Assessment of site-specific greenhouse gas emissions of chemical producers: case studies of propylene and toluene diisocyanate

Richard C. Müller[(a)], Andreas Schiessl[(a)], Rebekka Volk[(a)], Frank Schultmann[(a) (b)]

[(a)] Karlsruhe Institute of Technology (KIT), Institute for Industrial Production (IIP)
[(b)] University of Adelaide, Entrepreneurship, Commercialisation and Innovation Centre

Abstract

The chemical industry accounts for 20% of global industrial greenhouse gas (GHG) emissions and the plastics production is increasing worldwide by approx. 4% annually. To reduce GHG emissions and increase GHG transparency in chemical value chains despite industrial secrets, we developed an approach to estimate the product carbon footprint of chemicals site-specifically without using classified production data. The new approach, is applied to two comparative case studies: propylene and toluene diisocyanate (TDI) production in Germany. The case study analyses 23 crackers on 17 production sites and four TDI production sites in Germany. The results indicate significant GHG emissions variations between productions sites (Cradle-to-Gate) that could not be quantified before. Among the production sites, product-specific GHG emissions range between 0.95 and 1.51 $kgCO_2e/kg$ propylene (reduction potential of GHG emissions of 37.1%) and between 3.17 and 3.62 $kgCO_2e/kg$ TDI (reduction potential of GHG emissions of 12.4%). This indicates massive differences in GHG efficiency in the production of propylene and TDI and an immense GHG emission reduction potential in the manufacture of plastic-intensive products (e.g. in the automotive sector) by increased transparency and informed supplier selection and procurement decision making. The method is transferable to chemical sites worldwide and indicates an even higher GHG reduction potential worldwide.

Highlights

- New, generic and transferable method to estimate the carbon footprint of basic chemicals on a site-specific basis
- Method is applicable to all chemical sites and to all basic chemicals
- German propylene production shows a reduction potential of GHG emissions of 37.1%
- German toluene diisocyanate (TDI) production shows a reduction potential of GHG emissions of 12.4%

Keywords: LCA; CO_2e; carbon footprint; chemical industry; petrochemistry; product assessment; energy efficient production

Abbreviations

BAT	Best-Available Technique
CO_2e	CO_2 equivalent
DNT	Dinitrotoluene
$ECCO_2$	Evaluation tool to Compare CO_2e emissions
FCC	Fluid catalytic cracking
GHG	Greenhouse gas
GWP	Global warming potential
HVCs	High value petrochemical products from crackers (High Value Chemicals)
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
NI	Nelson index
PCF	Product Carbon Footprint
SC	Steam cracking
SEC	Specific energy consumption
SEF	Specific emission factor
TDA	Diaminotoluene
TDI	Toluene diisocyanate
VBA	Visual Basic for Applications

Nomenclature

Symbol	Definition	Symbol	Definition
$p \in \{1, \dots, P\}$	Set of all products. P is the final product up to which the emissions can be calculated product-specifically	$GWP_{p,s}^{\text{Steam}}$	GWP resulting from steam consumption for the production of p at site s [$kgCO_2/kg$]
$s \in \{1, \dots, S\}$	Set all modelled production sites.	$GWP_{p,s}^{\text{Elec}}$	GWP resulting from electricity consumption for the production of p at site s [$kgCO_2/kg$]
$c \in \{1, \dots, C\}$ $C \sqsubseteq \{1, \dots, P\}$	Set of all cracker products	$GWP_{p,s}^{\text{Fuel}}$	GWP resulting from fuel consumption for the production of p at site s [$kgCO_2/kg$]
$b \in \{1, \dots, B\}$	Set of all types of fuels	$SEC_{p,s}^{\text{Steam}}$	Specific energy consumption of steam generation to produce product p in site s [GJ/t p]
$x \in \{1, \dots, X\}$	Set of all modelled crackers	$g_{b,s}^{\text{Steam}} \in [0; 1]$	Share of a fuel b at production site s to generate steam [%]
$x \in X_{FCC}$ $X_{FCC} \sqsubseteq \{1, \dots, X\}$	Set of all FCC-crackers	$SEF_{b,s}^{\text{Steam}}$	Emission factor of fuel b used to generate steam at site s [$kgCO_2e/kWh$]
$f \in \{1, \dots, F\}$	Set of all raw types of feedstock in cracker	$\eta_s^{\text{Steam}} \in [0; 1]$	Efficiency of steam generation in site s [%]
$e \in \{1, \dots, E\}$	Set of all educts	$EFF_{p,s}^{\text{Site, Prod}} \in [0; 1]$	Efficiency of production of product p at site s [%]
$z \in \{1, \dots, Z\}$	Set of all intermediate products (intermediates)	$SEC_p^{\text{Steam, Ecoinvent}}$	Specific energy consumption of steam generation for the production of p based on Ecoinvent database (natural gas) [MJ/kg]
$h \in \{1, \dots, H\}$	Set of all main products	SEF_s^{NG}	Emission factor of natural gas at site s [$kgCO_2e/kWh$]

$y \in \{1, \dots, Y\}$	Set of all by-products
$E \subseteq Z, H \subseteq \{1, \dots, P\}$	Educts are a subset of all intermediates and main products. Intermediates and main products are a subset of all products.
$Edc_e \in Edc$	Set of all educts in which all educts are described by name
$CrPr_c \in CrPr$	Set of all cracker products in which all cracker products are described by name
$ImPr_z \in ImPr$	Set of all intermediates in which all intermediates are described by name
$MPr_h \in MPr$	Set of all main products in which all main products are described by name
$GWP^{\text{Ecoinvent}}$	Set containing the GWPs [in $kgCO_2e/kg$] of educts and products from the Ecoinvent V.2.2 database
$GWP^{\text{Ecoprofiles}}$	Set that contains the GWPs [in $kgCO_2e/kg$] of products and products from PlasticsEurope's Eco-profiles
$SEC_p^{\text{Elec, min}}$	Minimum specific consumption of electrical energy to produce product p [GJ/t]
$SEC_p^{\text{Fuel, Ecoinvent}}$	Specific energy consumption of fuels for production of p according to Ecoinvent [MJ/kg]
$GWP_{p,s}^{\text{Prechain}}$	GWP of processes in the upstream chain for the production of product p at site s [$kgCO_2e/kg$]
SEF_s^{Fuel}	Emission factor of the fuels which are used in site s [$kgCO_2e/kWh$]
$SEF_s^{\text{Fuel,SuppData}}$	Emission factor for fuels of site s, if primary data are available [$kgCO_2e/kWh$]
$SEF_{x,s}^{\text{HVC}}$	Emission factor of the raw materials used in cracker x in site s for the production of HVCs in [$kgCO_2e/kWh$]
A	Sum of crackers in all production sites implemented in the model (equals X)
A_s	Number of crackers in production site s
β	Correction value ($\beta = 10^6$) for the calculation of A_s, if $SEF_{x,s}^{\text{HVC}}$ has very small values
$SEC_p^{\text{Fuel, max}}$	Maximum specific energy consumption of fuels for the production of p [GJ/t]
$SEC_p^{\text{Fuel, min}}$	Minimum specific energy consumption of fuels for the production of p [GJ/t]
w^{INTL}	Weighting of the level of integration to calculate production efficiency [%]
w^{INNL}	Weighting of the level of integration to calculate production efficiency [%]
$SEC_p^{\text{Steam, max}}$	Maximum specific energy consumption of steam generation to produce product p [MJ/kg]
$SEC_p^{\text{Steam, min}}$	Minimum specific energy consumption of steam generation to produce product p [MJ/kg]
$SEC_{p,s}^{\text{Elec}}$	Specific energy consumption of electrical energy for the production of product p in site s [GJ/t]
$w_s^{\text{Elec, selfprod}}$	Share of self-generated electrical energy at the site s [%]
$SEC_p^{\text{Elec, Ecoinvent}}$	Specific energy consumption of electricity generation for the production of p according to Ecoinvent database [kWh/kg]
$SEF_{b,s}^{\text{Elec}}$	Emission factor of the fuel b used to generate electricity at site s [$kgCO_2e/kWh$]
$GWP_s^{\text{CountryElecMix}}$	Emission factor of the electricity mix of the country where the production site s is located [$kgCO_2e/kWh$]
η_s^{Elec}	Efficiency of the power plant at production site s [%]
$SEC_p^{\text{Elec, max}}$	Maximum specific consumption of electrical energy to produce product p [GJ/t]
$SEC_{p,s}^{\text{Fuel}}$	Specific energy consumption of fuels for production of product p at site s [GJ/t]
$GWP_{c,x,s}^{\text{Prechain, Cr}}$	GWP of the upstream chain of product c produced in cracker x at site s [$kgCO_2e/kg$]
$SEC_{c,x,s}^{\text{HVC}}$	Specific energy consumption for the production of a product c in cracker x in site s in [GJ/t]
$SEC_x^{\text{HVC, max}}$	Maximum specific energy consumption of cracker x to produce HVCs in [GJ/t]
$SEC_x^{\text{HVC, min}}$	Minimum specific energy consumption of cracker x to produce HVCs in [GJ/t]
$EFF_{c,x,s}^{\text{Cr}}$	Production efficiency of product c in cracker x in site s in [%]
$SEC_f^{\text{FCC,max}}$	Maximum specific energy consumption for FCC crackers, if raw material f is the cracker feed [GJ/t]
SEC_f^{max}	Maximum specific energy consumption for steam crackers, if raw material f is the cracker feed [GJ/t]
f	Raw material/feed type (e.g. ethane, propane, etc.)
$SEC_f^{\text{FCC,min}}$	Minimum specific energy consumption for FCC crackers, if raw material f is the cracker feed [GJ/t]
SEC_f^{min}	Minimum specific energy consumption for steam crackers, if raw material f is the cracker feed [GJ/t]
$w_{x,f}$	Relative shares of the feed f in the cracker x [%]

$w^{\text{LF,FA,UR,etc..}}$	Weighting of the factors/criteria of cracker and production efficiency [%]		$v_x^{\text{UR, Cr}}$	Utilization rate of the cracker x [%]	
$LF_s \in [0;10]$	Location factor of site s		$CrPrC_{c,x}$	Production capacity of product c in cracker x [t/a]	
FA_s	Area of the site s [km²]		$FC_{s,x}$	Total production Site capacity of all products of site s to which cracker x belongs [t/a]	
$Output_{p,s}$	Production quantity of product p in site s [t/a]		$FA_{s,x}$	Site area of site s to which the cracker x belongs [km²]	
$PC_{p,s}$	production capacity of product p in site s [t/a]		$NI_{s,x}$	Nelson index of the production site s where the cracker x is located	
FL_s	Flexibility of production at site s [number of production plants at the site]		$CrAge_x$	Age of the cracker x	
$PY_{p,s}$	Production yield of the product p at site s [%]	-	$SEF_x^{\text{HVC, min}}$	Minimum emission factor of the raw materials used in cracker x to produce HVCs [kgCO2e/kWh]	
LL	Lower limit - is defined for each factor/criterion used to calculate the cracker or production efficiency (e.g. LF_{LL})	%	$SEF_x^{\text{HVC, max}}$	Maximum emission factor of the raw materials used in cracker x to produce HVCs [kgCO2e/kWh]	
UL	Upper limit - is defined for each factor/criterion used to calculate the cracker or production efficiency (e.g. LF_{UL})		$SEF_f^{\min}$	Minimum emission factor of the raw material f fed into the cracker [kgCO2e/kWh]	
$GWP_{c,x,s}^{\text{CrPr}}$	GWP of a high value chemical product c from cracker x in site in [kgCO2e/kg]		$SEF_f^{\max}$	Maximum emission factor of the raw material f fed into the cracker [kgCO2e/kWh]	
$GWP_{c,x,s}^{\text{Energy, Cr}}$	GWP of the consumed energy by cracker x to produce c in site s in [kgCO2e/kg]		CR_x	Raw material conversion rate of the cracker x [%]	
$GWP_{c,x,s}^{\text{Prechain,Cr}}$	GWP of the upstream chain of the product c in cracker x in site s [kgCO2e/kg]		M_e^{Edc}	Molar mass of educt e [kg/mol]	
$GWP_f^{\text{Ecoprofiles}}$	GWP of raw material f from the Eco-profiles of PlasticsEurope [kgCO2e/kg]		$n_{y,p,s}^{\text{byPr}}$	Amount of substance of by-product y produced at site s during the production of product p [mol]	
$GWP_f^{\text{Ecoinvent}}$	GWP of raw material f from Ecoinvent database [kgCO2e/kg]		M_y^{byPr}	Molar mass of by-product y [kg/mol]	
$GWP_{p,s}^{\text{Pr}}$	GWP of product p produced in site s [kgCO2e/kg]		$m_{e,p,s}^{\text{Edc}}$	Mass of educt e required to produce the product p in site s [kg]	
$GWP_{p,s}^{\text{Energy, Prod}}$	GWP of the required Energy to produce p in site s [kgCO2e/kg]		$m_{p,s}^{\text{Pr}}$	Mass of product p resulting from the reaction during production in site s [kg]	
$GWP_{p,s}^{\text{Prechain}}$	GWP of processes in the upstream chain for the production of product p in site s [kgCO2e/kg]		$m_{y,p,s}^{\text{byPr}}$	Mass of by-product y resulting from the reaction during production of p in site s [kg]	
$RE(p,s)$	Reaction equation for the production of product p in site s		M_p^{Pr}	Molar mass of product p [kg/mol]	
$n_{e,p,s}^{\text{Edc}}$	Describes the amount of substance of an educt e required for production of p in site s [mol]		$n_{p,s}^{\text{Pr}}$	Resulting amount of substance of product p when produced at site s [mol]	
$m_{e,y,p,s}^{\text{Edc, byPr}}$	Part of the mass of an educt e that is processed into the by-product y that is produced during the production of p in site s [kg]		$GWP_{e,s}^{\text{Supp, Data}}$	GWP of an educt e in site s if primary data from the supplier is available [kgCO2e/kg]	
$GWP\_PE_{p,s}^{\text{Pr}}$	Energy-related GHG emissions caused in the "Gate-to-Gate" production system to produce product p [kgCO2e/kg]				

47

1 Introduction

Massive anthropogenic emissions of carbon dioxide and other greenhouse gases (GHG) are regarded as one of the main causes of climate change on Earth (IPCC, 2013). The Paris Climate Convention of 2015 set the goal of limiting global warming to 1.5°C to 2°C compared to the pre-industrial level (European Commission, 2015). To ensure comparability of the GHG's impact on global warming, all emissions are standardized to CO_2 equivalents (CO_2e) (IPCC, 2013).
To achieve these objectives, transparency and appropriate incentives and instruments must be created such as a CO_2 emission tax[1] or an effective emissions trading system (Mihatsch, 2014).

According to Christian Doppler Research Association in Vienna, approximately 100 large international corporations already use internal CO_2 prices as a preliminary stage to take account of this possible financial "risk" in their operations or investments (Mihatsch, 2014). A fixed pricing of CO_2 for all industrial companies will have a major influence on the decision making along the entire value chain, e.g. in material selection or the planning of the production chain. By taking a CO_2 tax into account, procurement or manufacturing costs could suddenly be reduced by choosing other suppliers or manufacturing processes that were previously too expensive from a purely economic point of view. Especially in the automotive industry, there are specific considerations to reduce CO_2 emissions in the value chain of vehicle production. Possible approaches are, for example, the consideration of CO_2 emissions in transport, in supplier development or in supplier selection (MHP, 2016). In addition, the European Commission has identified the embedded emissions for vehicle manufacturing as one future field of activity (EPSC, 2016).

Particularly, the global annual production of steel (6.7%), aluminium (2%) and chemical products (7%) constitute around 16% of the global annual GHG emissions (Hasanbeigi, 2018; Saevarsdottir et al., 2020; World Steel Association, 2014). Basic chemicals and plastics contribute with 20% to the global industrial GHG emissions (Hasanbeigi, 2018) and doubly rely on fossil resources – from a material and energy point of view. Furthermore, the plastics production is increasing worldwide by approx. 4% annually (Statista, 2018).
In order to reduce CO_2e emissions within the manufacturing of products, the selection of more efficient[2] raw material suppliers in procurement may constitute a promising opportunity (MHP, 2016, Schiessl et al., 2020). Especially in procurement, social and ecological factors are becoming increasingly important, apart from cost and quality targets (Büyüközkan, 2012; Guinée et al., 2011; Roy et al., 2009; Schiessl et al., 2020; Zimmer, 2016; Zimmer et al., 2015). A change in current procurement and supplier selection practices is unavoidable, once transparency as well as specific limits and exceedance penalties are established for CO_2e emissions from production. Thus, information on site[3]-specific GHG emissions of raw material production (e.g. steel and chemical production sites) is required (Schiessl et al., 2020). For steel, an approach is available to estimate the carbon footprint of steel production sites (CO_2e/t crude steel) in Europe (Schiessl et al., 2020).
However, for the chemical industry such transparency and site-specific assessment does not exist, yet. This is highly needed due to the increasing relevance of basic chemicals and plastics in global production volumes and their associated GHG emissions. This is a particular challenge due to the complexity of chemical sites, the large number of different products and co-products (Saygin, 2012) and a respective allocation of GHG emissions. In recent decades, chemical sites have grown to integrated chemical parks to increase energy and resource efficiency. For example, the radiating residual heat or by-products of one process is used to preheat, fuel or feed another process to save energy or raw materials (Fleiter et

[1] For example, in Germany a CO_2 tax of 25 €/tCO_2 will apply to petrol, diesel, heating oil and gas starting from 2021 onwards, affecting all citizens and companies in Germany (BMWi, 2019).
[2] Efficient production is defined here as low greenhouse gas emissions and energy-efficient production.
[3] In this study, "site" is the short form for "production site". The term "production site" refers to the entire "plant"/"factory" of a producer. "Plant", "site" and "factory" are therefore used synonymously. However, "plant" must be distinguished from "production plant". In this study "production plant" is one specific production plant (e.g. a cracker) out of many production plants in a chemical plant/site.

al., 2013; Saygin, 2012). In contrast to other industries, not just one but several different products can be produced at the same time (Saygin, 2012), e.g. in steam cracking or chloralkali electrolysis (Fleiter et al., 2013).[4] This increases complexity of GHG emission assessment and assignment considerably. The use of company internal primary data[5] could increase transparency of the complex integrated production systems and thus simplify calculations, but the primary data are usually confidential and not accessible to the public (Saygin, 2012).

This study aims at developing a highly innovative approach to estimate the carbon footprint of basic chemicals on a site-specific basis, without the need of primary producer data. The new generic calculation logic and assessment model is transferable to all chemical sites and to all basic chemicals. The main advantage of the developed assessment model is the provision of transparency regarding GHG emissions within specific chemical value chains on product and site level that is not available today. This transparency can have a game-changing influence in procurement and resulting embodied GWP of manufactured products of the chemical industry. The main contributions of this paper can be summarized as follows:

- Novel, transparent, site-specific and generic assessment method to quantify a site-specific product carbon footprint (instead of average values based on confidential data)
- Transferable assessment method to all chemical sites and to all basic chemicals produced worldwide
- Establishment of a valuable, open database for chemicals PCF assessment
- Increase of transparency in chemical value chains and procurement networks regarding GHG emissions per production site

In the following, the relevant literature on the assessment of GHG emissions in the chemical industry is discussed (chapter 2). This is followed by the research approach and the model concept (chapter 3). The focus of the paper lies in the development of the model (chapter 4), its application on producers for selected basic chemicals as well as the obtained results (chapter 5). Finally, we summarize the most important conclusions (chapter 6).

2 Literature review

A widely used method for evaluating GHG emissions and other environmental impacts of products is Life Cycle Assessment (LCA) (e.g. Rieckhof and Guenther, 2018; Rebitzer, 2002; Klöpffer and Renner, 2008). LCA is standardized in ISO 14040 and 14044 standards and is defined as an environmental management method that systematically assesses the environmental aspects and potential environmental impacts of product systems throughout their life cycle (from raw material acquisition through production, use, end-of-life treatment, recycling and final disposal, i.e. "from Cradle-to-Grave") (ISO, 14040:2006; ISO, 14044:2006).

2.1 Review of LCA and bottom-up analysis methods

In literature, two main LCA methods are distinguished and frequently discussed: the process method (bottom-up) and the input-output analysis (top-down). Both methods can also be combined to so-called hybrid methods (Guinée et al., 2011), which use both bottom-up and top-down data (Zimmer, 2016). In the process method, all environment-related input and output flows of product-specific processes are determined and quantified by a process flow diagram and the defined functional unit (Kndungu and Molavi, 2014; Sonnemann et al., 2004). In contrast, the input-output approach assumes an

[4] This so-called joint production (integrated production) is characteristic of the chemical industry. In chlor-alkali electrolysis for the production of caustic soda, the co-products chlorine and hydrogen are produced. In addition to main products such as ethylene and propylene, steam cracking produces a wide range of other products such as butadiene and pyrolysis benzene (BASF, 2017d; Saygin, 2012; Fleiter et al., 2013).

[5] Company internal primary data are defined here as technically and economically production-related raw data of a producer.

interdependence between the sectors of an economy and uses national economic input–output data in combination with sector-level environmental impacts (Bilec et al., 2006; Leontief, 1936; Suh et al., 2004). A whole economy as a system boundary and aggregated data at sector level is unsuitable for direct comparisons of specific products (Bilec et al., 2006; Suh et al., 2004; Zimmer et al., 2017). The process LCA, however, has the disadvantage that results of the entire LCA depend significantly on the data availability and quality (Bilec et al., 2006; Yellishetty et al., 2011). In addition, researching the required data is very time-consuming and restricted as primary data of the processes are often not or hardly accessible (Saygin, 2012). Due to the lack of primary data (cf. chapter 1), Life Cycle Inventory (LCI) and Life Cycle Impact Assessment (LCIA) databases such as Ecoinvent (e.g. Ecoinvent V2.2, 2007-2013) or GaBi (Thinkstep, 2019) are often used and represent industry average values for specific processes. But, this approach is being criticised as average values can significantly affect LCA results (Lang-Koetz et al., 2006).

In LCA, the evaluation of the environmental impact of a system under study (e.g. life cycle of a product) is carried out in the LCIA using different impact categories (ISO, 14040; 14044), e.g. global warming potential, acidification, ozone depletion (Heijungs and Guinée, 1992). For the LCIA, various impact models[6] exist in literature.

To reduce the above-mentioned time and economic effort of LCA's, various simplification approaches were developed, so-called "simplified LCAs" (S-LCA[7]) or "streamlining" approaches (Graedel and Saxton, 2002; Weitz et al., 1996).[8] Mainly, S-LCA consciously excludes specific phases of the life cycle or focuses on specific impact categories (Hochfeld and Jenseits, 1998; Schrack, 2016), such as the impact category *Global Warming Potential* (GWP) (Schrack, 2016). The GWP is typically considered over a period of 20 or 100 years and expressed in CO_2 equivalents (CO_2e). In the Kyoto Protocol, the GWP over a period of 100 years was defined as the key performance indicator. (IPCC, 2013) When assessing the environmental impact of a products' production, simplification results automatically due to the reduced scope by exclusion of the life cycle phases of *use* and *end-of-life*. Thus, the system boundary of the assessment is usually set to "Cradle-to-Gate", from raw material acquisition to the final product ready for distribution at the producer's factory exit gate.

The association PlasticsEurope[9] publishes regularly updated "Eco-profiles" for many chemical products with LCA "Cradle-to-Gate" information (PlasticsEurope, 2018). PlasticsEurope uses primary data on production processes provided by participating chemical sites in Europe. The individual LCA results (e.g. GWP100 of a product) are confidential and only the average value of the different producers is provided. Furthermore, numerous other "Cradle-to-Gate" studies assess the required energy input and resulting direct and indirect GHG emissions from the production of chemical products (e.g. for olefins)based on detailed techno-ecological analyses. For instance, Ren et al. (2006) assessed and compared different naphtha cracking technologies for olefin production, Xiang et al. 2014 the oil-to-olefins and coal-to-olefins production, Chen et al. 2017 the natural gas-to-olefins (ethylene) and coal-to-olefins (ethylene) production and Amghizar et al. 2017 several different technologies of olefin production based on naphtha, ethane, methane, biomass and coal.

