entering a planet's atmosphere will lose most of their energy due to collisions with gas-phase species. With increasing atmospheric depth, the likelihood that energetic CRs collide with the atmospheric species increases. Secondary particles form a beam of scattered secondary energetic electrons, or, if the energy of the primary precipitating particle is large enough to initiate nuclear reactions, and atmospheric air showers (Dorman et al. 2004). As the particles lose their energy on their way through the atmosphere, a sufficiently dense atmosphere will efficiently shield the surface from potentially harmful radiation.

A critical quantity describing the effect of energetic particles on life is the radiation dose (see, e.g., Horneck 2001; Zeitlin et al. 2011) which depends on both the atmospheric density and the particle species. Thus, it is essential to calculate the radiation environment for different atmospheres and different particles such as muons, neutrons, protons, electrons, gamma rays, and even heavy nuclei (see, e.g., Banjac et al. 2019a). Recently, the impact of CRs on the formation of secondary particles, ionization and radiation dose in the terrestrial, Martian, and Venusian atmospheres have been discussed, for example, in Banjac et al. (2019b), Guo et al. (2019), and Herbst et al. (2020a); Herbst et al. (2019a), respectively.

1.3 | Cosmic-ray-induced ion and neutral chemistry

Energetic particles precipitating into planetary atmospheres will collide with atmospheric constituents, leading to excitation, dissociation, and ionization of the atmospheric species. In CO_2-dominated (Venusian/Mars-like) atmospheres, ions and excited-state dissociation products of CO_2 would likely be the primary products, for example, CO_2^+, CO^+, C^+, and O^+ (Molina-Cuberos et al. 2001, 2002). In N_2—O_2 dominated (modern Earth-like) atmospheres, the most abundant species are N_2, O_2, in the Thermosphere also $O(^3P)$, and reaction products are excited atomic states such as $N(^2D)$ and $O(^1D)$, or ions such as N_2^+, O_2^+, or O^+ (Nieder et al. 2014; Sinnhuber et al. 2012; Sinnhuber & Funke 2019). Excitation and ionization of the atmosphere lead to chains of very fast chemical reactions significantly affecting the atmospheric composition.

In an Earth-like atmosphere, primary excitation and ionization leads to the formation of neutral reactive radicals such as NO, H, and OH. These contribute to catalytic reaction chains such as:

$$NO + O_3 \rightarrow NO_2 + O_2, \quad (1)$$

$$NO_2 + O\left(^3P\right) \rightarrow NO + O_2, \quad (2)$$

which overall destroy ozone. Since ozone is the main contributor to stratospheric radiative heating, this leads to changes in the net radiative heating and cooling rates (e.g., Sinnhuber et al. 2018), which can affect atmospheric temperatures and circulation down to the surface. Catalytic reaction chains are well as sources of nitric oxides NOx (NO, NO_2) and ozone loss in the Earth's middle and upper atmosphere, particularly related to large solar particle events following solar CMEs (e.g., Jackman et al. 2000, 2001, 2009) and electron precipitation related to geomagnetic storms and auroral substorms (e.g., Funke et al. 2014; Sinnhuber et al. 2018; Sinnhuber et al. 2016; P. T. Verronen et al. 2011) see also recent review by Sinnhuber & Funke (2019). Large ion clusters usually are typically formed by incorporating molecules such as H_2O, HNO_3, N_2O_2, or HCl, hence changing the partitioning of hydrogen, nitrogen-, and chlorine-containing species (e.g., P. Verronen et al. 2008; Winkler et al. 2009), also affecting the O_3 content. Such processes have been reviewed, for example, by Sinnhuber et al. (2012) and Sinnhuber & Funke (2019) for the atmosphere of Earth.

For rocky exoplanets only a few studies addressing air shower physics in Earth-like atmospheres exist (e.g., Grenfell et al. 2012; Scheucher et al. 2018; Tabataba-Vakili et al. 2016). Herbst et al. (2019b) discussed for the first time a model suite developed to model the impact of GCRs and SEPs on exoplanetary atmospheres. A first exoplanetary application has been discussed in Scheucher et al. (2020a).

2 | INCREASE

Figure 1 shows the interplay between physical and chemical effects in our model suite, which are further discussed at the end of this section. The following text discusses the models used and, where applicable, updates to the model suite discussed in Herbst et al. (2019b).

2.1 | PLANETOCOSMICS

PLANETOCOSMICS, the GEANT4-based simulation code developed by Desorgher et al. (2006), is utilized to model the transport of CRs in planetary magnetic fields.