[6] A detailed consideration of possible models can be found in Prammer (2009), who carried out an extensive analysis of available scientifically based environmental impact models. For this study, it should be sufficient to mention the impact assessment method of the "Centrum voor Milieukunde" (CML method), based in Leiden, as this method is also used in the ISO 14040 series. Since the mid-1990s, the CML method has become established in industry and is also the most widely accepted impact assessment model in the scientific community (Prammer, 2009; Schrack, 2016).

[7] Do not confuse this abbreviation with social life cycle assessment approaches (SLCA) in which social impact categories are integrated into the assessment (e.g. Chhipi-Shrestha et al., 2015, Zimmer, 2016 and Zimmer et al., 2017).

[8] Arzoumanidis et al. (2017) showed that the demand from industry and science for simplified LCA is very high: In 2016, there were about 80 new contributions in Scopus and Web of Science , while in 2006 there were only 12. An analysis of almost 20 simplified LCA approaches was published in Pigosso and Sousa (2011), to which reference is made for more detailed information.

[9] PlasticsEurope is a leading pan-European association and represents its member plastics manufacturers (Plastics Europe, 2020).

A very substantial study by Fleiter et al. (2013) investigated the energy consumption for the production of many various basic chemicals via bottom-up analyses. The actual chemical process was regarded as a black box by Fleiter et al. (2013); the focus was on the so-called "secondary energy", i.e. the measuring of input and output flows for electricity, steam and fuel. The input and output flows were transformed into the original form, as primary energy, using up-to-date conversion factors[10]. But in none of the mentioned publications the results are assigned to specific plants or sites of a chemical producer.

2.2 Review of site-specific assessment methods

Literature on the site-specific assessment of GHG emissions shows that there are already numerous studies[11] on site-specific LCAs: Pereira et al. (2013) model and assess the GHG emissions of a petrochemical plant in Brazil in detail with specific producer data (primary data), which rarely are reported/available (see chapter 1). Hannouf and Assefa (2017) conducted an LCA for the production of high density polyethylene for a site in Alberta, Canada, also based on primary data. Kanchanapiya et al. (2015) developed a CO_2 assessment model for seven Thai chemical sites also based on primary data. Although they used site-specific primary data for the calculation, no site-specific but average results were published, which indicates that the site-specific data were classified. Thus, only national Thai average values for selected products are available for international comparison. Zhao et al. (2017) evaluate GHG emissions from four propylene production pathways in China (catalytic cracking (FCC), steam cracking (SC), coal-to-olefins and coal-to-propylene, with CC and SC being petroleum-based processes and coal-to-olefins and coal-to-propylene being coal-based processes). A simplified LCA is carried out for the production phases of raw material extraction, raw material transport, raw material preparation and propylene production. These calculations provide a good comparison of the possible production paths of propylene and show that FCC and SC have the lowest GHG emissions. Zhao et al. (2017) used primary data from several Chinese production sites and average values from the literature (e.g. from Ou et al., 2011 and Wang, 2014).

Although there are many site-specific assessments of GHG emissions of chemical products in literature, there is no site-specific approach that works independently of confidential producer data (primary data). Moreover, by making the primary data anonymous, it is not possible to allocate the studies' results to specific production sites.

Also, numerous studies[12] on site-specific LCAs of basic chemicals have been conducted using flowsheeting simulations. Flowsheeting simulation is a widely used computer-aided instrument to simulate chemical engineering processes (Bauer et al., 2015). The starting point are flow diagrams of the process to be analysed with its basic operations and their material and energy flows (Trippe, 2013). A common software is for example Aspen Plus, which already contains numerous basic operations[13]. Due to the complex parameterisation of these simulation models to realistically simulate the characteristics of the processes under study, the application of flowsheeting simulation is usually limited to smaller observation levels such as individual production plants, processes or production sites (Breun, 2016). A site-specific but at the same time generic calculation logic for the simulation of all chemical sites as desired in this study is not feasible with this instrument (see also Breun, 2016; Fröhling et al., 2009).

2.3 Review of generic site-specific assessment methods

[10] Fleiter et al. (2013) do not provide any further details on the conversion factors. We assume that this refers, for example, to the efficiency of electricity generation, e.g. by a specific power plant (e.g. gas and steam combined cycle power plant).

[11] e.g. Pereira et al. (2013), Hannouf and Assefa (2017), Kanchanapiya et al. (2015) or Zhao et al. (2017)

[12] e.g. Mendivil et al. (2006), Nitzsche et al. (2016), Kikuchi et al. (2017), Bello et al. (2020) or Keller et al. (2020).

[13] such as reactors or those for splitting or heating flows, which can be manually adjusted if necessary.

Only a few site-specific approaches use a generic[14] methodology. Kanchanapiya et al. (2015) developed such a generic CO_2 assessment model, but the model requires primary data. Posen et al. (2015) developed an approach using Monte-Carlo simulation to estimate the GHG emissions from the conventional polyethylene production route via natural gas in the US. However, this approach only provides country-specific values for the US. Therefore, it would be applicable to other countries but not to specific sites. Patel (2003) calculated the cumulative energy demand and the cumulative CO_2 emissions "Cradle-to-Gate" for organic chemical products. He mainly used industrial averages to calculate the energy demand of production processes; to estimate the energy demand of energy generation he integrated a site-specific approach. Furthermore, Patel investigated power plants on German chemical sites to identify which portion of steam and energy is produced for own consumption and how much is purchased. Based on the power plant type, the efficiency of the self-produced electricity is calculated to better estimate the specific energy demand (Patel, 2003).

Only Breun (2016) and Schiessl et al. (2020) developed both a site-specific and generic approach, which also does not require confidential original production data from manufacturers. Breun (2016) developed a model to simulate metal plants on individual process level in order to evaluate future climate policies. The approach combines a non-linear programming model with an input–output model by Leontief (1936) and uses technological restrictions as well as plant specific data on GHG emissions.

Schiessl et al. (2020) follow the model of Breun (2016), but use a sequential step-by-step calculation in contrast to a simultaneous calculation applied by Breun (2016). They developed a combined model based on the process LCA method using both bottom-up and top-down site-specific publicly available data to fill data gaps (Schiessl et al., 2020). However, both methods only cover the iron and steel industry and only work if the reported top-down producer data refer to a single product (e.g. the crude steel produced by a steel mill).[15] In the chemical industry, many different products are produced simultaneously (Saygin, 2012; Fleiter at al., 2013), hence the approach of Breun (2016) cannot be transferred.

2.4 Research gaps

Despite many available product-specific and site-specific LCA studies, only very few approaches with a generic site-specific model have been developed. Such models are heavily dependent on confidential data and therefore cannot be used publicly.

A major research gap is the lack of a generic methodology that enables customers, companies and the public to assess the GHG efficiency of different chemical sites on a product-specific basis using only publicly available data. Particularly, companies in the packaging, construction or automotive sectors, currently have no means to integrate site-specific carbon footprints of products as a criterion in their purchase decision. Site-specific product carbon footprints (PCF) are not reported by chemical producers; only average PCF are available. Thus, it is the question how such a generic evaluation approach could be methodically structured, fed with respective approximate and publicly available data and implemented within real value chains of highly integrated chemical production sites. This arises further challenges of adequate system boundary definition and environmental and economic impact allocation. Furthermore, it is not apparent from the literature whether site-specific assessments play a major role in product carbon footprints (PCF) and how big the site-specific PCF differences of chemical products are. Answers to these questions will play a major role for an increased transparency and the reduction of GHG emissions in industrial value chains in the future by a more informed supplier selection. This contribution is intended to close this research gap.

[14] i.e. one that could be applied to several different sites or different products.

[15] Such top-down data used in Schiessl et al. (2020) are for example the reported GHG emissions of a site, which are published in the EPRTR (European Pollutant Release and Transfer Register of the European Environment Agency e.g. EEA (2007-2016)) and in this case can be linked to the single product "crude steel".

3 Research approach and method

3.1 Energy-based assessment and focus on basic chemicals

In the chemical industry, GHG emissions are almost proportional to final energy consumption and its energy consumption accounts for about 85% of its total GHG emissions (McKinsey, 2006). The calculation of the GHG emissions of a production system for the production of a chemical product is therefore based on an energy-related approach. The required energy is then transformed into GWP respectively into CO_2e via emission factors (e.g. [$kgCO_2e/GJ$] or [$kgCO_2e/kWh$]).

The products of the chemical industry are divided into six chemical divisions according to EU Regulation No. 1893 (EU, 2006)[16]. Among these divisions, basic chemicals represented 60.4% of total EU chemical sales in 2018 (cefic, 2020). In addition, basic chemicals are also the main cause of GHG emissions, as they consume 460.1 PJ/year of energy and account for around 84% of the chemical industry's total energy consumption (AGEB, 2009; Fleiter et al., 2013). Basic chemicals include "other organic basic chemicals" (with a share of 57%), "plastics in primary forms" (also called polymers) (24%), "fertilisers and nitrogen compounds" (7%), "other inorganic basic chemicals" (6%), "dyes and pigments" (3%), "industrial gases" (2%) and "synthetic rubber in primary forms" (1%) (EU, 2006); own calculation based on VCI (2018). Basic chemicals supply the entire manufacturing industry with chemicals and plastics in primary forms (polymers) (Fleiter et al., 2013) and is therefore of particular interest to purchasing units of companies, e.g. from the automotive, electronic, construction or packaging industry. For these reasons, the model is primarily developed for basic chemicals.

Organic basic chemicals are mainly produced in the petrochemical industry (VCI, 2018), by cracking natural gas and petroleum fractions such as naphtha (Behr et al., 2010). For this purpose, stream crackers are primarily used. Since the 1950s, however, FCC (fluid catalytic cracking) crackers have also been increasingly used (Behr et al., 2010). Thus, both cracking variants are modelled.

We distinguish between energy-related and process-related GHG emissions. Energy-related GHG emissions are the amount of CO_2e released during combustion. Process GHG emissions, are generated by certain industrial production processes as by-products, for example from a chemical reaction (Fleiter et al., 2013; Weber, 2014). Only approx. 15% are emitted process-related (McKinsey, 2006); of these approx. 74% relate to ammonia, approx. 13% to carbon black and approx. 8% to sodium carbonate production (own calculation according to data from EEA (2017)). The entire petrochemical industry only contributes to approx. 4% of these process-related emissions, and the production of high value petrochemical products from crackers (HVCs)[17] do not cause any process-related CO_2 emissions according to EEA (2017). Therefore, HVCs will be in the focus of this approach. For other organic or inorganic chemicals, apart from those mentioned above (e.g. ammonia), as well as for polymers, no process-related emissions are listed (EEA 2017). Therefore, an energy-based approach can be used without restriction for HVCs and most other organic and inorganic chemicals (e.g. toluene diisocyanate (TDI) or chlorine) as well as for polymers (e.g. polyethers[18]).

3.2 Model structure

As described in chapters 1 and 2, the availability of primary data is a major problem, as these data are usually highly confidential and it is very unlikely that they will ever be made public (Saygin, 2012). Therefore, this approach aims to enable the estimation of site-specific product carbon footprints (PCFs) independent of classified primary data. In addition, the new methodology is intended to be as generic as

[16] For classification and description of economic divisions in the chemical industry and weighting of the share of the production index in the chemical industry in Germany see appendix **Figure A. 1**.

[17] HVCs (high value chemicals) denotes higher value chemicals produced by the cracking process. The best known and most commonly produced HVCs are propylene and ethylene (Amghizar et al., 2017).

[18] In plastics processing, for example, TDI and polyethers are processed into polyurethane (Europur, 2015).

possible so that it can be applied to many different chemical sites and basic chemicals. This allows, for example, to identify the site with the lowest PCF to produce a specific product. Established software models such as Aspen Plus are not suitable for such a generic approach, so that new models are required. The new model for calculating the site-specific PCFs of HVCs is called "ECCO$_2$-HVC" (**E**valuation tool to **C**ompare **CO$_2$**e emissions of **HVC**s). Analogously, the model for other basic chemicals is called "ECCO$_2$-Basic Chemicals". **Figure 1** illustrates the basic model concept.

To assess the product carbon footprint of a chemical product, a calculation of the GHG emissions is carried out for a "Cradle-to-Gate" system as an S-LCA (see chapter 2) in accordance with the LCA guidelines in ISO 14040 and 14044. GHG emissions are assessed bottom-up along the processes (process LCA) and technologies used. This includes on the one hand the "Cradle-to-Gate" GHG emissions caused in upstream processes (upstream chain) and on the other hand the "Gate-to-Gate" GHG emissions of a production system to the final product. The functional unit of the model is defined as the production of one ton of a specific basic chemical product (e.g. propylene) at a specific production site. The impact assessment of the product carbon footprint [in CO_2e] is carried out according to the CML2001 method for the impact category global warming using the characterization factor "Global Warming Potential" (GWP) over 100 years (GWP100). The characterization factors or CO_2 equivalence factors [kgCO_2e/kg] of the gases used in the CML2001 method are derived from Ecoinvent (e.g. for 1 kg carbon dioxide (CO_2) = 1 kgCO_2e; 1 kg methane (CH_4)= 25 kgCO_2e and 1 kg nitrous oxide (N_2O) = 298 kgCO_2e (Ecoinvent V2.2, 2007-2013).

The Life Cycle Impact Assessment (LCIA) values for products of the upstream chain, i.e. in the "Cradle-to-Gate" system, by Ecoinvent are used to determine the GWP according to CML2001. For products produced in the "Gate-to-Gate" production system, GHG emissions are assessed using the energy-based approach as described above (see section 3.1).

To calculate the GWP not only product-specific but also site-specific, a site-specific energy efficiency is estimated for the "Gate-to-Gate" production system, which is integrated into the LCA model. For high-value cracker products (HVCs), this is done by estimating the energy efficiency of the cracker used onsite, and analogously for other basic chemicals (except for cracker products), the energy efficiency of the respective other required production plant at the site is estimated. In the following, the energy efficiency of a cracker is also called cracker efficiency and the energy efficiency of the production of other basic chemicals (not produced in the cracker) is called production efficiency.

The new approach requires detailed research in technical literature in order to identify and select suitable criteria[19] for estimating the energy efficiency of production sites. The challenge in selecting these criteria is on the one hand that the influence of a criterion on the energy efficiency of a production plant must be significant and scientifically proven. This means that there must be a close correlation between the energy consumption of the plant (e.g. cracker) and the criterion (the proxy variable). On the other hand, a criterion can only be used if the required data are publicly available. In addition to the available technical literature (e.g. Best Available Techniques (BAT) reference documents of the European Commission), we use producer-specific reports and studies (e.g. annual reports, sustainability reports, company websites and registered patents). Possible and finally selected criteria (see section 4.1 for HVCs and section 4.2 for other basic chemicals) were discussed, verified and weighted with experts[20] from the chemical industry. Once the criteria had been defined, an extensive data research was carried out to find site-specific data. Furthermore, a site-specific emission factor for electricity generation is calculated. For this purpose, existing power plants on a chemical site are examined with regard to its type, efficiency and amount of electricity generated.

[19] In the following also called “factors”.

[20] In 2017, three expert interviews were conducted with large chemical companies as well as a telephone interview with a management consultancy.

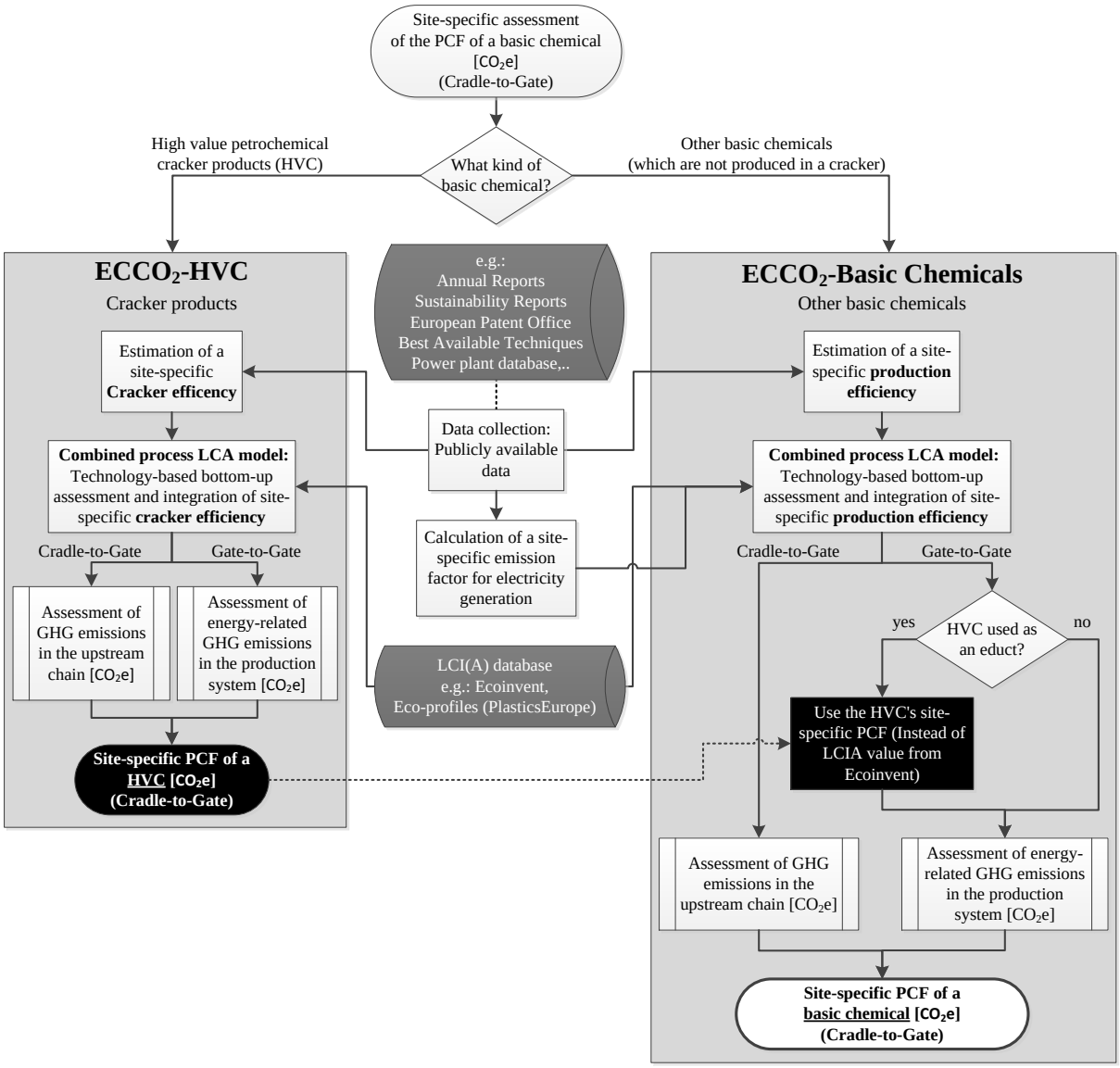


Figure 1: Model concept for estimating site-specific product carbon footprints.

3.3 System boundaries and modelling approach

A big challenge for the assessment of the GWP of the production of specific chemical products is the analysis of the existing energy data on the production of chemical products in the literature. The analyst is often confronted with the fact that different sources provide different values for the energy or steam required to produce a product. Thus, deviations of up to 50% occur between different sources. This is due to the fact that authors set different system boundaries, use different data sets or investigate different regions with different production technologies (Ayres, 1995; Worrell et al., 1994). Therefore, it is important to ensure that the sources and data obtained are used diligently and consistently, especially in the area of system boundaries, in order to avoid double counting due to overlapping system boundaries. Therefore, our model approach sharply separates the system "upstream chain" from the system "production system studied" (see **Figure 2**). All products that are not produced in the production system of a chemical site under study, but in upstream processes are allocated to the upstream chain. Production processes and logistics of the upstream chain are assumed to be unknown, since it is unclear to the model user in which country, for example, crude oil was extracted or by which modes of transport it was delivered. Therefore, the GWP of upstream products can only be assessed using average data from LCI or LCIA databases (e.g. Ecoinvent). Emissions from transports in the upstream chains are included in these average values and are taken into account (see **Figure 2**).

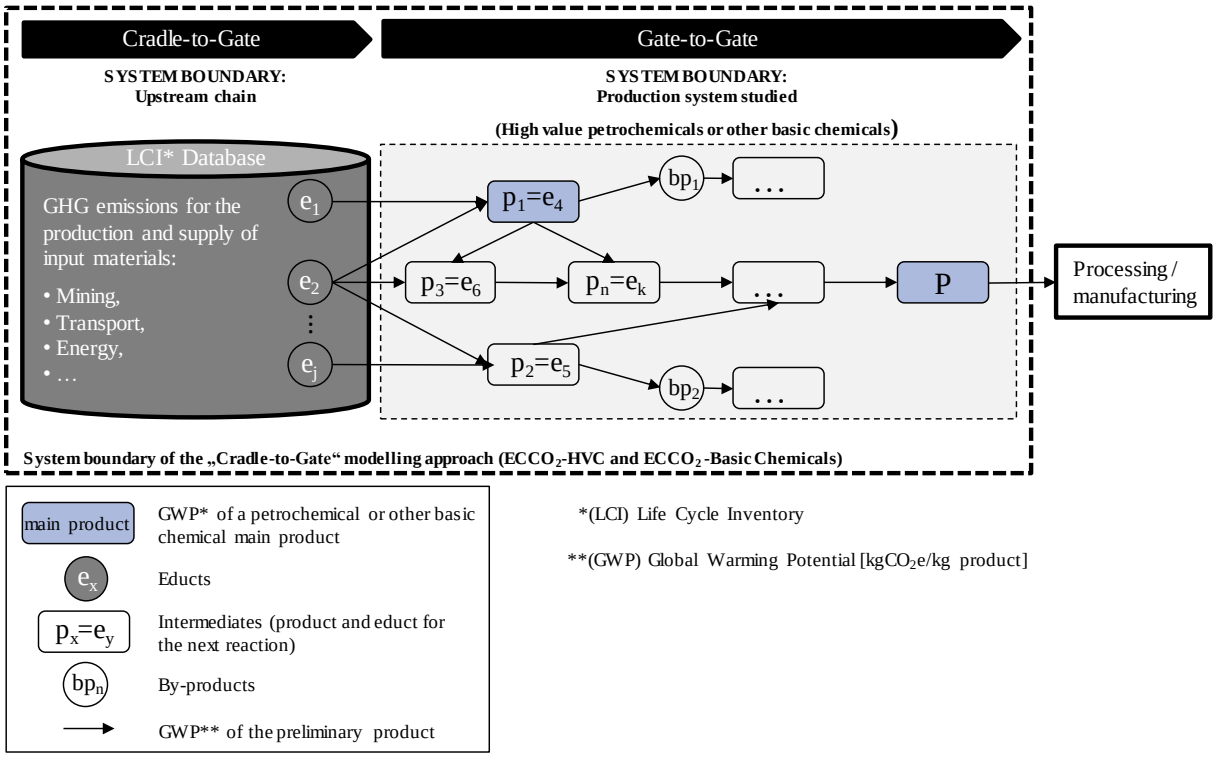


Figure 2: System boundaries of the modelling approach and distinction between main-product, intermediate-product and by-product.

In the model, main, intermediate and by-products are defined. **Main products** are defined as products where the specific energy consumption (SEC) for their production (production energy) are publicly available. This energy includes the required amount of electrical energy, steam and fuels. Often, the SEC is given in intervals with minimum and maximum required quantities (cf. IEA, 2009; Enviros Consulting, 2006; European Commission, 2003). The new developed approach uses these deviations resp. intervals from the SEC to integrate the site-specific energy efficiency (of the cracker or production plant) into the LCA model (section 3.2). To estimate the energy consumption of a specific chemical site within the interval, linear interpolation is performed based on the calculated cracker or production energy efficiency onsite. In this way, it is possible to determine precisely how much energy (SEC) a site requires for producing a product. Due to the dependence of the model on publicly available production energy data, the calculation of a product- and site-specific PCF is therefore by definition only possible for main products.

The model also takes into account that, depending on the boundaries of the production system, several main products must be assessed. This is the case when a main product is directly or indirectly used as an educt (also called reactant) in another main product (see **Figure 2**, e.g. "$p_1=e_4$" is indirectly used in "P"; compare also **Figure 1**, e.g. an HVC can be used as an educt in other basic chemicals). For example, the main product $\mathbf{p_1}$ could be propylene produced in a steam cracker, which is used as educt $\mathbf{e_4}$ in a subsequent process to produce $\mathbf{p_n}$ (e.g. propylene oxide) and is further processed to produce a main product **P**. In this case, $\mathbf{e_1}$ and $\mathbf{e_2}$ would be the educts (the cracker feed) for the production of main product $\mathbf{p_1}$. The GWP for the educts e_1 and e_2 would in this case come from a LCI database (e.g. Ecoinvent). **P** represents the last main product to be assessed and thus also the last step of a value chain under study.[21]

The specific energy consumption (SEC) of intermediate products is already included in the system boundary of the production of a certain main product, i.e. the energy-related GHG emissions. For example, this applies to the production of the basic chemical toluene diisocyanate (TDI) via the

[21] p_2, p_3 and p_n are not main products according to the example in Figure 2 (the SEC of the production of these products is unknown, see introduced definition) and can therefore not be assessed on a site-specific basis.

intermediates dinitrotoluene (DNT) and diaminotoluene (TDA). The SEC for the entire production process of TDI (average value) is known from studies by the International Energy Agency (e.g. IEA, 2009), so that TDI can be defined as a main product. Therefore, DNT and TDA are intermediate products whose SEC is included in the SEC of TDI. However, this does not yet include GHG emissions from the upstream chain, i.e. all processes that occurred prior the production system for the production of TDI. Thus, the GHG emissions (resp. the GWP) from the upstream processes of these intermediates have to be calculated additionally. This includes the GWP of all products respectively educts of the upstream chain of an intermediate product, e.g. sulphuric acid among other educts for the production of the intermediate product DNT.

To calculate the GWP, all products in the production system are balanced on a mass basis. The mass-based approach established for pragmatic reasons and is used by most energy analysis and LCA experts (Kindler and Nikles, 1980; Peereboom et al., 1998; Zhao et al., 2017). This means that the proportions of a reactant in the product are calculated stoichiometrically based on the chemical reaction equations. So, only the part of a substance is considered that is actually further processed; it is assumed that resulting substance surpluses and by-products can be fully and equivalently further used. This assumption relates to today's highly integrated chemical sites, where any by-product emitted in a process can be used as a fuel or raw material for another process (see chapter 1; Fleiter et al., 2013; Saygin, 2012).

4 Mathematical model

In this chapter, the developed calculation logic is presented for determining site-specific product carbon footprints (based on the GWP) of chemical base materials. First, the calculation logic of the methodology of the $ECCO_2$-HVC model for the assessment of high value cracker products (HVC) is explained (section 4.1). Second, section 4.2 introduces the calculation logic of the $ECCO_2$-Basic Chemicals model, which can be used to evaluate all those chemical products that are produced in production plants except for crackers. The input for these other production plants can be the previously assessed HVCs or other educts within or outside the system boundaries of a production site (cf. section 3.3). In our model, both approaches were formulated both generically and independently of original primary production data, so that they can be applied not only to different chemical products but also to all producers. Depending on the product and the availability and currentness of its data, the calculation logic operates as site-specific and up-to-date as possible using case distinctions (see e.g. formula (14)). Both approaches were also programmed as applicable software models: $ECCO_2$-HVC was programmed in Microsoft Visual Basic for Applications and $ECCO_2$-Basic Chemicals in Mathworks Matlab. The generic calculation logic of both approaches is presented in the following (see nomenclature section for the notation).

4.1 Site-specific calculation of the GWP of the production of high value chemicals (HVC)

The GWP of a high value chemical product c from cracker x in site s ($GWP_{c,x,s}^{\mathrm{CrPr}}$) in [kgCO₂e/kg c] depends on the energy required by the cracker onsite ($GWP_{c,x,s}^{\mathrm{Energy,\,Cr}}$) and the corresponding upstream chain of product c produced in cracker x at site s ($GWP_{c,x,s}^{\mathrm{Prechain,\,Cr}}$) (cf. (1)).

$$GWP_{c,x,s}^{\mathrm{CrPr}} = GWP_{c,x,s}^{\mathrm{Energy,\,Cr}} + GWP_{c,x,s}^{\mathrm{Prechain,\,Cr}} \quad (1)$$

The GWP of the consumed energy to produce p ($GWP_{c,x,s}^{\mathrm{Energy,\,Cr}}$) is calculated according to formula (2). $SEC_{c,x,s}^{\mathrm{HVC}}$ denotes the specific energy consumption [GJ/t c] for the production of a product c in cracker x in site s. The conversion factor for [GJ/t] to [kWh/kg] is K=0.277778 and constant. $SEF_{x,s}^{\mathrm{HVC}}$ is the emission factor of the raw materials for the cracker x of the production site s for the production of HVCs in [kgCO₂e/kWh] and is calculated according to (4).

$$GWP_{c,x,s}^{\mathrm{Energy,\,Cr}} = SEC_{c,x,s}^{\mathrm{HVC}} \cdot \mathrm{K} \cdot SEF_{x,s}^{\mathrm{HVC}} \quad (2)$$

To calculate $SEC_{c,x,s}^{\mathrm{HVC}}$ [GJ/t] site-specifically, the cracker efficiency $EFF_{c,x,s}^{\mathrm{Cr}}$ is used to interpolate linearly between the minimum ($SEC_{x}^{\mathrm{HVC,\,min}}$) and maximum specific energy consumption ($SEC_{x}^{\mathrm{HVC,\,max}}$) (cf. (3)). $EFF_{c,x,s}^{\mathrm{Cr}}$ is a site-specific factor between [0;1] to estimate the efficiency of the production of product c in cracker x in site s (cf. (5)). $SEC_{FCC,max}^{f}$ defines the maximum and $SEC_{FCC,min}^{f}$ the minimum specific energy consumption for FCC crackers. X_{FCC} is the set of FCC crackers in the model and is a subset of all crackers. SEC_{max}^{f} is the maximum and SEC_{min}^{f} the minimum specific energy consumption for steam crackers (SC). The variable f denotes the feed, i.e. the raw material feed of the cracker (e.g. ethane, propane, etc.). Accordingly, w_x^f indicates the relative shares of the feed f in the cracker x. To keep the mass balance for all calculations, the sum of the shares of the feed streams must be 1 ($\sum_{f\in F} w_x^f = 1$).

$$SEC_{c,x,s}^{\mathrm{HVC}} = SEC_{x}^{\mathrm{HVC,\,max}} + \left(SEC_{x}^{\mathrm{HVC,\,min}} - SEC_{x}^{\mathrm{HVC,\,max}}\right) \cdot EFF_{c,x,s}^{\mathrm{Cr}}$$

$$\text{with} \quad SEC_{x}^{\mathrm{HVC,\,max}} = \begin{cases} \sum_{f\in F} w_x^f \cdot SEC_{FCC,max}^{f} & , x \in X_{FCC} \\ \sum_{f\in F} w_x^f \cdot SEC_{\mathrm{max}}^{f} & , otherwise \end{cases} \quad (3)$$

$$\text{and} \quad SEC_{x}^{\mathrm{HVC,\,min}} = \begin{cases} \sum_{f\in F} w_x^f \cdot SEC_{FCC,min}^{f} & , x \in X_{FCC} \\ \sum_{f\in F} w_x^f \cdot SEC_{\mathrm{min}}^{f} & , otherwise \end{cases}$$

In the calculation of the raw material emission factor $SEF_{x,s}^{\mathrm{HVC}}$ in (4), $SEF_{x}^{\mathrm{HVC,\,min}}$ is the minimum and $SEF_{x}^{\mathrm{HVC,\,max}}$ is the maximum emission factor [kgCO₂e/kWh] of the raw materials for the cracker x producing HVCs. SEF_{min}^{f} denotes the minimum and SEF_{max}^{f} the maximum specific emission factor [kgCO₂e/kWh] of the raw material f fed into the cracker.

$$SEF_{x,s}^{\text{HVC}} = SEF_x^{\text{HVC, max}} + \left(SEF_x^{\text{HVC, min}} - SEF_x^{\text{HVC, max}}\right) \cdot EFF_{c,x,s}^{\text{Cr}}$$

$$\text{with} \quad SEF_x^{\text{HVC, max}} = \sum_{f \in F} w_x^f \cdot SEF_{max}^f \tag{4}$$

$$\text{and} \quad SEF_x^{\text{HVC, min}} = \sum_{f \in F} w_x^f \cdot SEF_{min}^f$$

In the following, the calculation logic of the cracker efficiency $EFF_{c,x,s}^{\text{Cr}}$ (cf. (5)) is explained. The energy consumption of a cracker depends on several factors such as the mixture of the feed (cf. (4)), the age of the plant (cracker), the utilization rate or the heat integration efficiency (Benchaita, 2013; European Commission, 2017; Fleiter et al., 2013; IEA, 2007). While some factors, such as the age of a cracker, can be researched specifically, heat integration efficiency is not specifically researchable and has to be represented by other factors that have a scientifically proven influence on heat integration efficiency and have publicly available data (cf. section 3.2). Such factors include the production capacity of the production plant, the production capacity of the entire site, the area of the site or the Nelson index of the site. The used factors to determine the cracker efficiency $EFF_{c,x,s}^{\text{Cr}}$ are:

1. $CrPrC_{c,x}$, the production capacity of HVC product c in cracker x [t/a], since CO_2e emissions per ton are decreasing with increasing cracker output (Benchaita, 2013).[22]
2. $FC_{s,x}$, the total production site capacity to process all products of site s to which the cracker x belongs [t/a]. The total site capacity is taken into account, since a higher production volume offers a higher potential for energy savings through economies of scale (Fleiter et al., 2013).
3. $FA_{s,x}$, the site area of site s to which the cracker x belongs [km²]. It is assumed that the size of the area of the site generally correlates with the number of production plants or facilities at the site. Therefore, a large chemical production site is assumed to have more product diversity and production flexibility than a small site where co-products and heat can be better re-integrated into the production of other products (cf. Fleiter et al., 2013).
4. $NI_{s,x}$, the Nelson index of the production site s where the cracker x is located. The Nelson index (*NI*)[23] is an index to measure the complexity of a refinery. The complexity of a refinery is defined by its ability to process crude oil into higher-value products. The simple crude oil distillation is defined with a complexity factor of 1.0 and serves as the reference value. Further plant components and thus longer value chains increase the complexity and consequently the *NI*. For example, a *NI* of 10 means that a refinery is ten times more complex than a pure crude oil distillation plant. The world's highest *NI*s are between 14 and 15 (see Reliance Industries Ltd. (2009) and literature used for Table A. 2 in the appendix). The index is also used in industry as a measure of the investment costs and value added potential of a refinery. A refinery with a high *NI* is therefore more expensive to build and operate, but produces higher value products (Nelson, 1976a, 1976b, 1976c, 1961, 1960a, 1960b; Reliance Industries Ltd., 2009). Based on the definition of the *NI* and analogous to 3. that large and highly integrated sites have better possibilities for energy supply and heat integration (Fleiter et al. 2013), it is deduced that a high *NI* of a site also implies a high degree of integration.
5. $CrAge_x$, the age of the cracker *x*. According to the Best Available Techniques (BAT) in the chemical industry, no correlation can be detected between the age of a cracker and its energy consumption. This is due to the fact that crackers are constantly being upgraded to save energy costs (European Commission, 2003). According to Yao et al. (2016), however, new crackers are usually more energy-efficient than older crackers due to the adoption of state-of-art technologies for the entire processes. Considering that the energy efficiency of a cracker depends on many different technical systems and parameters (e.g. steam turbine efficiency, compressor efficiency or steam system efficiency) (cf. Yao et al., 2015), it also seems unlikely that older crackers will be state-of-the-art in all related technical systems despite investments. In this study, it is therefore assumed that older crackers tend to have a higher energy consumption than newer ones. However, due to the vague

[22] This is illustrated in appendix **Figure A. 2** using the example of the HVC ethylene.
[23] Also known as Nelson complexity index (NCI).

correlation between the age of a cracker and its energy efficiency, the age is weighted less in the model application (cf. chapter 5).

6. $v_x^{\mathrm{UR,\,Cr}}$ denotes the utilization rate of the cracker x. The specific energy consumption is lowest if the plant operates close to the design capacity (cf. section 4.2.2. and Fleiter et al., 2013).

A lower limit (LL) and an upper limit (UL) are defined for all factors, representing a minimum and a maximum possible value. For example, the lower limit for the Nelson index is 1 ($NI_{LL} = 1$) and the upper limit is 14 ($NI_{UL} = 14$). The cracker efficiency for product c of cracker x in site s ($EFF_{c,x,s}^{\mathrm{Cr}}$) is determined in formula (5) by linear interpolation and weighting (w) the factors.

$$\begin{aligned} EFF_{c,x,s}^{\mathrm{Cr}} = {} & w^{\mathrm{CrPrC}} \cdot \max\left(0; \min\left(1; \frac{CrPrC_{c,x} - CrPrC_{c,LL}}{CrPrC_{c,UL} - CrPrC_{c,LL}}\right)\right) \\ & + w^{\mathrm{FC}} \cdot \max\left(0; \min\left(1; \frac{FC_{s,x} - FC_{LL}}{FC_{UL} - FC_{LL}}\right)\right) \\ & + w^{\mathrm{FA,Cr}} \cdot \max\left(0; \min\left(1; \frac{FA_{s,x} - FA_{LL}}{FA_{UL} - FA_{LL}}\right)\right) \\ & + w^{\mathrm{NI}} \cdot \max\left(0; \min\left(1; \frac{NI_{s,x} - NI_{LL}}{NI_{UL} - NI_{LL}}\right)\right) \\ & + w^{\mathrm{CrAge}} \cdot \max\left(0; \min\left(1; \frac{CrAge_x - CrAge_{LL}}{CrAge_{UL} - CrAge_{LL}}\right)\right) \\ & + w^{\mathrm{UR,\,Cr}} \cdot v_x^{\mathrm{UR,\,Cr}} \end{aligned} \tag{5}$$

Finally, to calculate the total GWP for the production of a cracker product c according to formula (1) the GWP from upstream processes is needed. The GWP of the upstream chain of the product c in cracker x in site s ($GWP_{c,x,s}^{\mathrm{Prechain,\,Cr}}$) is calculated according to formula (6) and is indicated in [kgCO_2e/kg c]. $GWP_f^{\mathrm{Ecoprofiles}}$ specifies the GWP of the raw material f from the Eco-profiles of PlasticsEurope [kgCO_2e/kg f]. $GWP_f^{\mathrm{Ecoinvent}}$ denotes the GWP of the raw material f from Ecoinvent [kgCO_2e/kg f] and is used if no GWP exists for f in the Eco-profiles. The variable CR_x is used to describe the raw material conversion rate of the cracker x ($CR_x = Input/Output$). This defines the total yield of the cracker by indicating how much of the total input can be used or reused for later products.

$$GWP_{c,x,s}^{\mathrm{Prechain,\,Cr}} = \left(\sum_{f \in F} w_x^f * \begin{cases} GWP_f^{\mathrm{Ecoprofiles}} & , \exists GWP_f^{\mathrm{Ecoprofiles}} \\ GWP_f^{\mathrm{Ecoinvent}} & , otherwise \end{cases}\right) * CR_x \tag{6}$$

4.2 Site-specific calculation of the GWP of the production of other basic chemicals

In section 4.2.1, we present the entire generic calculation logic to determine the GWP of a basic chemical on a site-specific level. Essential components are the site-specific energy consumption for the production process of the assessed basic chemical and the complex calculation of the corresponding energy-related site-specific GWP. For reasons of clarity, the calculations regarding the specific production energy are presented separately in section 4.2.2.

4.2.1 Calculation of the total GWP

The total GWP of a product is calculated based on an iterative matrix calculation depending on the value-adding steps i to calculate the i-th product (i=1,..., P) in a value-added chain (formula (7)). B_i is the CO_2e balance of step i and includes the GWP "Cradle-to-Gate" of all previous steps [kgCO_2e/kg p]. Matrix $\bar{A}$ represents the mass proportions of educts in the products, up to the i-th product. Matrix B_{i-1} consists of the products' GWPs of the previous value chain step. Vector a_i (12) ensures that only the

corresponding GWPs of the value chain of the i-th product are added to the resulting vector B_i in each iteration. The vector t_0 (13) stores the PCF (respectively the GWP) of each product that is used to produce a product p in site s, but cannot be calculated site-specifically ($GWP^{\mathrm{Edc}}_{e,p,s}$). This does not apply to educts which are cracker products, as their GWP can be calculated according to the developed cracker specific approach (section 4.1). The vector PE (15) contains the calculated GWP of the required production energy for each product that can be calculated site-specifically. PE is calculated in the following section 4.2.2. A detailed description of the formula components is given below.

$$B_i = (\bar{A} \cdot B_{i-1}) \circ a_i + (t_0 + PE) \circ a_i + B_{i-1} = (\bar{A} \cdot B_{i-1} + t_0 + PE) \circ a_i + B_{i-1} \quad (7)$$

Methodically, in this calculation the Hadamard product is used to multiply two matrices component-wise. For this, the Hadamard product requires that the dimensions of two matrices are equal (Chakrabarty, 2017). Matrices B_{i-1} B_i, describe the GWP of i -th product in the production process and matrix $\bar{A}$ the mass proportions of the chemical reaction. By applying formula (7) iteratively along the chemical reaction steps to the final product P (which we want to assess), the vector B_P (8) with the GWP of the desired product is obtained. Due to the iterative application, this resulting vector contains all the GWPs of the previous educts or products of all chemical processing steps i from site s ($GWP^{\mathrm{Pr}}_{p,s}$) to the end product P ($GWP^{\mathrm{Pr}}_{P,s}$) in [kgCO_2e/kg].

$$B_P = \begin{pmatrix} GWP^{\mathrm{Pr}}_{1,s} \\ \vdots \\ GWP^{\mathrm{Pr}}_{p,s} \\ \vdots \\ GWP^{\mathrm{Pr}}_{P,s} \end{pmatrix};\ B_P\colon \{1,\dots,P\} \times \{1\} \quad (8)$$

To produce a product p , different educts e are needed. Matrix $\bar{A}$ (9) represents the mass proportions of educts in the products, whereby all products (except the end product), can also be educts. The mass fraction of an educt e is in the produced product p in site s is calculated (cf. an entry in matrix $\bar{A}$). $m^{\mathrm{Edc}}_{e,p,s}$ denotes the mass of the educt e required to produce the product p in site s. $m^{\mathrm{Pr}}_{p,s}$ specifies the mass of the product p resulting from the reaction during production in site s. During the production of p, the by-products $y \in Y$ are also produced. The part of the mass of an educt e that is processed into the by-product y that is produced during the production of p in site s ($m^{\mathrm{Edc,\,byPr}}_{e,y,p,s}$) is subtracted, since by-products can be fully and equivalently further used (cf. chapter 3).

$$\bar{A} = \begin{pmatrix} \frac{m^{\mathrm{Edc}}_{e,p,s} - \sum_{y=1}^{Y} m^{\mathrm{Edc,\,byPr}}_{e,y,p,s}}{m^{\mathrm{Pr}}_{p,s}} & \cdots & \frac{m^{\mathrm{Edc}}_{E,p,s} - \sum_{y=1}^{Y} m^{\mathrm{Edc,\,byPr}}_{E,y,p,s}}{m^{\mathrm{Pr}}_{p,s}} & 0 \\ \vdots & \ddots & \vdots & \vdots \\ \frac{m^{\mathrm{Edc}}_{e,P,s} - \sum_{y=1}^{Y} m^{\mathrm{Edc,\,byPr}}_{e,y,P,s}}{m^{\mathrm{Pr}}_{P,s}} & \cdots & \frac{m^{\mathrm{Edc}}_{E,P,s} - \sum_{y=1}^{Y} m^{\mathrm{Edc,\,byPr}}_{E,y,P,s}}{m^{\mathrm{Pr}}_{P,s}} & 0 \end{pmatrix};\ \bar{A}:\ \{1,\dots,P\} \times \{1,\dots,E+1\} \quad (9)$$

Matrix $\bar{A}$ is generated from mass balances (10) based on product-specific reaction equations (11). These product-specific reaction equations depend on producer-specific recipes (e.g. accessible at the European Patent Office).

$$\sum_{e=1}^{E} m_{e,p,s}^{\mathrm{Edc}} = m_{p,s}^{\mathrm{Pr}} + \sum_{y=1}^{Y} m_{y,p,s}^{\mathrm{byPr}} \tag{10}$$

$$\sum_{e=1}^{E} n_{e,p,s}^{\mathrm{Edc}} \cdot M_e^{\mathrm{Edc}} \overset{(=)}{\rightarrow} n_{p,s}^{\mathrm{Pr}} \cdot M_p^{\mathrm{Pr}} + \sum_{y=1}^{Y} n_{y,p,s}^{\mathrm{byPr}} \cdot M_y^{\mathrm{byPr}} \tag{11}$$

Analogue to $m_{p,s}^{Pr}$, $m_{y,p,s}^{byPr}$ denotes the mass of the by-product y resulting from the reaction during production of p in site s. $n_{e,p,s}^{\mathrm{Edc}}$ describes the amount of substance [mol] of an educt e required for production of p in site s and M_e^{Edc} indicates the molar mass [kg/mol] of the educt e. Similarly, $n_{p,s}^{\mathrm{Pr}}$ denotes the amount of substance of p produced at site s and $M_p^{\mathrm{Pr}}$the molar mass of p. Likewise, $n_{y,p,s}^{\mathrm{byPr}}$ is the amount of substance of the by-product y produced at the production site s during the production of product p and M_y^{byPr} the molar mass of the by-product y.