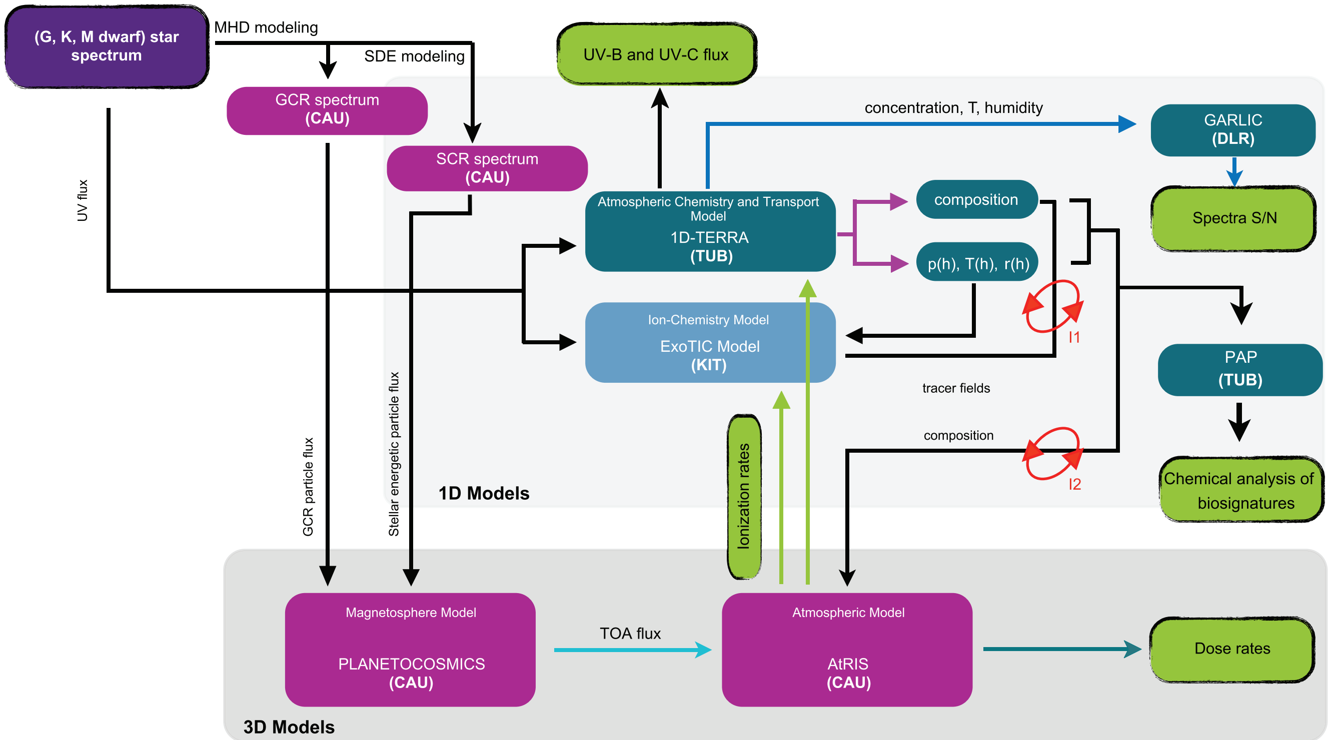

FIGURE 1 Interplay and output of our updated model suite INCREASE (based on figure 3 of Herbst Grenfell, et al., 2019). Purple boxes highlight parts derived and utilized at the University of Kiel (CAU), petrol ones represent the models utilized by DLR Berlin and the Technical University Berlin (DLR/TUB). The blue box represents the ExoTIC model maintained at the Karlsruher Institute of Technology (KIT). Green boxes show the output of our model suite

2.2 | AtRIS

The *Atmospheric Radiation Interaction Simulator (AtRIS)* is a GEANT4-based code recently developed by Banjac et al. (2019b) to compute the hadronic and electromagnetic interactions of energetic particles within planetary atmospheres, enabling simulations of the atmospheric (a) secondary particle environment, (b) ionization, and (c) radiation dose of arbitrary exoplanetary atmospheres over a wide variety of conditions.

2.3 | ExoTIC

ExoTIC is an adapted version of the University of Bremen Ion Chemistry column model (UBIC Nieder et al. 2014; Sinnhuber et al. 2012; Winkler et al. 2009). It is a state-of-the-art 1D stacked box model of the neutral and ion atmospheric composition initially developed to investigate the impact of energetic particle precipitation on ion and neutral chemistry in the terrestrial D- and E-regions. *ExoTIC* considers 60 neutral and 120 charged species, which interact due to neutral, neutral-ion, and ion-ion gas-phase reactions, as well as photolysis and photo-electron attachment and detachment reactions (see, e.g., Sinnhuber et al. 2012). The *ExoTIC* model extends the applicability of UBIC to atmospheres of (rocky) planets other than Earth.