The vector a_i (12) in formula (7) ensures that in each iteration only the corresponding GWPs of the considered value chain of the i-th product are added to the resulting vector B_i.

$$a_i = \begin{pmatrix} f_1 \\ \vdots \\ f_k \\ \vdots \\ f_P \end{pmatrix};\ a_i\colon \{1,\dots,P\} \times \{1\} \text{ with: } f_1 = \begin{cases} 1 & ,1 = i \\ 0 & ,1 \neq i \end{cases},\ f_2 = \begin{cases} 1 & ,2 = i \\ 0 & ,2 \neq i \end{cases}, \dots,\ f_k = \begin{cases} 1 & ,k = i \\ 0 & ,k \neq i \end{cases} \tag{12}$$

In vector t_0 (13), the $GWP_{e,p,s}^{\mathrm{Edc}}$ is determined according to the case distinction in Equation (14).

$$t_0 = \begin{pmatrix} GWP_{1,1,s}^{\mathrm{Edc}} \\ \vdots \\ GWP_{e,p,s}^{\mathrm{Edc}} \\ \vdots \\ GWP_{E,p,s}^{\mathrm{Edc}} \\ \vdots \\ GWP_{E,P,s}^{\mathrm{Edc}} \end{pmatrix};\ t_0\colon \{1,\dots,E+P\} \times \{1\} \tag{13}$$

$$GWP_{e,p,s}^{\mathrm{Edc}} = \begin{cases} GWP_{e,s}^{\mathrm{Supp,\,Data}} & ,1. \\ \dfrac{1}{A_s}\displaystyle\sum_{x=1}^{X} GWP_{c,x,s}^{\mathrm{CrPr}} & ,2. \\ \dfrac{1}{A}\displaystyle\sum_{s=1}^{S}\sum_{x=1}^{X} GWP_{c,x,s}^{\mathrm{CrPr}} & ,3. \\ 0 & ,4. \\ 0 & ,5. \\ GWP_e^{\mathrm{Ecoprofiles}} & ,6. \\ GWP_e^{\mathrm{Ecoinvent}} & ,7. \end{cases}$$

Cases:

1.: $\exists GWP_{e,s}^{\mathrm{Supp,\,Data}} \in GWP^{\mathrm{Supp,\,Data}}$

2.: $A_s \geq 1 \wedge Edc_e = CrPr_c \wedge \nexists GWP_{e,s}^{\mathrm{Supp,\,Data}} \in GWP^{\mathrm{Supp,\,Data}}$

3.: $A_s = 0 \wedge Edc_e = CrPr_c \wedge \nexists GWP_{e,s}^{\mathrm{Supp,\,Data}} \in GWP^{\mathrm{Supp,\,Data}}$

4.: $Edc_e = ImPr_z \wedge \nexists GWP_{e,s}^{\mathrm{Supp,\,Data}} \in GWP^{\mathrm{Supp,\,Data}}$

5.: $Edc_e = MPr_h \wedge \nexists GWP_{e,s}^{\mathrm{Supp,\,Data}} \in GWP^{\mathrm{Supp,\,Data}}$

6.: $\exists GWP_e^{\mathrm{Ecoprofiles}} \in GWP^{\mathrm{Ecoprofiles}} \wedge \nexists GWP_{e,s}^{\mathrm{Supp,\,Data}} \in GWP^{\mathrm{Supp,\,Data}} \wedge \nexists Edc_e = ImPr_z \wedge \nexists Edc_e = MPr_h \wedge \nexists Edc_e = CrPr_c$

7.: $\nexists GWP_e^{\mathrm{Ecoprofiles}} \in GWP^{\mathrm{Ecoprofiles}} \wedge \nexists GWP_{e,s}^{\mathrm{Supp,\,Data}} \in GWP^{\mathrm{Supp,\,Data}} \wedge \nexists Edc_e = ImPr_z \wedge \nexists Edc_e = MPr_h \wedge \nexists Edc_e = CrPr_c$ (14)

In Equation (14), $GWP_{e,s}^{\mathrm{Supp,\,Data}}$ describes the GWP of an educt e in site s if primary data from the supplier is available (case 1). A_s specifies the number of crackers in production site s and A the sum of crackers in all production sites implemented in the model (equals X). $GWP_{c,x,s}^{\mathrm{CrPr}}$ is the GWP of a cracker product c from the cracker x in site s. Case 2 occurs if at least one cracker exists at site s, educt e is a cracker product and no primary data on the GWP of this educt is given. Case 3 covers the GWP of an educt e (=cracker product) when no cracker is located onsite. In this case, the GWP of the cracker

product is the average value of all modelled crackers ($GWP_{c,x,s}^{\mathrm{CrPr}}$) (section 4.1). In cases 4 and 5, $GWP_{e,p,s}^{\mathrm{Edc}}$ is 0 if the educt is an intermediate or main product because in this case the site-specific approach has to be applied. $CrPr$ stands for the quantity of cracker products, $ImPr$ for the quantity of intermediate products and MPr for the quantity of main products that are included in the model. If no primary data is available and none of cases 2 to 5 occurs to specifically determine the educt, the GWP of an educt is taken from PlasticsEurope's Eco-profiles ($GWP_e^{\mathrm{Ecoprofiles}}$) (case 6). If no Eco-profile of p is available either, data from the Ecoinvent database V2.2 is used ($GWP_e^{\mathrm{Ecoinvent}}$) (case 7). The Eco-profiles are preferred because they are usually more up-to-date.

Vector PE (15) contains the GWP of the required production energy (PE) for each intermediate or main product that is produced at site s. $GWP\_PE_{p,s}^{\mathrm{Pr}}$ is determined according to the case distinction in formula (16). $GWP\_PE_{p,s}^{\mathrm{Pr}}$ is 0 if the product is not an intermediate and main product, but an educt and has therefore already been calculated in $GWP_{e,p,s}^{\mathrm{Edc}}$ (case 1). If the product p is not produced at site s, the mean value of the GWP of the production energy of all locations producing p is used for this site (case 3). $GWP_{p,s}^{\mathrm{Energy,\,Prod}}$ determines the specific energy needed to produce p in site s (section 4.2.2).

$$PE = \begin{pmatrix} GWP\_PE_{1,s}^{\mathrm{Pr}} \\ \vdots \\ GWP\_PE_{p,s}^{\mathrm{Pr}} \\ \vdots \\ GWP\_PE_{P,s}^{\mathrm{Pr}} \end{pmatrix}; PE: \{P\} \times \{1\} \tag{15}$$

$$GWP\_PE_{p,s}^{\mathrm{Pr}} = \begin{cases} 0 & , GWP_{e,p,s}^{\mathrm{Edc}} \neq 0 \\ GWP_{p,s}^{\mathrm{Energy,\,Prod}} & , \exists GWP_{p,s}^{\mathrm{Energy,\,Prod}} \in GWP^{\mathrm{Energy,\,Prod}} \\ \dfrac{1}{|\tilde{s}|} \sum_{\tilde{s} \in \tilde{S}} GWP_{p,\tilde{s}}^{\mathrm{Energy,\,Prod}} & , \nexists GWP_{p,s}^{\mathrm{Energy,\,Prod}} \in GWP^{\mathrm{Energy,\,Prod}} \end{cases} \tag{16}$$

with
$\tilde{S} = \{s \mid p \text{ is produced at } s\}$

4.2.2 Sub-calculation: GWP of the production energy used onsite

The total GHG emissions (Cradle-to-Gate) resulting from the production of the product p at production site s ($GWP_{p,s}^{\mathrm{Pr}}$) are calculated according to formula (7) or (8). $GWP\_PE_{p,s}^{\mathrm{Pr}}$ in vector PE (15) includes the energy-related GHG emissions caused in the production system to produce the product p "Gate-to-Gate". All other GHG emissions that occur in preliminary stages onsite or in upstream chains off-site are included in the GWPs of the pre-products B_{i-1} (7) or in vector t_0 (13).

GHG emissions from the production of p at site s ($GWP_{p,s}^{\mathrm{Energy,\,Prod}}$) are calculated based on the required steam, electricity and fuels according to formula (17). Here, only the production energy used for the product to be balanced is calculated (mass-based approach, cf. section 4.2). m_p^{Pr} is the mass of the product p and $m_{y,p,s}^{\mathrm{byPr}}$ is the mass of a by-product y resulting from the production of p .

$$GWP_{p,s}^{\mathrm{Energy,\,Prod}} = \left(GWP_{p,s}^{\mathrm{Steam}} + GWP_{p,s}^{\mathrm{Elec}} + GWP_{p,s}^{\mathrm{Fuel}}\right) \cdot \left(\frac{m_p^{\mathrm{Pr}}}{m_p^{\mathrm{Pr}} + \sum_{y=1}^{Y} m_{y,p,s}^{\mathrm{byPr}}}\right) \tag{17}$$

The GWP triggered by the generation of the required steam for the production of p at site s ($GWP_{p,s}^{\mathrm{Steam}}$) is calculated according to formula (18).

$$GWP_{p,s}^{\text{Steam}} = \begin{cases} \left(SEC_{p,s}^{\text{Steam}} \cdot \text{K} \cdot \sum_{b=1}^{B} (g_{b,s}^{\text{Steam}} \cdot SEF_{b,s}^{\text{Steam}}) \right) \cdot \frac{1}{\eta_s^{\text{Steam}}} & ,1. \\ SEC_p^{\text{Steam, Ecoinvent}} \cdot \text{K} \cdot SEF^{\text{NG}} \cdot \frac{1}{\eta_s^{\text{Steam}}}, & ,2. \\ 0 & ,3. \end{cases} \quad (18)$$

1.: $\exists p \in \{1, \dots P\}, h \in \{1, \dots H\}$: $Pr_p = MPr_h$
2.: $\nexists p \in \{1, \dots P\}, h \in \{1, \dots H\}$: $Pr_p = MPr_h$
3.: $\nexists p \in \{1, \dots P\}, h \in \{1, \dots H\}$: $Pr_p = MPr_h \wedge \nexists SEC_p^{\text{Steam, Ecoinvent}} \in SEC^{\text{Steam, Ecoinvent}}$

$SEC_{p,s}^{\text{Steam}}$ describes the specific energy consumption of steam generation to produce product p in production site s in [GJ/t p]. $g_{b,s}^{\text{Steam}}$ is the share of a fuel b [%] at production site s to generate steam. To comply with mass balances, shares of all fuels used must sum up to 1 ($\sum_{b \in B} g_{b,s}^{\text{Steam}} = 1$). $SEF_{b,s}^{\text{Steam}}$ stands for the emission factor of fuel b used to generate steam at production sites s in [kgCO_2e/kWh]. η_s^{Steam} denotes the efficiency of steam generation onsite. The specific energy consumption of steam generation in [MJ/kg p] for the production of p based on Ecoinvent data is labelled $SEC_p^{\text{Steam, Ecoinvent}}$. SEF^{NG} in [kgCO_2e/kWh] is the emission factor of natural gas, which is generally used for steam generation (according to Evoinvent). The calculation distinguishes between a main product with publicly available product-specific energy data (case 1), and no defined main product (case 2). In case 2, Ecoinvent data is used. If Ecoinvent does not provide any information either, it is assumed that no steam is required (case 3). This case distinction applies analogously to the specific GWP of the required electricity ($GWP_{p,s}^{\text{Elec}}$) in formula (23) and the required site-specific GWP from fuel use for production of product p in site s ($GWP_{p,s}^{\text{Fuel}}$) described in the following equations (19, 20, 21).

$$GWP_{p,s}^{\text{Fuel}} = \begin{cases} SEC_{p,s}^{\text{Fuel}} \cdot \text{K} \cdot SEF_s^{\text{Fuel}} & ,1. \\ SEC_p^{\text{Fuel, Ecoinvent}} \cdot \text{K} \cdot SEF_s^{\text{Fuel}} & ,2. \\ 0 & ,3. \end{cases} \quad (19)$$

1.: $\exists p \in \{1, \dots P\}, h \in \{1, \dots H\}$: $Pr_p = MPr_h$
2.: $\nexists p \in \{1, \dots P\}, h \in \{1, \dots H\}$: $Pr_p = MPr_h$
3.: $\nexists p \in \{1, \dots P\}, h \in \{1, \dots H\}$: $Pr_p = MPr_h \wedge \nexists SEC_p^{\text{Fuel, Ecoinvent}} \in SEC^{\text{Fuel, Ecoinvent}}$

with

$$SEF_s^{\text{Fuel}} = \begin{cases} SEF_s^{\text{Fuel, SuppData}} & , \exists SEF_s^{\text{Fuel,SuppData}} \in SEF^{\text{Fuel,SuppData}} \\ \frac{1}{A_s} \cdot \sum_{x=1}^{X} SEF_{x,s}^{\text{HVC}} & , A_s \geq 1 \wedge \nexists SEF_s^{\text{Fuel,SuppData}} \in SEF^{\text{Fuel,SuppData}} \\ \frac{1}{A} \cdot \sum_{\tilde{s}=1}^{\tilde{S}} \sum_{x=1}^{X} SEF_{x,s}^{\text{HVC}} & , A_s = 0 \wedge \nexists SEF_s^{\text{Fuel,SuppData}} \in SEF^{\text{Fuel,SuppData}} \end{cases} \quad (20)$$

and

$$A = \sum_{s=1}^{S} \sum_{x=1}^{X} \min\{1; SEF_{x,s}^{\text{HVC}}\} \text{ and } A_s = \sum_{x=1}^{X} \min\{1; SEF_{x,s}^{\text{HVC}} \cdot \beta\} \quad \forall s \in \{1, \dots S\} \quad (21)$$

To calculate $SEC_{p,s}^{\text{Steam}}$ site-specifically (22), $EFF_{p,s}^{\text{Site, Prod}}$ is used to interpolate linearly between the minimum ($SEC_p^{\text{Steam, min}}$) and maximum specific energy consumption ($SEC_p^{\text{Steam, max}}$) based on consistent literature (e.g. the Best Available Techniques (BAT) of the European Commission (2003, 2017)). The production efficiency $EFF_{p,s}^{\text{Site, Prod}}$ is a site-specific factor (cf. (26)) between [0;1] to estimate the efficiency of production of product p at site s.

$$SEC_{p,s}^{\text{Steam}} = SEC_{p}^{\text{Steam, max}} + \left(SEC_{p}^{\text{Steam, min}} - SEC_{p}^{\text{Steam, max}}\right) \cdot EFF_{p,s}^{\text{Site, Prod}} \quad (22)$$

The GWP resulting from the electricity consumption for the production of p at site s ($GWP_{p,s}^{\text{Elec}}$) is calculated in (23):

$$GWP_{p,s}^{\text{Elec}} = \begin{cases} SEC_{p,s}^{\text{Elec}} \cdot K \cdot \omega & ,1. \\ SEC_{p}^{\text{Elec, Ecoinvent}} \cdot \omega & ,2. \\ 0 & ,3. \end{cases}$$

$$\begin{aligned} &1.: \exists p \in \{1, \dots P\}, h \in \{1, \dots H\}: \ Pr_p = MPr_h \\ &2.: \nexists p \in \{1, \dots P\}, h \in \{1, \dots H\}: \ Pr_p = MPr_h \\ &3.: \nexists p \in \{1, \dots P\}, h \in \{1, \dots H\}: \ Pr_p = MPr_h \wedge \nexists SEC_{p}^{\text{Elec, Ecoinvent}} \in SEC^{\text{Elec, Ecoinvent}} \end{aligned} \quad (23)$$

with

$$\omega = \left(\left(w_s^{\text{Elec, selfprod}} \cdot \sum_{b \in B}\left(g_{b,s}^{\text{Elec}} \cdot SEF_{b,s}^{\text{Elec}}\right)\right) \cdot \frac{1}{\eta_s^{\text{Elec}}} + \left(1 - w_s^{\text{Elec, selfprod}}\right) \cdot GWP_s^{\text{CountryElecMix}}\right)$$

$SEC_{p,s}^{\text{Elec}}$ is the specific energy consumption of electrical energy for the production of product p at site s [GJ/t p]. $SEC_{p}^{\text{Elec, Ecoinvent}}$ stands for the specific energy consumption of electricity generation in [kWh/kg p] for the production of p according to Ecoinvent. ω is used to calculate a site-specific emission factor for electricity [kgCO_2e/kWh]. $w_s^{\text{Elec, selfprod}}$ indicates the share of self-generated electricity onsite [%] and $SEF_{b,s}^{\text{Elec}}$ denotes the emission factor of the fuel b used to generate electricity onsite. To comply with mass balances, the sum of the shares of all fuels used to produce energy must be 1 ($\sum_{b \in B} g_{b,s}^{\text{Elec}} = 1$). The efficiency of the power plant at production site s is indicated with η_s^{Elec}. $GWP_s^{\text{CountryElecMix}}$ in [kgCO_2e/kWh] denotes the emission factor of the electricity mix of the country where the production site s is located. If electricity is not produced onsite, the GWP of the respective national average electricity mix is assumed.

For the site-specific calculation of $SEC_{p,s}^{\text{Elec}}$ (24), the factor $EFF_{p,s}^{\text{Site, Prod}}$ is used analogously to (22) to interpolate linearly between the minimum and maximum consumption of electrical energy. $SEC_{p}^{\text{Elec, max}}$ is the maximum and $SEC_{p}^{\text{Elec, min}}$ the minimum specific consumption of electrical energy to produce product p [GJ/t].

$$SEC_{p,s}^{\text{Elec}} = SEC_{p}^{\text{Elec, max}} + \left(SEC_{p}^{\text{Elec, min}} - SEC_{p}^{\text{Elec, max}}\right) \cdot EFF_{p,s}^{\text{Site, Prod}} \quad (24)$$

In analogy to the calculation of the GWP resulting from the use of steam and electrical energy, a site-specific calculation logic for the corresponding GWP of fuel use $GWP_{p,s}^{\text{Fuel}}$ is formulated in (19). In formula (19), $SEC_{p,s}^{\text{Fuel}}$ describes the specific energy consumption of fuels for the production of product p at site s in [GJ/t]. $SEC_{p}^{\text{Fuel, Ecoinvent}}$ stands for the specific energy consumption of fuels for the production of p according to Ecoinvent in [MJ/kg], if no site-specific value is available. SEF_s^{Fuel} quantifies the emission factor of the fuels in [kgCO_2e/kWh], which are used in production site s. $SEF_s^{\text{Fuel,SuppData}}$ indicates the emission factor for fuels of the production site s, if primary data are available. $SEF_{x,s}^{\text{HVC}}$ denotes the emission factor [kgCO_2e/kWh] of the raw materials or fuels used in cracker x at site s for the production of high value chemical products (HVC). The use of $SEF_{x,s}^{\text{HVC}}$ as an emission factor for the used fuels assumes that the used fuels are mainly those that are also used in the cracker (if there is a cracker onsite). $SEF_{x,s}^{\text{HVC}}$ is described in formula (4) (section 4.1). A is the number of crackers considered in the model and A_s is the number of crackers at site s. $\tilde{s}$ is an auxiliary variable

and is equivalent to s. β is a necessary correction value ($\beta = 10^6$) for the calculation of A_s if $SEF_{x,s}^{\mathrm{HVC}}$ has very small values, but has no influence on the result.

As in (22) and (24), the factor $EFF_{p,s}^{\mathrm{Site,\ Prod}}$ is also used in (25) to calculate the specific energy consumption of a site for the production of product p ($SEC_{p,s}^{\mathrm{Fuel}}$). $SEC_{p,s}^{\mathrm{Fuel,\ max}}$ is the maximum and $SEC_p^{\mathrm{Fuel,\ min}}$ the minimum specific energy consumption [GJ/t] of fuels for the production of p.

$$SEC_{p,s}^{\mathrm{Fuel}} = SEC_p^{\mathrm{Fuel,\ max}} + \left(SEC_p^{\mathrm{Fuel,\ min}} - SEC_p^{\mathrm{Fuel,\ max}}\right) \cdot EFF_{p,s}^{\mathrm{Site,\ Prod}} \quad (25)$$

The production efficiency $EFF_{p,s}^{\mathrm{Site,\ Prod}}$ according to formula (26) is composed of various factors that estimate both the level of integration and the level of innovation of a production plant. Like for crackers (section 4.1), the factors are put into relation to a lower limit (LL) and an upper limit (UL) and weighted (w) in order to determine the site-specific efficiency of the production of a product.

<u>Factors for determining the level of production integration are:</u>

1. LF_s, the location factor of the production site s. This serves as an indicator of how suitable the location of a site is for contributing to a low PCF. The more upstream products are produced onsite or nearby, the shorter the transport distances. Therefore, the assessment of the LF_s takes into account whether a refinery is located on the site and with which Nelson index it is rated, how short the transport distances to refineries and other chemical sites are and which modes of transport (e.g. river, road, sea, pipeline) can be used to supply a site. LF_s is evaluated with a value between 0 (bad location) and 10 (very good location) [0;10].
2. FA_s, the area of the site s [km²]. (Explanation is identical like for factor $FA_{s,x}$ used to calculate cracker efficiency cf. (5)).
3. The utilization rate of the production plant depends on the production quantity of product p in site s [t/a] ($Output_{p,s}$) and the production capacity of product p in site s [t/a] ($PC_{p,s}$). The utilization rate is taken into account, as energy consumption is lowest when the plant operates at its design capacity. Capacities above and below the design capacity increase the specific energy consumption of the plant. (Fleiter et al., 2013)
4. FL_s, the flexibility of production at site s [number of production plants at the site]. Analogous to the explanation of the factor of the factory area $FA_{s,x}$ (cf. cracker efficiency (5)), the number of production facilities is used to estimate the heat integration potential.
5. $PC_{p,s}$, the production capacity of the product p at site s [t/a] is taken into account, as a higher production volume leads to a higher potential for energy savings due to economies of scale (Fleiter et al., 2013).

<u>Factors for describing the level of innovation are:</u>

1. $PY_{p,s}$, the production yield of the product p at site s [%]. The use of innovative production processes, solvents or, for example, nanoscale catalysts increase the yield and result in a higher output quantity with the same energy input (UBA, 2009).
2. TE_s, the technical equipment (software and hardware) of site s. This involves evaluating the state of the art of the machines used. For example, the use of frequency-controlled pumps increases energy efficiency (Leimkühler, 2010). In general, new or modernised production plants are generally more energy-efficient than older plants (Schönbucher, 2002; BMLFUW, 2010). A very high state of the art is rated 10 and a very low one 0 [0;10].

$$
\begin{aligned}
EFF_{p,s}^{\text{Site, Prod}} = \Bigg[& \left(\max\left(0, \min\left(1, \frac{LF_s - LF_{LL}}{LF_{UL} - LF_{LL}}\right)\right) \cdot w^{\text{LF}}\right) + \left(\max\left(0, \min\left(1, \frac{FA_s - FA_{LL}}{FA_{UL} - FA_{LL}}\right)\right) \cdot w^{\text{FA}}\right) \\
& + \left(\frac{Output_{p,s}}{PC_{p,s}} \cdot w^{\text{UR}}\right) + \left(\max\left(0, \min\left(1, \frac{FL_s - FL_{LL}}{FL_{UL} - FL_{LL}}\right)\right) \cdot w^{\text{FL}}\right) \\
& + \left(\max\left(0, \min\left(1, \frac{PC_s - PC_{p,LL}}{PC_{p,UL} - PC_{p,LL}}\right)\right) \cdot w^{\text{PC}}\right)\Bigg] \cdot \; w^{\text{INTL}} \\
& + \left[\left(PY_{p,s} \cdot w^{\text{PY}}\right) + \left(\max\left(0, \min\left(1, \frac{TE_s - TE_{LL}}{TE_{UL} - TE_{LL}}\right)\right) \cdot w^{\text{TE}}\right)\right] \cdot w^{\text{INNL}}
\end{aligned}
\tag{26}
$$

5 Model application and case study results

In this chapter, the models developed in sections 4.1 and 4.2 are applied to the production of basic chemicals propylene and TDI in German production sites.

In Germany, 21% of GHG emissions are industry-related, i.e. caused by the production and processing of products (UBA, 2018a). The majority of these emissions are caused by the production of raw materials (GFSO, 2018a). These are mainly steel and basic chemicals which can be processed into end products such as vehicles (Bauer et al., 2015; Ducker, 2015). The steel and chemical[24] industries account for 23% and 25% respectively of the industry-related GHG emissions in Germany. Particularly the production of basic and mass chemicals requires a high level of energy input and therefore induces high energy-related GHG emissions. In 2016, the chemical industry in Germany[25] accounts for approx. 27% of the energy consumption in the manufacturing sector (GFSO, 2018b).

After ethylene, propylene is the most important petrochemical basic chemical worldwide and is used for the production of bulk chemicals such as propylene oxide, cumene, acrylic acid and especially polypropylene (Ceresana Market Research, 2014). Polypropylene has the largest share (32%) of all plastics used in the automotive industry (Patil et al., 2017), making the results of this case study particularly interesting for the automotive industry. To assess the site-specific product carbon footprint (Cradle-to-Gate) [CO_2e] of propylene production, the ECCO$_2$-HVC model (section 4.1) is used, since propylene is mainly produced in steam and FCC crackers (Lei and Bao, 2014; Zhao et al., 2017). The propylene case study (section 5.1) includes the assessment of 23 crackers at 17 production sites in Germany (see **Figure 3**).

TDI is chosen as an example for the application of the ECCO$_2$-Basic Chemicals model because TDI is an important basic chemical for the production of polyurethane (Kaiser, 2015), which has the second largest share (17%) among the plastics used in the automotive industry (Patil et al., 2017). In addition, polyurethane is also used in the production of mattresses and upholstered furniture as well as for acoustic noise reduction purposes, carpet underlays, sponges, clothing and packaging (Kaiser, 2015). The assessment of the site-specific product carbon footprint (Cradle-to-Gate) [CO_2e] of TDI production is carried out for four chemical sites in Germany (see **Figure 3**).

[24] The latter covers the production of mineral oil and chemical products in Germany (GFSO, 2018b).

[25] The German chemical industry is the largest in Europe with a 25% share of turnover. That is about 8% of global chemical production (Fleiter et al., 2013).

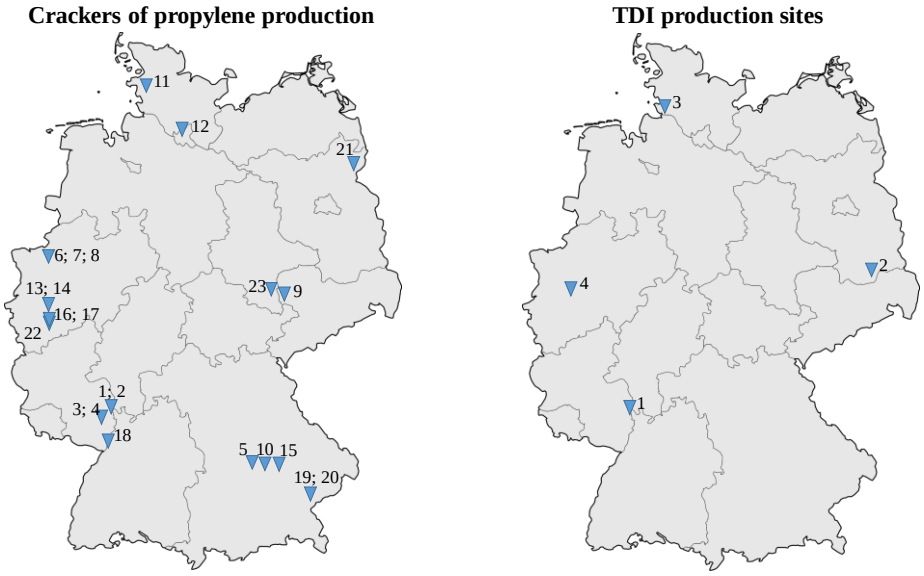


Figure 3: Assessed crackers of propylene production sites and assessed TDI production sites[26] in Germany.

5.1 Case study on propylene production

5.1.1 Background and assumptions

For the GWP calculation it is necessary to define the interval for the specific energy consumption (SEC) for the production of one ton of propylene and the specific emission factor (SEF) of the raw materials/fuels used in the model (cf. **Table 1**). A good approximation for the SEC can be found in the BAT (Best Available Technique) documents on Large Volume Chemicals. The BAT documents specifies the SEC for steam crackers in Gigajoule per ton of HVC [GJ/t HVC] (European Commission, 2003, 2017). Propylene is one of the main HVCs, produced by the cracking process (Amghizar et al., 2017). Since there is no specific data for propylene in the BAT document or elsewhere, the BAT data per ton of HVC is the best approximation. There are sources with more recent SEC data, e.g. Enviros Consulting (2006), but these values are derived from the same used European Commission (2003) and European Commission (2017) sources. However, the BAT documents only contain values for ethane, naphtha and gas oil. Data are missing for the liquid gases butane and propane, which are also used as raw materials in stream crackers. According to Worrell et al. (2008), the real SEC values of butane and propane are somewhere between the SEC values of ethane and naphtha. Based on this information, the SEC values for butane and propane for this study are generated by taking the mean value of the SEC values of ethane and naphtha. For the SEC of FCC crackers, the data are taken from Ren et al. (2006, 2008). Catalytic cracking is assumed to consume between 8-12 [GJ/t HVC], depending on the technology. Typical raw materials are ethane, naphtha and mainly gas oil (Ren et al., 2008, 2006). The data for the specific emission factors of the feedstock fractions in the cracker are derived from a study by Enviros Consulting (2006). Similar values for the emission factors could also be found in Neelis et al. (2005), who also calculated specific emission factors for naphtha- and ethane-based steam crackers.[27]

[26] Site 3 was transformed to an MDI production site in 2018.

[27] Enviros Consulting (2006) gives these specific emission factors in the unit [kgCO_2e/kWh] and Neelis et al. (2005) in [kgCO_2e/GJ]. For ethane, for example, Neelis et al. (2005) calculate a specific emission factor of 0.047 [kgCO_2e/GJ], which corresponds to approx. 0.169 [kgCO_2e/kWh].

Table 1:
Specific emission factors and specific energy consumption of the cracker feed (European Commission, 2003, 2017; Ren et al., 2006, 2008; Enviros Consulting, 2006; Neelis et al., 2005).

	Ethane		Propane		Butane		Naphtha		Gas oil		Natural gas	
	min	**Max**	**min**	**max**	**min**	**max**	**min**	**max**	**min**	**max**	**min**	**max**
Specific emission factor (SEF) [kgCO_2e/kWh]	0.115	0.192	0.133	0.200	0.147	0.220	0.153	0.245	0.158	0.198	0.171	0.209
SEC SC [GJ/t HVC]	12.50	21.00	13.25	21.50	13.25	21.50	14.00	22.00	18.00	23.00	12.50	21.00
SEC FCC [GJ/t HVC]	8.00	12.00	-	-	-	-	8.00	12.00	8.00	12.00	-	-

As described in section 4.1, the SEC of a cracker results from the feedstock mix (section 5.1.2) and the cracker efficiency (section 0), which is estimated on the basis of different factors. The raw material conversion rate CR_x (Input/Output) is set to 1=(100%) for all crackers, since almost no emissions are released during cracking (EEA, 2017) (cf. section 3.1). This is also confirmed by the company BASF, as unusable substances such as methane, propane and butane are refed as raw materials or used for heating (BASF, 2019).

5.1.2 Data of the feedstock mix

Information on the feedstock mix of some of the crackers under consideration can be found in the Ethylene Reports of the Oil & Gas Journal, e.g. in Koottungal (2015). For 2015, these are listed in appendix **Table A. 1.** Missing values for the remaining crackers are filled with average values for European steam crackers according to PlasticsEurope (2012a). The values of 12% for Liquefied Petroleum Gas, are split into 6% propane and 6% butane. Due to lacking values for FCC crackers, gas oil is assumed to be the only raw material, as is usually the case (Vogt and Weckhuysen, 2015).
Data on the GWPs of feedstock fractions (Cradle-to-Gate) are listed in **Table 2**.[28] Since Ecoinvent does not contain a GWP for ethane, the value of propane and butane is assumed instead. Also, for the missing value for gas oil, the average of the medium distillates diesel and light heating oil from Ecoinvent v.2.2 is used as an approximation.

Table 2:
GWP of the feedstock fractions (Cradle-to-Gate).

	Naphtha	**Natural gas**	**Ethane**	**Propane**	**Butane**	**Gasoil**
GWP (kgCO_2e/kg Product)	0.34	0.52	0.60501	0.60501	0.60501	0.48539
Source	(PlasticsEurope, 2005a)	(PlasticsEurope, 2005b)	(assumed)-	(Ecoinvent v.2.2)	(Ecoinvent v.2.2)	(Ecoinvent v.2.2)

5.1.3 Data to calculate the cracker efficiency

The factors for the calculation of the cracker efficiency are listed in appendix **Table A. 2** for each site. However, producers provide information about their crackers or production sites to the public to a different extent. For this, expert interviews and discussions were conducted to close data gaps. For example, it was possible to obtain information about propylene capacities on a producer-specific basis (light grey cells in **Table A. 2**). If a data gap could not be filled by expert interviews, average values were used (dark grey cells in **Table A. 2**). For the average site capacity, the average of the considered sites was calculated. The average for the Nelson index was set to 6.5, which is according Raffinerie Heide GmbH (2012) the European average. The average value for the year of construction of the crackers is taken from the BAT document of the European Commission (2003). The average capacity utilization of the crackers corresponds to the German average value for the year 2015 (VCI, 2018). The lower and upper limits of the interval of the factors as well as for their selected weightings (cf. section 4.1) were defined on the basis of the literature and in consultation with experts (**Table 3**).

[28] According to the calculation logic in section 4, the GWP for products outside the system boundary is obtained from the Eco-profiles. If it is not available there, the value from Ecoinvent is used.

Due to diverging opinions in the literature, the year of construction of the cracker and the propylene capacity is less weighted in the calculation (10%) (cf. section 4.1). A weighting of 15% is assumed both for the site area and the site capacity. The Nelson index is weighted higher (25%), as it is a well-founded and established indicator for assessing the complexity and innovation of a site. The cracker utilization rate is also taken into account, as energy consumption correlates directly with it (cf. section 4.1).

Table 3:
Weightings and lower and upper limits for calculating the cracker efficiency (BASF, 2017c; BAYERNOIL, 2016; Enviros Consulting, 2006; European Commission, 2017, 2003; Reliance Industries Ltd., 2009; Ren et al., 2006).

	Propylene capacity [t/a]	Site area [km²]	Site capacity [kt/a]	Nelson-index	Year of construction (age) of the cracker	Cracker utilization rate
Weightings	10%	15%	15%	25%	10%	25%
Lower limit	30,000	0.82	2,800,000	1	1955	
Upper limit	395,000	10.00	11,840,000	14	2003	

The lower and upper limits for propylene capacity, site area and site capacity are based on the minimum and maximum values of European propylene producers.[29] For the Nelson index, he minimum value of 1 is chosen as the lower limit and the upper limit is set at 14, as the most innovative and complex production sites worldwide are rated at this level (Reliance Industries Ltd., 2009).
For the year of construction of the cracker, the year 1955 was chosen as the lower limit assuming that even older crackers are by now at least as efficient as a cracker from 1955. The upper limit was set to 2003, because the most recent data on the cracker's energy consumption originate from that year (cf. European Commission, 2003; Ren et al., 2006; Enviros Consulting, 2006).

5.2 Case Study on toluene diisocyanate (TDI)

5.2.1 Background and assumptions

The production scheme for TDI production is illustrated in **Figure 4**. The individual production processes, such as the processing of Dinitrotoluene (DNT), depend on the recipes of the individual producers, which can be modelled based on patents. As an example, the production process of DNT is examined in detail (**Figure A. 3**, appendix). For the DNT production, the same recipes are assumed for all four German production sites.

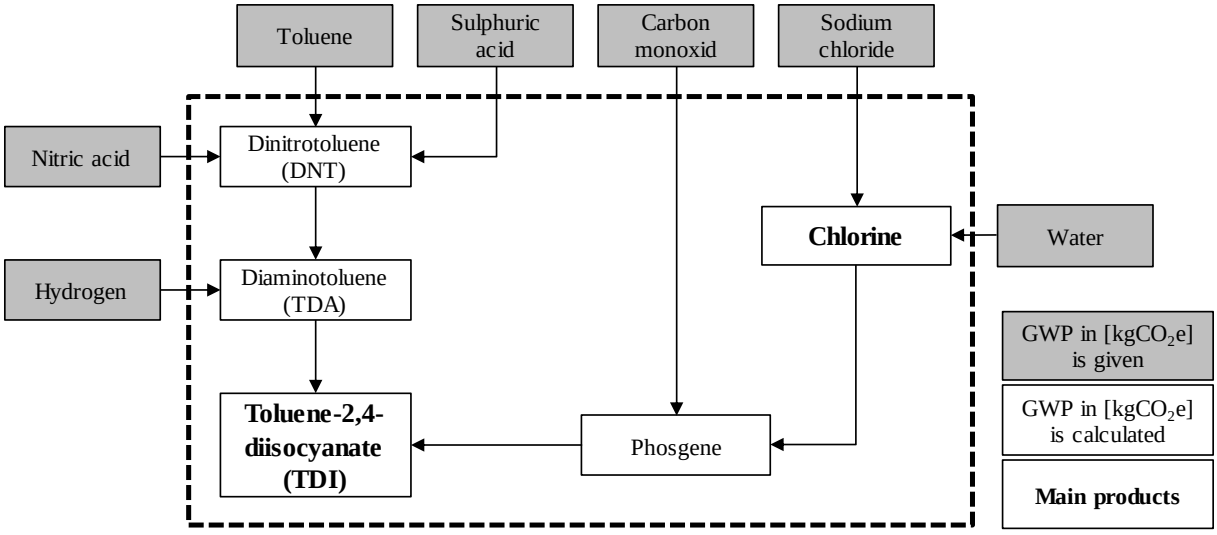


Figure 4: Simplified input-output production scheme for toluene-2,4-diisocyanate (TDI) (based on PlasticsEurope, 2012b).

[29] For the definition of the limits, the European producers are considered both here and also for TDI in the following section, since the BAT documents (European Commission, 2003, 2017) refer to all European producers as well.

For this assumption, current patents for the production of DNT were compared and show the same raw materials and similar mixing ratios (cf. patents Büttner et al., 2005 and Lorenz et al., 2006). In any case, differences in the mixing ratios would remain without consequence in the calculation, since in the highly integrated chemical sites in Germany it is assumed that all surpluses are reused without losses (see section 3.3).

5.2.2 Data on the production process and recipes

According to the production scheme (**Figure 4**) and the individual production recipes (e.g. DNT production, in appendix **Figure A. 3**), reaction equations and mass balances are set up in order to create matrix $\bar{A}$. The resulting matrix $\bar{A}$ [fraction of an reactant for the production of a product] of this case study is shown in **Figure 5**.

$\bar{A} =$

	Sulphuric acid	Nitric acid	Toluene	DNT	Hydrogen	TDA	Sodium chloride	Chlorine	Carbon monoxid	Phosgene	TDI
Sulphuric acid	0	0	0	0	0	0	0	0	0	0	0
Nitric acid	0	0	0	0	0	0	0	0	0	0	0
Toluene	0	0	0	0	0	0	0	0	0	0	0
DNT	**0.39**	**0.36**	**0.25**	0	0	0	0	0	0	0	0
Hydrogen	0	0	0	0	0	0	0	0	0	0	0
TDA	0	0	0	**0.967**	**0.033**	0	0	0	0	0	0
Sodium chloride	0	0	0	0	0	0	0	0	0	0	0
Chlorine	0	0	0	0	0	0	**1**	0	0	0	0
Carbon monoxid	0	0	0	0	0	0	0	0	0	0	0
Phosgene	0	0	0	0	0	0	0	**0.71**	**0.29**	0	0
TDI	0	0	0	0	0	**0.678**	0	0	0	**0.322**	0

Figure 5: Mass proportions of educts in products along the production process of TDI [kg/kg].

DNT is further processed with hydrogen to TDA (**Figure 4**). According to formula (9), the proportions of DNT and hydrogen for the production of TDA are calculated according to the reaction equation in **Figure 6**.

DNT		Hydrogen		TDA		Water
$\mathbf{C_7H_6N_2O_4}$	+	$\mathbf{6H_2}$	→	$\mathbf{C_7H_{10}N_2}$	+	$\mathbf{4H_2O}$
182.14u		12u		122.7u		72u

Figure 6: Reaction equation and mass balance of TDA production.

$$\frac{182.14u - 64u}{122.17u} = 0.967\ (see\ column\ 4, line\ 6)$$

$$\frac{12u - 8u}{122.17u} = 0.033\ (see\ column\ 5, line\ 6)$$

Figure 7: Exemplary calculation of the input values for matrix $\bar{A}$ on the basis of the reaction equation DNT to TDA.

Four oxygen atoms (4x16 - atomic mass of oxygen (O) = 16u) are split off from DNT and four hydrogen atoms (H = 1u) are additionally taken up. The split oxygen atoms also react with hydrogen to form water. Under the assumption of integrated sites (see above), i.e. that by-products can be reused completely, the mass fractions of educts that become by-products are not taken into account. Therefore, the mass of oxygen atoms is subtracted from DNT (cf. **Figure 7**). For hydrogen, only the four hydrogen atoms (12u-8u) that react with DNT to form Diaminotoluene (TDA) are taken into account, since the remaining

hydrogen reacts with oxygen to form water. The other values of the matrix $\bar{A}$ are calculated analogously depending on the respective reaction equation.

Based on the GWPs of the reactants and the system boundaries, vector t_0 is generated for site no. 4[30] as an example (see **Table 4**).[31]

Table 4:
Vector t_0 exemplary for production site 4.

Educt/Reactant	[kgCO₂e/kg]	Source	Vector t_0
Sulphuric acid	0.12395	Ecoinvent V2.2	0.12395
Nitric acid	3.1742	Ecoinvent V2.2	3.1742
Toluene	0.87	Supp.Database	0.87
DNT	0	To be calculated	0
Hydrogen	4.2	Eco-profiles	4.2
TDA	0	To be calculated	0
Sodium chloride	0.06	Eco-profiles	0.06
Chlorine	0	To be calculated	0
Carbon monoxid	1.5541	Eco-profiles	1.5541
Phosgene	0	To be calculated	0
TDI	0	To be calculated	0

The vector *PE* of the production energy is calculated according to section 4.2.2 and the resulting vector is shown for production site 4 (**Table 5**).

Table 5:
Vector *PE* exemplary for production site 4.

Educt/Reactant	Vector *PE* [kgCO₂e/kg]
Sulphuric acid	0
Nitric acid	0
Toluene	0
DNT	0
Hydrogen	0
TDA	0
Sodium chloride	0.7369
Chlorine	0
Carbon monoxid	0.3019
Phosgene	1.9471
TDI	0

5.2.3 Data to calculate the production efficiency

The data for calculating the production efficiency ($EFF_{p,s}^{\text{Site, Prod}}$) for TDI by formula (26) for all sites located in Germany are listed in **Table 6**. The capacity, production volume, site area, the number of production facilities and the proportion of electricity generated at the respective site could be obtained from publicly available sources. For the site area, the size of the entire chemical park is used, since local companies are integrated with each other in order to jointly use the advantages of logistics and heat integration (ChemCoastPark Brunsbüttel, 2018b; CHEMCologne, 2018). The location factor of a site was presented, discussed and determined within the expert interviews with three chemical companies

[30] The TDI production plant in site no. 4 represents one of the four modelled TDI plants (cf. map in **Figure 3**) and serves as an example for the calculations.
[31] The GWP for hydrogen (4.2 [kgCO₂e/kg]) refers to reformer hydrogen (according to the expert interviews, steam reforming is the most economical and widely used method).

and a management consultancy. The evaluation focused primarily on the aspects presented in section 4.2.2 (e.g. transport distances, possible modes of transportation, refinery on-site). The efficiency of electricity production is based on data from the Federal Grid Agency (2018). For the efficiency of steam production, no site-specific information could be found, so that an average value was assumed according to Ren et al. (2006).

Table 6:
Data basis for calculation of site-specific production efficiency of TDI (BASF, 2017a, 2017c, 2017e, 2015; Bundesnetzagentur Deutschland, 2018; ChemCoastPark Brunsbüttel, 2018a; CHEMPARK, 2017, 2016; Covestro Deutschland AG, 2018a, 2018b, 2018c; Hüthig GmbH, 2018b; Ren et al., 2006; SWR, 2018; UBA, 2016; Wirtschaftsregion Lausitz GmbH, 2018).

Site	Capacity TDI [t]	Production volume TDI [t]	Site area [km²]	Location factor [0;10]	Number of production plants at the location	Self-produced electricity	Electricity efficiency	Steam Efficiency
1	300,000	300,000	10.00	10	110	100%	42.41%	85%
2	80,000	80,000	2.90	6	10	100%	33.00%	85%
3	150,000	150,000	4.20	8	14	0%	34.34%	85%
4	300,000	300,000	3.60	9	60	0%	34.00%	85%

Similarly, the site-specific data for calculating the production efficiency of chlorine was collected, since chlorine is a pre-product in the value chain of TDI (see **Figure 4**) and also a main product that can be calculated site-specifically (see section 3.3). However, only the production capacity and the corresponding lower (4,000 t Kapachim, Greece) and upper limit (480,000 t) change in the calculation logic. In this case study, the site-specific approach to chlorine production can only be applied to sites 1 (capacity: 385,000 t) and 4 (capacity: 480,000 t), since no chlorine is produced at sites 2 and 3 (BASF, 2017b; Euro Chlor, 2015; NGZ, 2017). For sites 2 and 3, the value of the GWP for chlorine is taken from the Eco-profiles (0.9 $kgCO_2e/kg$ chlorine) (PlasticsEurope, 2013) and listed in vector t_0 accordingly.

The lower and upper interval limits as well as the selected factors weightings for calculating the production efficiency of TDI (according to section 4.2.2) were defined taking into account the literature and experts consultation (**Table 7**). In the expert interviews, no weightings preferences could be determined so that an equal weighting of all factors was assumed following Laplace and his principle of indifference. The weightings of the degree of integration (71%) and innovation (29%) were adjusted according to the equal weighting within each category ($0.71 \cdot 0.2 \approx 0.29 \cdot 0.5$). The interval restrictions for the TDI capacity, the number of production plants and the site area are based on the minimum and maximum values of European sites producers. For the technical equipment (e.g. frequency-controlled pumps), the maximum value of 10 is assumed for all German sites, since the German TDI production is located at highly integrated production sites. For the production yield, 98% is assumed for all locations on the basis of expert interviews.

Table 7:
Weightings and interval limits for calculating production efficiency (BASF, 2017c, 2017e, 2015; Hüthig GmbH, 2018a; Merchant Research & Consulting, 2013).

	Production capacity TDI [t]	Production flexibility (Amount of production plants at location)	Site area [km²]	Location factor [0;10]	Utilization	Yield	Techn. Equipment [0;10]
	Integration level					Innovation level	
Weightings	71%					29%	
	20%	20%	20%	20%	20%	50%	50%
Lower Limit	80,000	10	2.9	0			
Upper Limit	300,000	110	10.00	10			

For the SEC of electricity for the production of TDI there is only one specific value in the literature (2.76 [GJ/t TDI] in IEA (2009) (**Table 8**). For the required steam, the maximum value is calculated (31.68 [GJ/t]) by adding the difference between the BAT value of the IEA (21.7 [GJ/t] (IEA, 2009)) and the mean value of the Fraunhofer ISI (26.69 [GJ/t] (Fleiter et al., 2013)) to the latter. The International

Energy Agency explicitly mentions that the data on the required energy do not contain any information on the feedstock, since the energy used there has already been taken into account in the necessary pre-products (IEA, 2009). Emissions from the upstream chain are calculated and taken into account in accordance with section 4.2.1.

The SEC for the chlorine production focuses in this study on the state-of-the-art technology (membrane process).[32] The SEC of electrical energy required for the chlorine production with the membrane process ranges between 2,347 kWh/t and 3,796 kWh/t and includes 2,279 to 3,000 kWh/t for electrolysis and 68 to 796 kWh/t for auxiliary "equipment" or "processes" (Euro Chlor, 2010; European Commission, 2014). This corresponds to a total of 8.449 to 13.666 GJ/t chlorine. According to European Commission (2014) and Euro Chlor (2010), the SEC for steam in the membrane process is derived from the steam required for caustic evaporation (0.46 to 1.5 t steam/t caustic) and from auxiliary processes (0.138 to 2.1 t steam/t chlorine). Then, the steam consumption for caustic evaporation must be converted to the reference value for chlorine by multiplying it by the stoichiometric factor of 1.128 t caustic/t chlorine in accordance with BAT (European Commission, 2014). This means that 0.519 to 1.692 t steam/t chlorine are required for the caustic evaporation (European Commission, 2014). In total, a minimum of 0.657 and a maximum of 3.792 t steam/t chlorine are required. This corresponds to an SEC between 1.632 - 9.48 GJ/t chlorine, since according to European Commission (2014) and Euro Chlor (2011) an exergy of 2.5 GJ/t steam is assumed.

The emission factor of the electricity mix and the emission factor for natural gas for Germany are used for the year 2016 according to the Federal Environment Agency (UBA, 2018b, 2016).

Table 8:
Specific energy consumption of TDI and chlorine production and emission factors for electricity and natural gas (Fleiter et al., 2013; IEA, 2009; UBA, 2018b, 2016).

	Electricity		**Steam**	
	min	max	min	max
SEC TDI [GJ/t TDI]	2.76	2.76	21.70	31.68
SEC Chlorine [GJ/t Chlor]	8.45	13.67	1.63	9.48
Emission factor electricity mix [$kgCO_2e$/kWh]	0.516			
Emission factor natural gas [$kgCO_2e$/kWh]	0.199			

5.3 Case study results and discussion

This study showed for the first time the variability of product carbon footprints within production site of the same country. In this study, 2 products of 23 chemical production sites in Germany were investigated. We found that the product carbon footprint (PCF) (Cradle-to-Gate(out)) of propylene produced in 23 German crackers ranges between 0.95 (cracker 18) and 1.51 (cracker 11) [$kgCO_2e$/kg propylene], depending on the installed cracker technology and the operators knowhow (**Figure 8**). Referring to the motivation of this study, this means that companies can reduce their GHG emissions from propylene in their upstream supply chains by up to 37.1% by revising their procurement decisions and by procuring their future propylene from selected German producers with low or lowest PCF. It confirms the necessity of site-specific assessment models and more generally the need to foster technological improvements at chemical productions sites from a sustainable perspective. As currently not all customers can possibly source the material from the "best in class" supplier due to capacity restrictions, it represents only an individual perspective. However, a rising demand for 'greener' produced basic chemicals from several customers will urge suppliers to rethink and optimize existing processes in order to maintain or extend competitive advantages and market share.