2.4 | 1D-TERRA

The 1D-TUB model utilized in the model suite discussed in Herbst et al. (2019b) has been significantly updated to the new 1D Terrestrial Climate-Chemistry (1D-TERRA) column model (Scheucher et al. 2020b). The radiative scheme was recently updated significantly for the study of a wide range of exoplanetary atmospheric compositions up to temperatures of 1,000 K and pressures of 1,000 bar (e.g., Scheucher et al. 2020a). The new module is based on the k-distribution method using the correlated-k approach with the random overlap technique for the frequency integration between $\nu = 10^5\,\mathrm{cm}^{-1}$ (100 nm) and $0\,\mathrm{cm}^{-1}$ (∞), and the δ-two-stream approximation for the angular integration. In the visible and infra-red, we can choose from 20 absorbers and can add up to 81 UV/visible cross-sections; in addition, Rayleigh scattering and various continua can be added flexibly. Convective adjustment to a dry or wet adiabatic lapse rate can be performed for the condensible H_2O and CO_2, and the water profile can be parameterized following Manabe & Wetherald (1967) for planets with ocean reservoirs. The chemistry module of *1D-TERRA* was also recently updated (Wunderlich et al. 2020). The flexible chemical network now consists of 1,127 reactions for 115 species, including photolysis for 81 absorbers. The scheme can consider wet and dry deposition and biomass, volcanic, and lightning emissions and features an adaptive eddy-diffusion coefficient profile based on atmospheric conditions. For the photochemical effects induced by the precipitating high-energy cosmic rays, we have two possibilities, namely (a) an air shower approach using the Gaisser-Hillas method, as discussed in Tabataba-Vakili et al. (2016) and further developed as described in Scheucher et al. (2018), and (b) direct processing of the CR-induced ionization rate of the atmosphere as calculated by *AtRIS* and the CR-induced chemical production rates of atmospheric molecules calculated by *ExoTIC*. In both approaches, the photochemistry module then incorporates atmospheric profiles of these elaborate CR-induced changes in composition. The chemistry routine can also include biogenic and source gas emissions. Since we do not explicitly include an ion chemistry network in the *1D-TERRA* climate-chemistry column model, the effects of ion chemistry for exoplanetary scenarios are parameterized in our model by using input from *ExoTIC*.

2.5 | GARLIC

For spectral analysis, we use the *Generic Atmospheric Radiation Line-by-line Infra-red Code* (GARLIC, e.g., Schreier et al. 2014; Schreier et al. 2018a, 2018b). *GARLIC* uses output atmospheric profiles (p, T, composition) from the coupled model suite as input. We use *GARLIC* with the latest cross-section data, which is currently HITRAN 2016 (Gordon et al. 2017), MT_CKD continua for H_2O (currently in version 3.2[1]) derived from Mlawer et al. (2012), visible and near infra-red (IR) cross sections from the Mainz Spectral Atlas (Keller-Rudek et al. 2013), and Rayleigh scattering parameterization from Sneep & Ubachs (2005), Marcq et al. (2011) and Murphy (1977).

To build INCREASE, a close collaboration between KIT, DLR, and CAU is mandatory, and the following steps presented in Figure 1 are performed:

1. Measured stellar UV fluxes and the results of the *MHD* and *SDE* modeling are used as input for the *1D-TERRA* and *ExoTIC* models as well as to estimate the incoming cosmic ray fluxes at the close-in exoplanets, respectively.
2. The CR transport within the planetary magnetosphere is studied by utilizing *PLANETOCOSMICS* in order to provide top-of-the-atmospheres (TOA) particle fluxes as input for the computations performed with *AtRIS*.
3. Modeling of both the GCR and SEP induced altitude-dependent atmospheric ionization and the resulting atmospheric dose rates down to the exoplanetary surface by utilizing *AtRIS*.
4. Calculation of the surface UV-A, UV-B, and UV-C exposure with *1D-TERRA*.
5. Determination of the impact of changing atmospheric ionization for the different atmospheric compositions and parameterization of the neutral atmosphere (*1D-TERRA* and *ExoTIC*).
6. Parameterization of the neutral-ion chemistry and computation of the resulting atmospheric composition and climate (*1D-TERRA*).
7. Performance of a pathway analysis (utilizing the Pathway Analysis Program by Lehmann 2004) in order to understand the biosignature chemical responses.
8. Utilization of the global atmospheric composition and temperature fields to compute atmospheric transit (primary) and emission (secondary) spectra with GARLIC.

To ensure consistency between the calculations of *1D-TERRA*, *ExoTIC*, and *AtRIS*, we perform iterations between their output until the results converge (see red circles I1 and I2).

3 | PROJECT-RELATED INVESTIGATIONS

In the near future, we will consider CO_2, H_2, H_2O, and N_2—O_2 dominated exoplanetary atmospheres with a focus on key systems such as Proxima Centauri b, the TRAPPIST-1 planets, LHS-1140b, and K2-18b and will vary initial atmospheric masses ranging from 1 Earth mass up to 10 Venus masses. We will perform evolutionary temporal snapshots equally spaced over the age of the system varying key uncertainties like the CR fluxes. Further, we will calculate observables such as planetary radius, atmospheric albedo, as well as photometric and spectroscopic output by applying our updated unique model suite discussed above.

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