A comparison with Zhao et al. (2017) and Kanchanapiya et al. (2015) reveals that the GHG emission reduction potential in global propylene supply chains is even higher. Zhao et al. (2017) calculated a PCF

[32] The membrane process has been used in the construction of new plants for more than 20 years and also, older diaphragm and amalgam plants are successively being converted to membrane plants Behr et al. (2016).

(Cradle-to-Gate(out)) of approx. 2.00 $kgCO_2e/kg$ propylene for a single Chinese steam cracker. In this case, a reduction of the PCF by up to 52.5% would be possible (0.95 vs. 2.00 $kgCO_2/kg$ propylene) compared to the most efficient cracker in Germany. Kanchanapiya et al. (2015) calculated average GHG emissions from Thai crackers (Gate(in)-to-Gate(out)) of 1.33 $kgCO_2/kg$ propylene. Compared to the Gate(in)-to-Gate(out) GHG emissions calculated in this study (system: "propylene production") indicates a reduction potential of 65.5% (0.46 vs. 1.33 $kgCO_2/kg$ propylene).

If we compare the German crackers under study only with regard to the Gate-to-Gate system "propylene production", the differing CO_2e efficiencies of the crackers can be highlighted even more (green bars, **Figure 8**). Cracker 18 with 0.46 [$kgCO_2e/kg$ propylene] has the lowest CO_2e emissions and crackers 11 and 19 with 1.03 [$kgCO_2/kg$ propylene] the highest CO_2e cracker-specific emissions. Thus, in the cracking process for the production of propylene alone, there is a massive CO_2e reduction of 55.4% possible within German crackers.

The CO_2e emissions in the upstream chain (blue bars, **Figure 8**) range between 0.34 and 0.49 [$kgCO_2e/kg$ propylene]) and depend on the feedstock of the cracker (**Table 2**). Emissions in the upstream chain of a cracker are comparatively low if the cracker mainly processes the feedstock naphtha, as the GWP of naphtha production is lower than that of other cracker feedstock fractions such as natural gas, propane or butane (see **Table 2**).

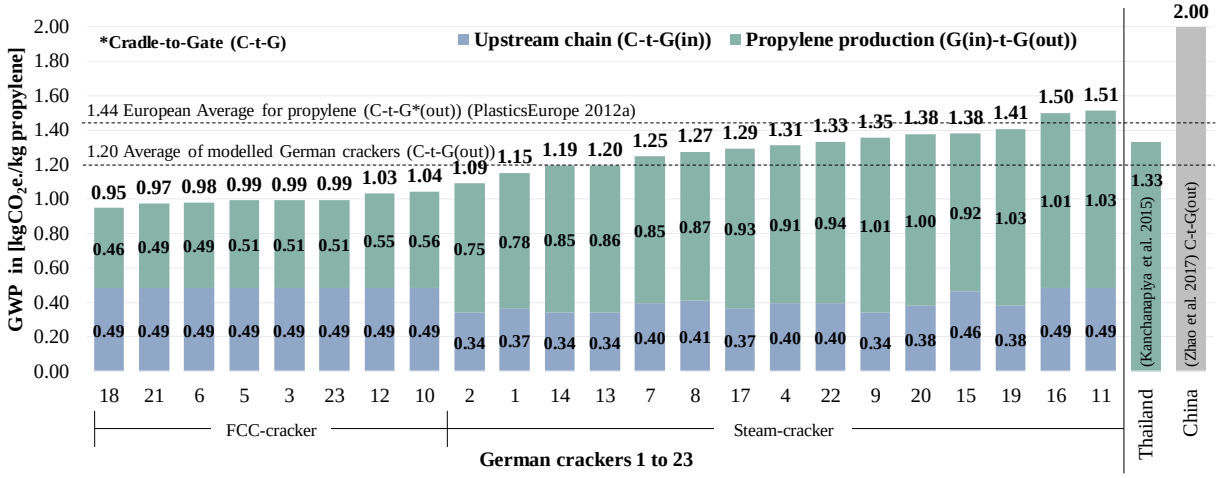


Figure 8: Cracker-specific CO_2e emissions from propylene production of 23 crackers in Germany and a cracker in China, together with European, German and Thai average values.

The average value for all modelled crackers in Germany is 1.20 [$kgCO_2/kg$ propylene]. The comparable European average value in the Eco-profiles is 1.44 [$kgCO_2/kg$ propylene] (Cradle-to-Gate(out)), based on 50 European steam crackers, whose data were collected in 2007 (PlasticsEurope, 2012a). The Ecoinvent V.2.2 value refers to the Eco-profiles and therefore also amounts to 1.44 [$kgCO_2/kg$ propylene] and also applies only to steam crackers. For better comparability and validation purposes, the mean value is therefore also calculated specifically for the modelled steam and FCC crackers in this study and results in 0.99 (FCC crackers) and 1.31 (steam crackers) [$kgCO_2/kg$ propylene]). In Germany, propylene produced in FCC crackers has a lower PCF than produced in steam crackers. Within the German FCC crackers, there is potential for improvement of 8.7% (0.95 = bic[33]; 1.04 = wic[34]). Within the German steam crackers, there is a higher potential for improvement of 27.3% (1.09 = bic; 1.5 = wic). The difference of 0.13 [$kgCO_2/kg$ propylene] (9%) between the mean value of the steam crackers from the Eco-Profiles (1.44) and from this study (1.31) can be explained by more recent data used in this study for the energy consumption and the raw material mix of the feedstock (e.g. European Commission, 2017; Koottungal, 2015) than used for the Eco-Profiles (from 2007). Moreover, this study only refers to German crackers. The results could lead to the

[33] Best in class
[34] Worst in class

hypothesis that German crackers tend to be more efficient than the European average. However, no references are known to the authors that could support this hypothesis.

In 2017, 4,243 [kt] of propylene were produced in Germany (VCI, 2019a) and 14,432 [kt] in Europe (Cefic, 2019). Using the average value calculated in the model (1.20 [kg CO_2e/kg propylene]) and the European average according to PlasticsEurope (1.44), the propylene production emitted approx. 5,092 [kt CO_2] in Germany and approx. 20,783 [ktCO_2e] in Europe. If all crackers were as GHG or as energy-efficient as the best German cracker 18, approx. 1,061 [ktCO_2e] could be saved annually in propylene production in Germany and approx. 7,072 [kt CO_2] respectively in Europe.

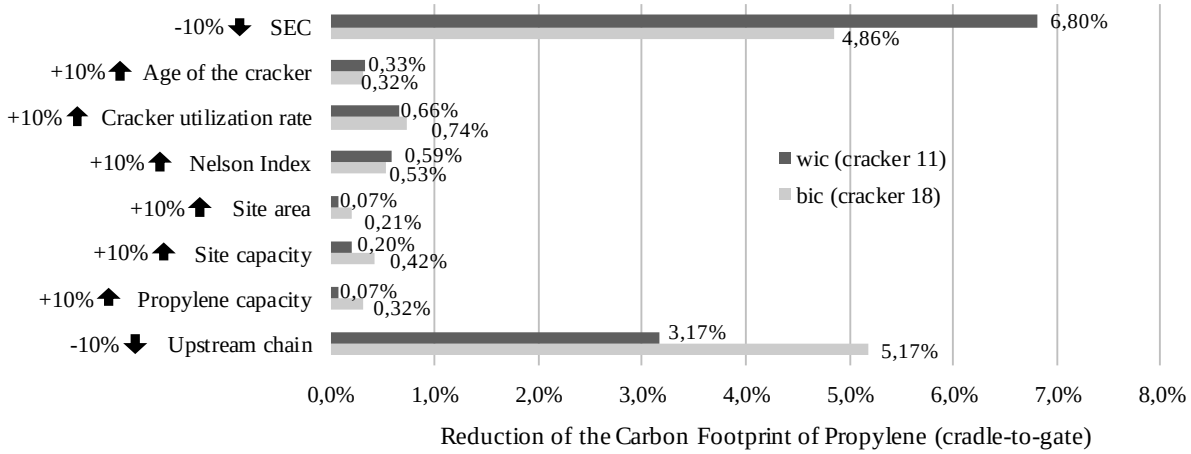


Figure 9: Sensitivity analysis results of the PCF of propylene from best (18) and worst in class cracker (11) when selected input variables are improved by 10%.

In a sensitivity analysis, important input parameters of the site-specific approach for HVC (see section 4.1) were examined. In this analysis, each value was individually improved by 10% (for the reference values see Table 1 and Table 3). As a consequence, the SEC and upstream chain PCF value were reduced by 10% each while the utilization rate, Nelson index, site area, site capacity and propylene capacity were increased by 10% and the cracker was assumed to be five years younger than originally built.

The sensitivity analysis was applied to the bic-cracker (18) and the wic-cracker (11) in order to identify GHG reduction potentials for both (see **Figure 9**). The result shows that energy saving measures (reduction of SEC) have the greatest impact on the PCF of propylene; a 10% reduction of the specific energy consumption (SEC) results in a 4.86% PCF reduction for cracker 18 and a 6.80% PCF reduction. Secondly, GHG emissions reduction in the upstream chain by 10% have the second largest impact and result in a 5.17% reduction in propylene PCF in cracker 18 and 3.17% in cracker 11. The influence of all other parameters is significantly lower (<<1%). The third largest influence would be an increase in the utilization rate by 10% that would reduce the PCF by 0.74% (Cracker 18) and by 0.66% (Cracker 11). A weakness of the model and thus also of the sensitivity analysis results is the dependency on the weightings of some of the input parameters that were defined with experts (see table 3). A misjudgement or another weighting of the experts could lead to different result and conclusions. In further research, a large survey among experts would be conceivable to in order to specify the currently used weightings.

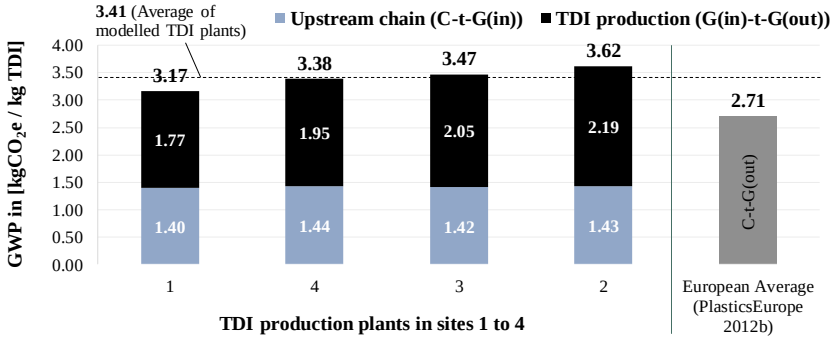


Figure 10: Site-specific CO2e emissions from TDI production in Germany.

The results of the case study on TDI (**Figure 10**) show that TDI in Germany is produced with a PCF between 3.17 [kg CO_2e/kg TDI] (site 1) and 3.62 [kg CO_2e/kg TDI] (site 2), depending on the production plant. Thus, in Germany there is a PCF-specific reduction potential in TDI production of up to 12.4%.

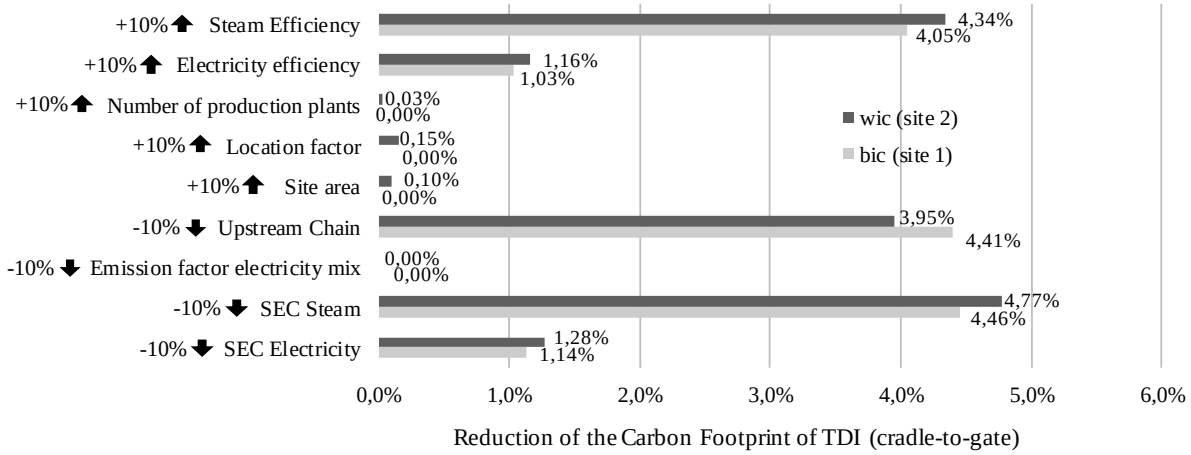


Figure 11: Sensitivity analysis results of the PCF of TDI from the best (located site 1) and worst in class plant (located site 2) when selected input variables are improved by 10%.

Likewise, a sensitivity analysis is performed for TDI for the best (site 1) and worst (site 2) site (see **Figure 11**). For this purpose, the values of most relevant input parameters of the site-specific model for other basic chemicals (see section 4.2) are improved by 10% and the model results are shown and analysed. Thus, the values of steam and electricity efficiency, upstream chain, emission factor of the electricity mix and the specific energy consumption (SEC) of steam and electricity are reduced by 10%, while the number of production plants onsite, the location factor and the plant area are increased by 10%. The sensitivity analysis results show that in particular energy savings in the generation of the required steam (SEC Steam) (PCF reduction by 4.46% at site 1 and by 4.77% at site 2) and an increased steam generation efficiency have a major impact on the PCF (PCF reduction by 4.05% at site 1 and by 4.34% at site 2). The third largest influence lies in the upstream chain: a reduction of GHG emissions in the upstream chain by 10% would reduce the PCF of TDI by 4.41% at site 1 and by 3.95% at site 2. This is followed by the amount of electrical energy required (SEC Electricity): a 10% reduction would reduce the PCF by 1.14% at site 1 and by 1.28% at site 2. The emission factor of the country-specific electricity mix has no influence in this case (0%), since the two TDI plants under consideration are each operated in sites that produce 100% of their own electricity (see Table 6). In this case, the sites should therefore aim to increase the efficiency of their power plants. An increase of 10% will result in a TDI-PCF reduction of 1.03% at site 1 and 1.16% at site 2. The number of production plants onsite, the size and the location factor of the site have almost no influence. In the HVC model (section 4.1), a main weakness remains in the calculation logic for other basic chemicals (section 4.2) since it also uses weightings for some of the input parameters that were defined by a small number of experts (see Table 7). Cumulating

the improvements of the individually analysed factors in **Figure 9** and **Figure 11** might lead to higher PCF reductions.

The average Carbon Footprint of TDI of the four production sites is 3.41 [$kgCO_2e$/kg TDI]. This value is 0.70 higher (26%) than the value stated in the Eco-profiles from 2012 (2.71 [$kgCO_2e$/kg TDI]) (PlasticsEurope, 2012b).

This difference can be traced back to the calculation of the GWP of the upstream chain, as the data used for the calculation was obtained from the Ecoinvent V.2.2 database, which is partly outdated. For example, the GWPs determined in Ecoinvent V.2.2 for sulphuric and nitric acid, which have a major impact on emissions in the upstream chain of TDI (see appendix **Figure A. 3**), mainly date back from studies in the 1990s and 2000-2001 where technologies were less integrated and efficient and where national energy mixes had higher carbon and GHG emission factors. This assumption is supported by the high value of the GWP from Ecoinvent V.2.2 of 6.39 [$kgCO_2e$/kg TDI]. This value is based on three European sites in Germany, France and Italy with data from 1995-2001 (Ecoinvent V.2.2). Thus, it becomes obvious how strongly the result varies depending on the currentness of the data, the technologies onsite and the emissions factors related to the national energy mix.

Furthermore, it should be noted, that the comparison of our results with LCA databases is limited because the used allocation methods may differ depending on the LCA database, resulting in inaccuracies and widely differing results. However, a comparison with the Eco-Profiles of PlasticsEurope is in any case valid, since both apply the same mass allocation method (see PlasticsEurope, 2012b). Furthermore, a comparison of the PCF of TDI with other studies is not possible, as no similar site-specific studies exist in literature.

The influence of the currentness of the data on the result is further demonstrated by an exemplary calculation on nitric acid. For this purpose, the current PCF of nitric acid 2.63 [$kgCO_2e$/kg] (Ecoinvent V.3) was inserted in the model instead of the previous value of 3.17 [$kgCO_2e$/kg] (Ecoinvent V.2.2). This change (-17%) alone reduces the average value of the modelled sites from 3.41 to 3.28 [$kgCO_2e$/kg TDI] by -3.8%. Another reason for the deviation in the results are the different emission factors used for the electricity supply. For example, if the emission factor of the German electricity mix (0.516 $kgCO_2$/kWh) is replaced by the European value (0.296 $kgCO_2$/kWh) (EEA, 2018) and thus reduced by -43%, the average value of the modelled sites changes also from 3.41 to 3.28 [$kgCO_2e$/kg TDI][35]. With these two changes alone, the deviation between our results and Ecoinvent V.2.2 PCF data on TDI can be reduced from 26% to 16%. The remaining deviation can be explained by the different data basis and different production processes. For example, some sites feed the required hydrogen into the TDI production process not only from reformers but also from chloralkali electrolysis. Due to the applied mass allocation method, hydrogen from chloralkali electrolysis has a PCF of only 1.14 [$kgCO_2e$/kg] (PlasticsEurope, 2013) compared to the PCF of 4.2 [$kgCO_2e$/kg] produced by the steam reformer. With 100% hydrogen supply from the more efficient chloralkali electrolysis, the modelled average value would be reduced from 3.41 to 3.34 [$kgCO_2e$/kg TDI] (by 2%). Also, biomass could be used as an energy source in the reformer to further reduce site-specific GHG emissions. However, since in our model the same data respectively GWPs were used for the inputs in the upstream chains for all sites, the absolute differences between the production sites remain constant and are comparable with each other. Due to the outdated data basis of Ecoinvent V2.2. in the upstream chain, we focus on assessing the processes within the system boundary "TDI production" (Gate(in)-to-Gate(out)). Within this system boundary "TDI production", we reveal site-specific variations in GHG emissions between 1.77 and 2.19 [$kgCO_2e$/kg TDI]. This corresponds to a possible PCF reduction potential of 19.2% between site 2 and site 1).

In addition, our model "$ECCO_2$-Basic Chemicals" calculates the result vector B_P (cf. section 4.2) for each considered site in tabular form (**Figure 12**), which contains the GWP of all precursors, intermediates and the end product. This way, not only end products but entire value chains can be compared on a site-specific basis.

[35] But as shown above, this has no effect on the plants in sites 1 and 2, as they use 100% self-produced electricity. The reduction in the average value is therefore achieved by improving the PCF of TDI plants from sites 3 and 4.

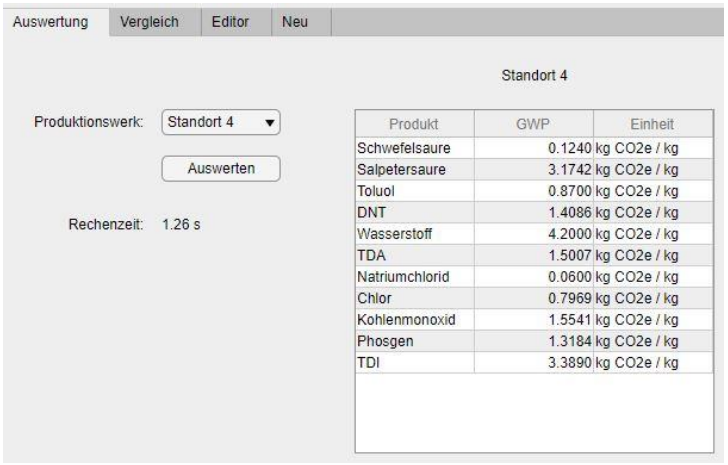


Figure 12: Result vector BP, exemplary for site 4 ("Standort 4")[36].

6 Conclusion and outlook

In this study, a new assessment model was developed to estimate the CO_2e emissions (Cradle-to-Gate) of basic chemicals from crackers (ECCO$_2$-HVC model) and other chemical production plants (ECCO$_2$-Basic Chemicals model) on a site-specific basis.

The new model combines the method of a technology-based bottom-up life cycle assessment with a newly developed method for estimating the energy efficiency of chemical production plants to assess the plant-specific product carbon footprint (PCF) of specific basic chemicals.

A novelty of this combined approach is that it allows a model application and PCF calculation only based on publicly available data, in order to avoid the limitation of confidential company internal production data that are not available to the public (cf. Saygin, 2012). However, if internal company production data is available, it can be easily integrated into the model to further improve the accuracy of the results. Similarly, data sets can be updated at any time as soon as they are available. Thus, this study results and the developed model are highly interesting and useful for a wide range of stakeholders along the basic chemical and plastic value chains (e.g. in the automotive, packing or construction industries), as well as authorities, policy makers and the interested public.

Two case studies on the bulk chemicals propylene and toluene diisocyanate (TDI) were performed and showed a considerable GHG emission reduction potential. The case studies' results are plausible and could be validated with LCA databases and literature sources. In the case of propylene, the product carbon footprint (Cradle-to-Gate) of propylene production in Germany shows variations between production sites from 0.95 to 1.51 [kgCO_2e/kg propylene]. In the Gate-to-Gate assessment, site-specific GHG emissions range between 0.46 to 1.03 [kgCO_2e/kg propylene]. This indicates a GHG reduction potential of 37% produced propylene (Cradle-to-Gate) by selection of the most efficient production site and upstream supplier. As currently not all customers can possibly source the material from the "best in class" supplier due to capacity restrictions, it represents only an individual perspective. If all crackers were as GHG or as energy-efficient as the "best in class" cracker, approx. 1,061 [ktCO_2e] could be saved annually in propylene production in Germany and approx. 7,072 [kt CO_2] in Europe, respectively. Worldwide, the GHG savings' potential is even much higher when considering that currently about 12% (14 kt) of the worldwide propylene production capacity is located in Europe (worldwide production capacity: 120 kt) (GlobalData, 2019).

The results calculated for TDI vary depending on the production sites between 3.17 and 3.62 [kgCO_2e/kg TDI] (Cradle-to-Gate) and between 1.77 and 2.19 [kgCO_2e/kg TDI] (Gate-to-Gate).

[36] The figure is in German, because it is a screenshot from the "ECCO$_2$-Basic Chemicals" model implemented in German (programmed in MATLAB).

From an ecological point of view, the case studies show that it makes a huge difference from which site chemical products are procured and delivered. Thus, for manufacturers of plastic-intensive products, such as companies in the automotive, packaging or construction industries, there is an immense GHG emission reduction potential by changing procurement decisions on basic chemicals and plastics in favour of CO_2e efficient producers respectively suppliers. Therefore, these companies should integrate the site-specific PCF of their suppliers as a decision criterion in their supplier selection process.

In total, this new site-specific assessment approach aims at making a contribution to the scientific field of sustainability management and enables a comparability among chemical production sites. Thus, it allows for informed purchase selection decisions and to reduce the GHG emissions within supply chains. The case study applications do not only confirm the necessity for a site-specific evaluation, but also show that a purchasing decision in favour of the most efficient producer can make a crucial contribution to the reinforcement of and investment in economically viable sustainable supply chains.

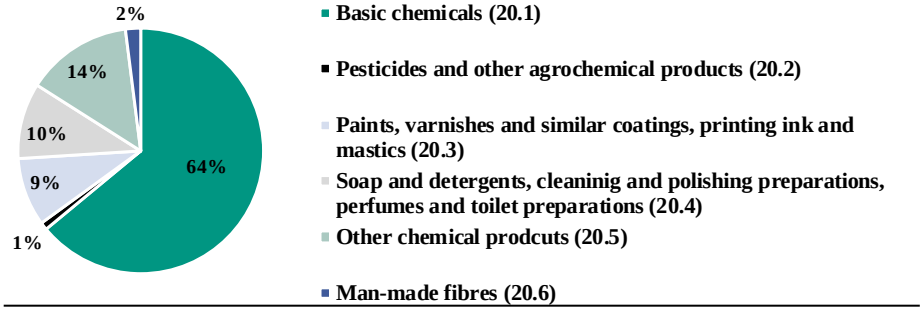
The presented model also opens up further research activities to extend and revise current decision support systems, for example by Multi Criteria Decision Making (MCDM) approaches. Worldwide, the GHG emissions from the production of basic chemicals could thus be reduced immensely if purchasing decisions are not only based on price, delivery time and quality, but also on the site-specific carbon footprint of the product.

In addition, current limitations of the model could also be explored in future research activities. Input raw materials and chemicals for the production system under study that were extracted or produced outside the system boundaries were considered with an average GWP taken from LCA databases. As well, for these input materials a site-specific approach would be desirable in the future to assess GHG emissions in the upstream chains as well (e.g. oil production) and provide further transparency along the value chains. Accordingly, an extension of the site-specific approach to downstream value chains in which basic chemicals are further processed is worthwhile, e.g. to assess a value chain-specific Product Carbon Footprint for the production of polypropylene or polyurethane.

Also, analysis of production sites in the EU or worldwide is required to make GHG emissions from basic chemicals production conditions more transparent in global supply chains. Furthermore, our new site-specific approach was primarily developed based on a simplified LCA and with a focus on the impact category GWP. Analogously, this approach could be transferred to other impact categories of the LCA and lead to even more ecological transparency in global and national supply chains.

Appendix

Figure A. 1: Classification and description of economic divisions in the chemical industry (data from EU (2006)) and weighting of the share of the production index in the chemical industry in Germany (based on data from VCI (2018)).



Shares of specific chemical divisions in the production index		
Basic chemicals (20.1)	**64%**	
Industrial gases (20.11)		1%
Dyes and pigments (20.12)		2%
Other inorganic basic chemicals (20.13)		4%
Other organic basic chemicals (20.14)		37%
Fertilisers and nitrogen compounds (20.15)		4%
Plastics in primary forms (20.16)		15%
Synthetic rubber in primary forms (20.17)		1%
Pesticides and other agrochemical products (20.2)	**1%**	
Paints, varnishes and similar coatings, printing ink and mastics (20.3)	**9%**	
Soap and detergents, cleaninig and polishing preparations, perfumes and toilet preparations (20.4)	**10%**	
Soap and detergents, cleaninig and polishing preparations (20.41)		6%
Perfumes and toilet preparations (20.42)		4%
Other chemical prodcuts (20.5)	**14%**	
Explosives (20.51)		1%
Glues (20.52)		1%
Essential Oils (20.53)		1%
Other chemical products n.e.c. (20.59)		11%
Man-made fibres (20.6)	**2%**	

Figure A. 2: CO_2e emissions from crackers using the example of ethylene production (cefic, 2008).

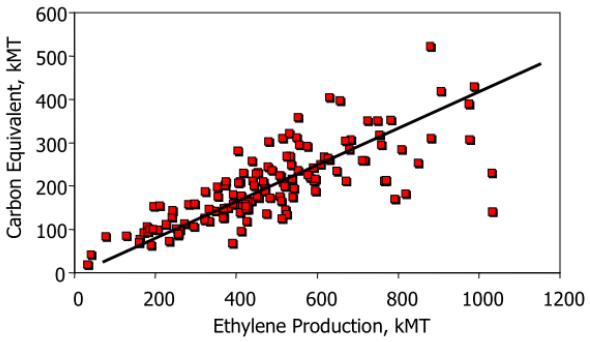


Figure A. 3: Production of DNT according to Lorenz et al. (2006).

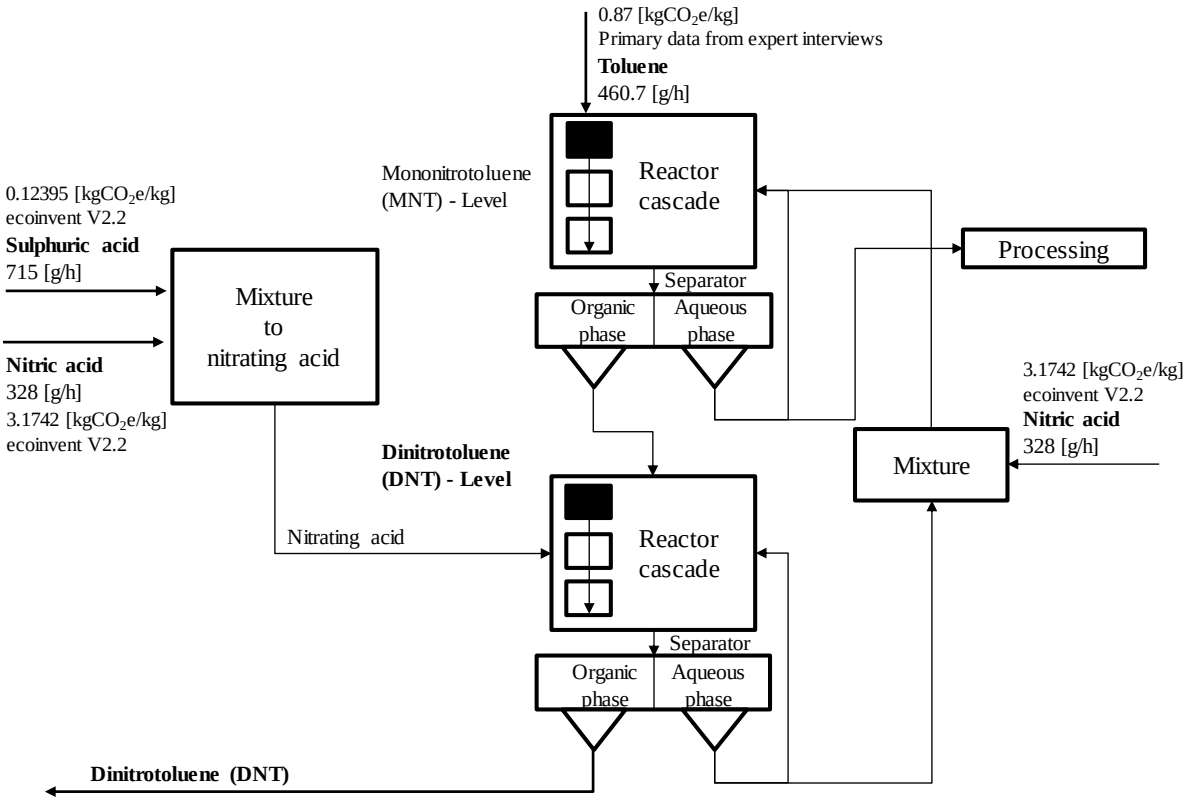


Table A. 1:
Feedstock mixture of the selected crackers (Data from Koottungal (2015)).

Cracker	Production path	Feedstock				
		Ethane	Propane	Butane	Naphtha	Gasoil
1	SC	0.0%	5.0%	5.0%	90.0%	0.0%
2	SC	0.0%	0.0%	0.0%	100.0%	0.0%
3	FCC					100.0%
4	SC	4.0%	6.0%	6.0%	74.0%	10.0%
5	FCC					100.0%
6	FCC					100.0%
7	SC	0.0%	2.0%	12.0%	73.0%	13.0%
8	SC	1.0%	1.0%	11.0%	64.0%	23.0%
9	SC	0.0%	0.0%	0.0%	100.0%	0.0%
10	FCC					100.0%
11	SC	0.0%	0.0%	0.0%	0.0%	100.0%
12	FCC					100.0%
13	SC	0.0%	0.0%	0.0%	100.0%	0.0%
14	SC	0.0%	0.0%	0.0%	100.0%	0.0%
15	SC	13.0%	17.0%	17.0%	53.0%	0.0%
16	SC	0.0%	0.0%	0.0%	0.0%	100.0%
17	SC	0.0%	0.0%	10.0%	90.0%	0.0%
18	FCC					100.0%
19	SC	2.5%	6.0%	6.0%	84.0%	1.5%
20	SC	2.5%	6.0%	6.0%	84.0%	1.5%
21	FCC					100.0%
22	SC	4.0%	6.0%	6.0%	74.0%	10.0%
23	FCC					100.0%
SC	No site-specific data available: Average feedstock of European steam crackers					
FCC	No site-specific data available: 100% gas oil					

Table A. 2:
Data basis to calculate the cracker efficiency (BASF, 2017d, 2016; BAYERNOIL, 2016, 2014; bp, 2008, 2008; bp Deutschland, 2018a, 2018b, 2018c; Burghausen, 2018; Chemie Technik, 2016; CHEMPARK, 2017; DOW, 2015; Evonik Industries AG, 2018; Gunvor Raffinerie Ingolstadt, 2018, 2017, 2016; Holborn Refinery, 2018; Hustede, 2018; Industriepark Schwedt, 2018; INEOS Köln GmbH, 2007; Lynondellbasell, 2017; MiRO Mineraloelraffinerie Oberrhein, 2018; OMV Deutschland GmbH, 2016; PCK, 2018; PKN ORLEN Capital Group, 2016; Raffinerie Heide GmbH, 2016, 2012; Rosneft, 2016; Shell Rheinland Raffinerie, 2018; Total Raffinierie Mitteldeutschland, 2018).

Cracker	Propylene Capacity [t/a]	Site capacity [kt/a]	Site area [km^2]	Nelson-index	Year of construction of the Cracker	Cracker utilization
1	125,000	7,113,116	10.00	14.0	1965	85.66%
2	220,000	7,113,116	10.00	14.0	1980	85.66%
3	30,000	10,533,000	4.27	6.8	1981	85.66%
4	30,000	10,533,000	4.27	6.8	1981	85.66%
5	70,000	10,533,000	4.27	6.8	1976	85.66%
6	75,000	11,840,000	1.60	8.4	1991	85.66%
7	335,000	11,840,000	2.50	8.4	1976	85.66%
8	310,000	11,840,000	2.50	8.4	1976	85.66%
9	310,000	2,800,000	3.20	6.5	1976	85.66%
10	55,000	4,174,000	1.28	7.5	1970	85.66%
11	60,000	4,500,000	1.34	9.6	1976	85.66%
12	40,000	4,500,000	3.75	6.1	1976	85.66%
13	325,000	7,113,116	3.60	13.0	1963	85.66%
14	335,000	7,113,116	3.60	13.0	1963	85.66%
15	190,000	7,113,116	1.25	6.5	1976	85.66%
16	150,000	7,113,116	2.70	6.5	1976	85.66%
17	395,000	7,113,116	2.70	6.5	1976	85.66%
18	320,000	11,160,000	4.58	9.4	1984	85.66%
19	210,000	4,433,041	0.82	7.3	1967	85.66%
20	260,000	4,433,041	0.82	7.3	1976	85.66%
21	250,000	10,078,000	2.20	9.8	1976	85.66%
22	195,000	7,113,116	4.40	6.5	1976	85.66%
23	140,000	7,113,116	3.20	7.1	1997	85.66%

Data from expert interviews
Average values

References

AGEB (2009): Energy balances of Germany 1990-2007 and evaluation tables 1990-2008. AG Energiebilanzen e.V, DIW Berlin, EEFA, Köln AG (in German).

Amghizar, Ismaël; Vandewalle, Laurien A.; van Geem, Kevin M.; Marin, Guy B. (2017): New Trends in Olefin Production. In Engineering 3 (2), pp. 171–178. DOI: 10.1016/J.ENG.2017.02.006.

Arzoumanidis, Ioannis; Salomone, Roberta; Petti, Luigia; Mondello, Giovanni; Raggi, Andrea (2017): Is there a simplified LCA tool suitable for the agri-food industry? An assessment of selected tools. In Journal of Cleaner Production 149, pp. 406–425. DOI: 10.1016/j.jclepro.2017.02.059.

Ayres, Robert U. (1995): Life cycle analysis. A critique. In Resources, Conservation and Recycling 14 (3-4), pp. 199–223. DOI: 10.1016/0921-3449(95)00017-D.

BASF (2015): News Release. BASF starts operations at 300,000-metric-ton TDI plant at Ludwigshafen site 17.11.2015.

BASF (2016): Ludwigshafen production site 2015 in figures. Available online at https://www.basf.com/documents/corp/de/about-us/publications/reports/2016/LU-in-Zahlen-2015_Infoblatt_A4_DE.pdf.

BASF (2017a): Chemical company takes positive stock. REGIONAL PRESS RELEASE 15.03.2017. Available online at https://www.basf.com/de/de/company/about-us/sites/Schwarzheide/Press/Presseinformationen-Schwarzheide/2017/03/PI-08.html. (in German).

BASF (2017b): Group management report - Products and investments - BASF Online Report 2016. BASF SE. Available online at https://bericht.basf.com/2016/de/konzernlagebericht/segmente/chemicals/produkte-und-investitionen.html, checked on 12/3/2018.

BASF (2017c): Ludwigshafen production site 2017 in figures. Available online at https://www.basf.com/documents/corp/de/about-us/publications/reports/2018/LU-in-Zahlen-2017.pdf, checked on 11/22/2015.

BASF (2017d): The Heart of the Verbund. Available online at https://www.basf.com/de/en/company/about-us/sites/ludwigshafen/production/the-production-verbund/Steamcracker.html, checked on 11/20/2018.

BASF (2017e): Environmental Report Data and Facts 2017 BASF Schwarzheide GmbH. (in German).

BASF (2019): Steam cracker. Environment. Edited by BASF SE. Available online at https://www.basf.com/global/de/who-we-are/organization/locations/europe/german-sites/ludwigshafen/gesellschaftliches-engagement/woran-wir-arbeiten/education/angebote-7-13/unterrichtsmaterialien/Steamcracker.html, updated on 1/25/2019, checked on 1/25/2019.

Bauer, Christian; Hofer, Johannes; Althaus, Hans-Jörg; Del Duce, Andrea; Simons, Andrew (2015): The environmental performance of current and future passenger vehicles. Life cycle assessment based on a novel scenario analysis framework. In Applied Energy 157, pp. 871–883. DOI: 10.1016/j.apenergy.2015.01.019.

BAYERNOIL (2014): Bayernoil journal - The magazine of BAYERNOIL Raffineriegesellschaft mbH (Ausgabe 2/2014). (in German).

BAYERNOIL (2016): Environmental Report 2016 of BAYERNOIL Raffineriegesellschaft mbH (in German).

Behr, Arno; Agar, David W.; Jörissen, Jakob (2010): Einführung in die Technische Chemie. (engl.: Introduction to Technical Chemistry) Heidelberg: Spektrum Akademischer Verlag. Available online at http://site.ebrary.com/lib/alltitles/docDetail.action?docID=10356129. (in German).

Behr, Arno; Agar, David W.; Jörissen, Jakob; Vorholt, Andreas J. (2016): Einführung in die Technische Chemie. (engl.: Introduction to Technical Chemistry). 2. Edition. Berlin: Springer Spektrum. Available online at http://dx.doi.org/10.1007/978-3-662-52856-3. (in German).

Bello, Sara; Méndez-Trelles, Pedro; Rodil, Eva; Feijoo, Gumersindo; Moreira, Maria Teresa (2020): Towards improving the sustainability of bioplastics. Process modelling and life cycle assessment of two separation routes for 2,5-furandicarboxylic acid. In Separation and Purification Technology 233, p. 116056. DOI: 10.1016/j.seppur.2019.116056.

Benchaita, T. (2013): Greenhouse Gas Emissions from New Petrochemical Plants. Background Information Paper for the Elaboration of Technical Notes and Guidelines for IDB Projects. Available online at https://publications.iadb.org/bitstream/handle/11319/5962/Greenhouse%20Gas%20Emissions%20from%20New%20Petrochemical%20Plants%20.pdf;sequence=1, checked on 11/20/2018.

Bilec, Melissa; Ries, Robert; Matthews, H. Scott; Sharrard, Aurora L. (2006): Example of a Hybrid Life-Cycle Assessment of Construction Processes. In J. Infrastruct. Syst. 12 (4), pp. 207–215. DOI: 10.1061/(ASCE)1076-0342(2006)12:4(207).

BMLFUW (2010): Bundesministerium für Land- und Forstwirtschaft, Umwelt und Wasserwirtschaft Österreich.

Leitfaden für das Klima- und Energiekonzept im Rahmen von UVP-Verfahren. Spezialteil Industrieanlagen. (engl.: Federal Ministry of Agriculture, Forestry, Environment and Water Management Austria. Guidelines for the climate and energy concept in the context of EIA procedures. Special part industrial plants.) (in German).

BMUB (2016): Bundesministerium für Umwelt, Naturschutz, Bau und Reaktorsicherheit (BMUB).

Klimaschutzplan 2050. Klimaschutzpolitische Grundsätze und Ziele der Bundesregierung. (engl: German Federal Ministry for the Environment, Nature Conservation, Construction and Nuclear Safety (BMUB). Climate Protection Plan 2050. Climate protection policy principles and objectives of the Federal Government.) 1. Edition. (in German).

BMWi (2019): Klimaschutzprogramm 2030. Edited by Bundesministerium für Wirtschaft und Energie. (engl.: Climate Protection Programme 2030 Edited by Federal Ministry of Economics and Energy in Germany). Available online at https://www.bmwi.de/Redaktion/DE/Artikel/Industrie/klimaschutzprogramm-2030.html, checked on 4/12/2020. (in German)

bp (2008): Financial and Operating Information 2004-2008. Refining and Marketing.

bp Deutschland (2018a): Historie. (engl.: bp Germany. History). Available online at http://www.bp.com/de_de/germany/ueber-bp/aktivitaeten-in-deutschland/raffinerie-gelsenkirchen/wer-wir-sind/historie.html. (in German).

bp Deutschland (2018b): Wo wir sind. (engl.: bp Germany. where we are). Available online at https://www.bp.com/de_de/germany/ueber-bp/aktivitaeten-in-deutschland/raffinerie-gelsenkirchen/wo-wir-sind.html, checked on 11/20/2018. (in German).

bp Deutschland (2018c): Zahlen und Fakten. (engl.: bp Germany. Figures and facts). Available online at http://www.bp.com/de_de/germany/ueber-bp/aktivitaeten-in-deutschland/raffinerie-gelsenkirchen/wer-wir-sind/zahlen-und-fakten.html. (in German).

Breun, Patrick (2016): Ein Ansatz zur Bewertung klimapolitischer Instrumente am Beispiel der Metallerzeugung und -verarbeitung. Dissertation (engl.: An approach for the evaluation of climate policy instruments using the example of metal production and processing). Karlsruher Institut für Technologie (KIT); Karlsruher Institut für Technologie, Karlsruhe. Available online at http://nbn-resolving.de/urn:nbn:de:0072-527140. (in German).

Bundesnetzagentur Deutschland (2018): Kraftwerksliste (engl.: Power plant list) 2018. (in german)

Burghausen (2018): Industriegebiet Nord - Zukunft des Industrie-Standorts (engl.: Industrial area north - future of the industrial location). Available online at https://www.burghausen.com/index.php?id=98, checked on 11/20/2018. (in German).

Büttner, J.; Mackenroth, W.; Hermann, H.; Konieczny, P.; Gebauer, J. (2005): Patent Herstellung DNT - WO2005075407A1 (engl.: Patent production DNT - WO2005075407A1). Available online at

https://patents.google.com/patent/WO2005075407A1/de?q=Herstellung&q=Dinitrotoluol&scholar&oq=Herstellung+Dinitrotoluol, checked on 11/21/2018.

Büyüközkan, Gülçin (2012): An integrated fuzzy multi-criteria group decision-making approach for green supplier evaluation. In International Journal of Production Research 50 (11), pp. 2892–2909. DOI: 10.1080/00207543.2011.564668.

Cefic (2008): An allocation method for petrochemicals. Available online at file:///C:/Users/vk1683/Downloads/14leuckx_sectoral_en%20(2).pdf, checked on 11/20/2018.

Cefic (2019): Propylene: Nameplate capactiy, production, consumption in EU15 + Norway. PetroChemicalsEurope. Available online at: https://www.petrochemistry.eu/about-petrochemistry/petrochemicals-facts-and-figures/european-market-overview/, checked on 05/12/2020.

cefic (2020): Facts & Figures of the European chemical industry. Hg. v. The European Chemical Industry Council. Available online at https://cefic.org/app/uploads/2019/01/The-European-Chemical-Industry-Facts-And-Figures-2020.pdf.

Ceresana Market Research (2014): Marktstudie Propylen (engl.: Market Study Propylene) (2. edition). Available online at https://www.ceresana.com/de/marktstudien/chemikalien/propylen/propylen-markt-anteil-kapazitaet-angebot-nachfrage-prognose-innovation-anwendung-wachstum-produktion-industrie.html, checked on 11/20/2018.

Chakrabarty, Arijit (2017): The Hadamard product and the free convolutions. In Statistics & Probability Letters 127, pp. 150–157. DOI: 10.1016/j.spl.2017.04.009.

ChemCoastPark Brunsbüttel (2018a): Unternehmen. (engl.: company). Available online at https://www.chemcoastpark.de/de/unternehmen/#sasol-germany, checked on 11/22/2018. (in German).

ChemCoastPark Brunsbüttel (2018b): Unternehmen. Covestro Deutschland - Gebündelte Kompetenz. (engl.: Company. Covestro Germany - combined competence). Available online at https://www.chemcoastpark.de/de/unternehmen/, checked on 11/23/2018. (in German).

CHEMCologne (2018): Erfolgsfaktor für die Region - Verbundproduktion. (engl.: Success factor for the region - integrated production). Available online at https://www.chemcologne.de/investieren-im-rheinland/verbundproduktion.html, checked on 11/23/2018. (in German).

Chemie Technik (2016): Erfolgreicher Turnaround in Traditions-Chemiewerk (Juni). (engl.: Successful turnaround in traditional chemical site (June)). Available online at https://www.chemietechnik.de/erfolgreicher-turnaround-in-traditions-chemiewerk/. (in German).

CHEMPARK (2016): Bilanz des CHEMPARK Dormagen für 2015. 271 Millionen Euro Investitionen stärken Standort. (engl.: Balance sheet of CHEMPARK Dormagen for 2015. 271 million euros investment strengthens site), updated on 4/6/2016, checked on 11/22/2016. (in German).

CHEMPARK (2017): Chempark Dormagen. Zahlen und Fakten. (engl.: Chempark Dormagen. Facts and figures). Available online at https://www.chempark.de/de/chempark-dormagen.html, updated on 12/31/2017, checked on 11/20/2018. (in German).

Chen, Qianqian; Lv, Min; Wang, Danfeng; Tang, Zhiyong; Wei, Wei; Sun, Yuhan (2017): Eco-efficiency assessment for global warming potential of ethylene production processes. A case study of China. In Journal of Cleaner Production 142, pp. 3109–3116. DOI: 10.1016/j.jclepro.2016.10.156.

Chhipi-Shrestha, Gyan Kumar; Hewage, Kasun; Sadiq, Rehan (2015): 'Socializing' sustainability. A critical review on current development status of social life cycle impact assessment method. In Clean Techn Environ Policy 17 (3), pp. 579–596. DOI: 10.1007/s10098-014-0841-5.

Covestro Deutschland AG (2018a): Hochwertige Materialien aus Brunsbüttel und vom Niederrhein. Hilfreich im täglichen Leben. (engl.: High quality materials from Brunsbüttel and the Lower Rhine. Helpful in daily life). Available online at https://www.covestro.de/de/products-and-services/overview, checked on 11/22/2018. (in German).

Covestro Deutschland AG (2018b): Nördlichster Produktionsstandort von Covestro. Kreuzfahrtschiffe und ein Schornstein als Kunstwerk. (engl.: Northernmost production site of Covestro. Cruise ships and a chimney as a work of art). Available online at https://www.covestro.de/de/sites/brunsbuettel/overview. (in German).

Covestro Deutschland AG (2018c): Zahlen und Fakten. An vier Standorten arbeiten rund 6.200 Menschen - Schwerpunkt Rheinschiene. (engl.: Facts and figures. Around 6,200 people work at four locations - focus on the Rhine region). Available online at https://www.covestro.de/de/company/facts-and-figures, checked on 11/22/2018. (in German).

DOW (2015): Dow, Dow Olefinverbund GmbH. Daten und Fakten. Dow in Mitteldeutschland. (engl.: Facts and figures. Dow in Central Germany). Available online at https://de.dow.com/de-de/standorte/mitteldeutschland, checked on 05/04/2020. (in German).

Ducker (2015): Anteile der bei der Produktion eines Pkws verwendeten Materialien im Jahr 2015. (engl.: Proportions of materials used in the production of a passenger car in 2015). Statistsa. Available online at https://de.statista.com/statistik/daten/studie/658683/umfrage/verwendete-materialien-in-der-automobilproduktion/, checked on 1/30/2019. (in German).

Ecoinvent V2.2 (2007-2013): Ecoinvent. Version V2.2: Swiss Federal Institute of Technology Zurich (ETH Zurich); EPF Lausanne; Paul Scherrer Institute (PSI); the Swiss Federal Laboratories for Materials Science and Technology (Empa); Agroscope, Institute for Sustainability Sciences. Available online at https://www.ecoinvent.org/database/older-versions/ecoinvent-version-2/ecoinvent-version-2.html.

EEA (2007-2016): European Pollutant Release and Transfer Register. Facility level. Edited by European Environment Agency. Available online at https://prtr.eea.europa.eu/#/facilitylevels.

EEA (2017): GHG Inventory EU 15-01-2017. DEU_2017_2015_11012017_101416.xlsx. Edited by European Environment Agency. Available online at http://cdr.eionet.europa.eu/de/eu/mmr/art07_inventory/ghg_inventory/envwhvj6g/index_html?&page=2, checked on 2/13/2019.

EEA (2018): CO2 emission intensity. Hg. v. European Environment Agency. Available online at https://www.eea.europa.eu/data-and-maps/daviz/co2-emission-intensity-5#tab-googlechartid_chart_11_filters=%7B%22rowFilters%22%3A%7B%7D%3B%22columnFilters%22%3A%7B%22pre_config_ugeo%22%3A%5B%22European%20Union%20(current%20composition)%22%5D%7D%7D, checked on 14.07.2020.

Enviros Consulting (2006): EU ETS Phase II new entrant benchmarks: Petrochemicals. Available online at http://ebooks.lib.ntu.edu.tw/1_file/moeaidb/013215/23_%E7%9F%B3%E5%8C%96%E7%94%A2%E5%93%81.pdf.

EPSC (2016): Towards low-emission mobility. Driving the modernisation of the EU economy. Edited by European Political Strategy Centre Brussels. Available online at https://www.actu-environnement.com/media/pdf/news-27258-mobilite-bas-carbone-ue.pdf.

EU (2006): Verordnung (EG) Nr. 1893/2006 Des Europäischen Parlaments und des Rates. Zur Aufstellung der statistischen Systematik der Wirtschaftszweige NACE Revision 2 und zur Änderung der Verordnung (EWG) Nr. 3037/90 des Rates sowie einiger Verordnungen der EG über bestimmte Bereiche der Statistik. (engl.: Regulation (EC) No 1893/2006 of the European Parliament and of the Council. establishing the statistical classification of economic activities NACE Revision 2 and amending Council Regulation (EEC) No 3037/90 and certain EC Regulations on specific statistical domains). (in German).

Euro Chlor (2010): Energy consumption data of chlor-alkali plants in the EU-27 and EFTA countries.

Euro Chlor (2011): Euro Chlor position on energy consumption in chlor-alkali production.

Euro Chlor (2015): Chlorine Industry Review 2014-2015. Maintaining Momentum in Uncertain Times.

European Commission (2003): Integrated Pollution Prevention and Control (IPPC) Reference Document on Best Available Techniques in the Large Volume Organic Chemical Industry.

European Commission (2014): Best Available Techniques Reference Document for the Production of Chlor-alkali. JRC Science and Policy Reports. Industrial Emissions Directive 2010/75/EU (Integrated Pollution Prevention and Control).

European Commission (2015): Paris Agreement. Edited by European Commission. Available online at https://ec.europa.eu/clima/policies/international/negotiations/paris_en#tab-0-0, checked on 11/15/2018.

European Commission (2017): Best Available Techniques (BAT) Reference Document in the Large Volume Organic Chemical Industry. Final Draft.

Europur (2015): Flexible Polyurethane (PU) Foam. Eco-profiles and Environmental Product Declarations of the European Plastics Manufacturers.

Evonik Industries AG (2018): Der Leitgedanke Poolbetrieb Münchsmünster. (engl.: The guiding principle of pool operation Münchsmünster). Available online at https://history.evonik.com/sites/geschichte/de/gesellschaften/skw-trostberg/muenchsmuenster/. (in German).

Federal Grid Agency (2018): List of power plants 2018 - Deutschland.

Fleiter, Tobias; Schlomann, Barbara; Eichhammer, Wolfgang (Eds.) (2013): Energieverbrauch und CO2-Emissionen industrieller Prozesstechnologien. Einsparpotenziale, Hemmnisse und Instrumente. Fraunhofer-Institut für Systemtechnik und Innovationsforschung. (engl.: Energy consumption and CO2 emissions of industrial process technologies. Savings potentials, obstacles and instruments. Fraunhofer Institute for Systems and Innovation Research). Stuttgart: Fraunhofer-Verl. (ISI-Schriftenreihe "Innovationspotenziale"). Available online at http://publica.fraunhofer.de/dokumente/N-234719.html. (in German).

Fröhling, M.; Bartusch, H.; Schwaderer, F.; Schultmann, F. (2009): An inter-company Approach to improve Resource and Energy Efficiency and reduce Greenhouse Gas Emissions in Metal Industries by linking Flow Sheet Models. In World of metallurgy - Erzmetall.

Georgii, Hans-Otto (2009): Stochastik. Einführung in die Wahrscheinlichkeitstheorie und Statistik. 4., überarb. und erw. Auflage (engl.: Stochastic. Introduction to probability theory and statistics. 4th, revised and expanded edition). Berlin: de Gruyter (De-Gruyter-Lehrbuch). Available online at http://www.reference-global.com/doi/book/10.1515/9783110215274. (in German).

GlobalData (2019): Global Propylene Capacity and Capital Expenditure Outlook, 2019 – China and India to Lead Globally in Terms of Propylene Capacity Additions. Hg. v. GlobalData.

Graedel, Thomas E.; Saxton, Elizabeth (2002): Improving the overall environmental performance of existing telecommunications facilities. In Int J LCA 7 (4), pp. 219–224. DOI: 10.1007/BF02978876.

Guinée, Jeroen B.; Heijungs, Reinout; Huppes, Gjalt; Zamagni, Alessandra; Masoni, Paolo; Buonamici, Roberto et al. (2011): Life cycle assessment: past, present, and future. In Environmental science & technology 45 (1), pp. 90–96. DOI: 10.1021/es101316v.

Guinée, Jeroen B.; Heijungs, Reinout; Udo de Haes, Helias A.; Huppes, Gjalt (1993): Quantitative life cycle assessment of products. In Journal of Cleaner Production 1 (2), pp. 81–91. DOI: 10.1016/0959-6526(93)90046-E.

Gunvor Raffinerie Ingolstadt (2016): Aktualisierte Umwelterklärung 2016. (engl.: Gunvor Refinery Ingolstadt (2016): Updated Environmental Statement 2016). (in German).

Gunvor Raffinerie Ingolstadt (2017): Pressmeldung: TÜV-Revision in der Gunvor Raffinerie. (engl.: Press release: TÜV inspection at the Gunvor refinery). (Nr. 1 / 13.02.2017). (in German).

Gunvor Raffinerie Ingolstadt (2018): 50 Jahre Raffinerie Ingolstadt. Wärme und Mobilität mit Perspektive! Die Geschichte der Raffinerie Ingolstadt. (engl.: 50 years refinery Ingolstadt. Heat and mobility with perspective! The history of the Ingolstadt refinery). (in German).

Hannouf, Marwa; Assefa, Getachew (2017): Life Cycle Sustainability Assessment for Sustainability Improvements. A Case Study of High-Density Polyethylene Production in Alberta, Canada. In Sustainability 9 (12), p. 2332. DOI: 10.3390/su9122332.

Hasanbeigi, Ali (2018): Chemical Industry's Energy Use and Emissions. Hg. v. Global Efficiency Intelligence. Available online at https://www.globalefficiencyintel.com/new-blog/2018/chemical-industrys-energy-use-emissions, checked on 09.07.2020.

Heijungs, Reinout; Guinée, J. B. (Eds.) (1992): Environmental life cycle assessment of products. [study carried out under the auspices of the National Reuse of Waste Research Programme (NOH)]. Rijksuniversiteit Leiden; Nederlandse Organisatie voor Toegepast-Natuurwetenschappelijk Onderzoek. Leiden: Centrum voor Milieukunde (NOH report).

Hochfeld, Ch.; Jenseits, W. (1998): Allokation in Ökobilanzen und bei der Berechnung des Kumulierten Energieaufwandes (KEA). Arbeitspapier im Rahmen des UBAF& E-Vorhabens Nr. 104 01 123. (engl.: allocation in life cycle assessments and in the calculation of the cumulative energy demand (KEA). Working paper within the framework of the UBAF&E project no. 104 01 123). (in German).

Holborn Refinery (2018): Holborn Refinery - Our operations. Available online at http://www.oilinvest.com/en/what-we-do/our-operations/holborn-refinery, checked on 11/20/2018.

Hustede, R. (2018): Gute Landung für Koloss von Knielingen. (engl.: Good landing for Koloss von Knielingen). Available online at https://bnn.de/lokales/karlsruhe/gute-landung-fuer-koloss-von-knielingen, checked on 11/20/2018. (in German).

Hüthig GmbH (2018a): Chemie Technik - Fachinformationen für Entscheider - Industrieparks Chemie, Pharma, Biotech. (engl.: Chemie Technik - Expert information for decision-makers - Chemical, pharmaceutical and biotech industrial parks). Port of Rotterdam (Havenbedrijf Rotterdam). Available online at https://marktuebersichten.chemietechnik.de/mu-industrieparks-chemie-pharma-biotech/2603/port-of-rotterdam-havenbedrijf-rotterdam/detail, checked on 11/23/2018. (in German).

Hüthig GmbH (2018b): PLASTVERARBEITER - Das Portal für den Kunststoffverarbeiter. (engl.: PLASTVERARBEITER - The portal for the plastics processor). Available online at https://marktuebersichten.plastverarbeiter.de/mu-industrieparks-chemie-pharma-biotech/2599/bayer-industriepark-brunsbuttel/detail, checked on 11/22/2018. (in German).

IEA (2007): Tracking Industrial Energy Efficiency and CO2 Emissions: OECD.

IEA (2009): Chemical and Petrochemical Sector - Potential of best practice technology and other measures for improving energy efficiency.

Industriepark Schwedt (2018): Industrie- und Energiestandort mit Zukunft. (engl.: Industrial and energy location with a future). Available online at http://www.ipsdt.de/, checked on 11/20/2018. (in German).

INEOS Köln GmbH (2007): INEOS Unternehmensbroschüre. (engl.: INEOS company brochure). (in German).

IPCC (Ed.) (2013): Climate change 2013. The physical science basis ; summary for policymakers, a report of Working Group I of the IPCC, technical summary, a report accepted by Working Group I of the IPCC but not approved in detail and frequently asked questions ; part of the Working Group I contribution to the fifth assessment report of the Intergovernmental Panel on Climate Change. With assistance of Stocker, T.F., D. Qin, G.-K. Plattner, M. Tignor, S.K. Allen, J. Boschung, A. Nauels, Y. Xia, V. Bex and P.M. Midgley. Intergovernmental Panel on Climate Change. New York: Intergovernmental Panel on Climate Change. Available online at http://www.ipcc.ch/.

IPCC (Ed.) (2015): Climate Change 2014. Mitigation of Climate Change ; Summary for Policymakers Technical Summary ; Part of the Working Group III Contribution to the Fifth Asessment Report of the Intergovernmental Panel on Climate Change. With assistance of Ottmar Edenhofer, Ramon Pichs-Madruga, Youba Sokona, Jan C. Minx, Ellie Farahani, Susanne Kadner et al. Intergovernmental Panel on Climate Change. Geneva, Switzerland: Intergovernmental Panel on Climate Change.

ISO 14044:2006: Environmental management – Life cycle assessment – Requirements and guidelines (ISO 14044:2006).

ISO 14040:2006: Environmental management – Life cycle assessment – Principles and framework (ISO 14040:2006).

Kaiser, W. (2015): Kunststoffchemie für Ingenieure. (engl.: Plastics chemistry for engineers). München: Carl Hanser Verlag GmbH & Co. KG. (in German).

Kanchanapiya, Premrudee; Limphitakphong, Nantamol; Pharino, Chanathip; Chavalparit, Orathai (2015): Evaluation of greenhouse gas emissions and reduction from the petrochemical industry in Thailand. In Greenhouse Gas Measurement and Management 4 (2-4), pp. 161–177. DOI: 10.1080/20430779.2015.1008362.

Keller, Florian; Lee, Roh Pin; Meyer, Bernd (2020): Life cycle assessment of global warming potential, resource depletion and acidification potential of fossil, renewable and secondary feedstock for olefin production in Germany. In Journal of Cleaner Production 250, p. 119484. DOI: 10.1016/j.jclepro.2019.119484.

Kikuchi, Yasunori; Oshita, Yuko; Mayumi, Kazuya; Hirao, Masahiko (2017): Greenhouse gas emissions and socioeconomic effects of biomass-derived products based on structural path and life cycle analyses. A case study of polyethylene and polypropylene in Japan. In Journal of Cleaner Production 167, pp. 289–305. DOI: 10.1016/j.jclepro.2017.08.179.

Kindler, H.; Nikles, A. (1980): Energieaufwand zur Herstellung von Werkstoffen - Berechnungsgrundsätze und Energieäquivalentzwerte von Kunststoffen. Kunststoffe. (engl.: Energy demand for the production of materials - calculation principles and energy equivalent values of plastics. Plastics). (in German).

Klöpffer, Walter; Renner, Isa (2008): Life-Cycle Based Sustainability Assessment of Products. In Stefan Schaltegger, Martin Bennett, Roger L. Burritt, Christine Jasch (Eds.): Environmental Management Accounting for Cleaner Production, vol. 24. Dordrecht: Springer Netherlands (Eco-Efficiency in Industry and Science), pp. 91–102.

Kndungu, Peter; Molavi, Jeffrey M. (2014): A Hybrid LCA Approach to Quantify the Environmental Impacts during Construction. In IJIRSET 03 (10), pp. 16402–16413. DOI: 10.15680/IJIRSET.2014.0310002.

Koottungal, L. (2015): International Survey of Ethylene From Steam Crackers - 2015. In Oil & Gas Journal.

Lang-Koetz, C.; Springer, S.; Beucker, S. (2006): Life Cycle e-Valuation - Produkt, Service, System. Stuttgart: Fraunhofer IRB.

Laplace, Pierre-Simon de (1812): Théorie analytique des probabilités.

Lei, L.; Bao, X. (2014): The forecast of propylene market supply pattern in China. In Chem. Ind. (32 (8), 19-21,28).

Leimkühler, Hans-Joachim (2010): Managing CO2 Emissions in the Chemical Industry. Weinheim, Germany: Wiley-VCH Verlag GmbH & Co. KGaA.

Leontief, Wassily W. (1936): Quantitative Input and Output Relations in the Economic Systems of the United States. In The Review of Economics and Statistics 18 (3), p. 105. DOI: 10.2307/1927837.

Lorenz, W.; Muenning, J.; Pennemann, B.; Pohl, F.; Wiechers, G. (2006): DE102006033722A1 - Verfahren zur Herstellung von Dinitrotoluol (engl.: Process for the production of dinitrotoluene). - Google Patents. Available online at https://patents.google.com/patent/DE102006033722A1/de?q=Herstellung&q=Dinitrotoluol&scholar&oq=Herstellung+Dinitrotoluol, checked on 11/21/2018. (in German).

Lübbers, Peter (2012): Berechnung von Produktionsindizes für das verarbeitende Gewerbe. (engl.: Calculation of indices of production for the manufacturing sector). In Statistische Monatshefte Rheinland-Pfalz (07/2012). (in German).

Lynondellbasell (2017): Nachbar Weltkonzern. In Wesseling stimmt die Chemie. (engl.: Neighbour global corporation. The chemistry is right in Wesseling). Available online at https://www.lyondellbasell.com/globalassets/lyb-around-the-world/plant-sites/eai/wesseling/german/lyondellbasell_corporate-brochure.pdf?id=19868, checked on 11/20/2018. (in German).

McKinsey (2006): Kosten und Potenziale der Vermeidung von Treibhausgasemissionen in Deutschland. Sektorenperspektive Industrie. (engl.: Costs and potentials of avoiding greenhouse gas emissions in Germany. Sector Perspective Industry). (in German).

Mendivil, Ramon; Fischer, Ulrich; Hirao, Masahiko; Hungerbühler, Konrad (2006): A New LCA Methodology of Technology Evolution (TE-LCA) and its Application to the Production of Ammonia (1950-2000) (8 pp). In Int J Life Cycle Assessment 11 (2), pp. 98–105. DOI: 10.1065/lca2005.08.222.

Merchant Research & Consulting (2013): TDI Manufacturers in Europe Restructure and Expand their Production Capacities. Available online at https://mcgroup.co.uk/news/20150505/tdi-manufacturers-europe-restructure-expand-production-capacities.html, checked on 11/23/2018.

MHP (2016): CO2 als Wettbewerbsfaktor im automobilen Wertschöpfungsnetzwerk. (engl.: CO2 as a competitive factor in the automotive value-added network). Available online at https://www.mhp.com/fileadmin/www.mhp.com/assets/downloads/studien/MHPeBook_CO2.pdf. (in German).

Mihatsch, Christian (2014): Wie die Wirtschaft mit "Schattenpreisen" kalkuliert. Bericht zum Weltklimabericht 2014. (engl.: How the economy calculates with "shadow prices" Report on the World Climate Report 2014). Edited by IPCC-Arbeitsgruppe 3. IPCC. (in German).

MiRO Mineraloelraffinerie Oberrhein (2018): Willkommen bei Miro. Miro in Zahlen. (engl.: Welcome to Miro. Miro in figures). Available online at http://www.miro-ka.de/de/portrait/miro-in-zahlen.htm, checked on 11/20/2018. (in German).

Neelis, M. L.; Patel, M.; Gielen, D. J.; BLOK, K. (2005): Modelling CO2 emissions from non-energy use with the non-energy use emission accounting tables (NEAT) model. In Resources, Conservation and Recycling 45 (3), pp. 226–250. DOI: 10.1016/j.resconrec.2005.05.003.

Nelson, W. L. (1960a): How complexity of a refinery affects costs of processing. In Oil & Gas Journal (Sept. 26), p. 216.

Nelson, W. L. (1960b): How to describe refining complexity. In Oil & Gas Journal (Mar. 14), p. 189.

Nelson, W. L. (1961): How to compute refinery complexity. In Oil & Gas Journal (June 19), p. 109.

Nelson, W. L. (1976a): Complexity-1: The concept of refinery complexity. In Oil & Gas Journal (Sept. 13), p. 81.

Nelson, W. L. (1976b): Complexity-2: Process unit complexity factors examined. In Oil & Gas Journal (Sept. 20), p. 202.

Nelson, W. L. (1976c): Complexity-3: How to apply complexity. In Oil & Gas Journal (Sept. 27), p. 83.

NGZ (2017): Seit 50 Jahren wird in Dormagen Chlor produziert. (engl.: Chlorine has been produced in Dormagen for 50 years). Available online at https://rp-online.de/nrw/staedte/dormagen/seit-50-jahren-wird-in-dormagen-chlor-produziert_aid-19472009, checked on 12/3/2018. (in German).

Nitzsche, R.; Budzinski, M.; Gröngröft, A.; Majer, S.; Müller-Langer, F.; Thrän, D. (2016): Process Simulation and Sustainability Assessment during Conceptual Design of New Bioeconomy Value Chains. In European Biomass Conference and Exhibition Proceedings (Volume 2016, Issue 24thEUBCE, 2016, Pages 1723-1726).

OMV Deutschland GmbH (2016): Fortschreibung Umwelterklärung 2016. (engl.: Update of Environmental Report 2016). (in German).

Ou, Xunmin; Xiaoyu, Yan; Zhang, Xiliang (2011): Life-cycle energy consumption and greenhouse gas emissions for electricity generation and supply in China. In Applied Energy 88 (1), pp. 289–297. DOI: 10.1016/j.apenergy.2010.05.010.

Patel, M. (2003): Cumulative energy demand (CED) and cumulative CO2 emissions for products of the organic chemical industry. In Energy 28 (7), pp. 721–740. DOI: 10.1016/S0360-5442(02)00166-4.

Patil, Akshat; Patel, Arun; Purohit, Rajesh (2017): An overview of Polymeric Materials for Automotive Applications. In Materials Today: Proceedings 4 (2), pp. 3807–3815. DOI: 10.1016/j.matpr.2017.02.278.

PCK (2018): Geschäftsfelder. Available online at https://www.pck.de/unternehmen/geschaeftsfelder.html, checked on 11/20/2018.

Peereboom, Eric Copius; Kleijn, René; Lemkowitz, Saul; Lundie, Sven (1998): Influence of Inventory Data Sets on Life-Cycle Assessment Results. A Case Study on PVC. In Journal of Industrial Ecology 2 (3), pp. 109–130. DOI: 10.1162/jiec.1998.2.3.109.

Pereira, C. P.; Prata, D. M.; Monteiro, L. P. C.; Mainier, F. B. (2013): Evaluation of the CO2 Emissions in a Petrochemical Plant. In ARPN Journal of Science and Technology (VOL. 3, NO. 8 August 2013).

Pigosso, Daniela Cristina Antelmi; Sousa, S. R. (2011): Life Cycle Assessment (LCA): Discussion on Full-Scale and Simplified Assessments to Support the Product Development Process. In 3rd International workshop on advances in cleaner production: Cleaner production initiatives and challenges for a sustainable world.

PKN ORLEN Capital Group (2016): Company Overview 2016.

PlasticsEurope (2005a): Eco-profiles of the European Plastics Industry: Naphtha.

PlasticsEurope (2005b): Eco-profiles of the European Plastics Industry: Natural Gas.

PlasticsEurope (2012a): Ethylene, Propylene, Butadiene, Pyrolysis Gasoline, Ethylene Oxide (EO), Ethylene Glycols (MEG, DEG, TEG). Eco-profiles and Environmental Product Declarations of the European Plastics Manufacturers.

PlasticsEurope (2012b): Toluene Diisocyanate (TDI) & Methylenediphenyl Diisocyanate (MDI).

PlasticsEurope (2013): Chlorine (The chloralkali process) Euro Chlor. An Eco-profile and Environmental Product Declaration of the European Chlor Alkali Industry.

PlasticsEurope (2018): Eco-Profiles. PlasticsEurope's Eco-profiles comprise Life Cycle Inventory datasets (LCI) and Environmental Product Declarations (EPD) for plastics.

Posen, I. Daniel; Griffin, W. Michael; Matthews, H. Scott; Azevedo, Inês L. (2015): Changing the renewable fuel standard to a renewable material standard: bioethylene case study. In Environmental science & technology 49 (1), pp. 93–102. DOI: 10.1021/es503521r.

Prammer, Heinz Karl (2009): Integriertes Umweltkostenmanagement. Bezugsrahmen und Konzeption für eine ökologisch nachhaltige Unternehmensführung. (engl.: Integrated environmental cost management. Reference framework and concept for ecologically sustainable corporate management). Zugl.: Linz, Univ., Habil.-Schr., 2008. Wiesbaden: Betriebswirtschaftlicher Verlag Gabler (neue betriebswirtschaftliche forschung (nbf), v.369). Available online at http://dx.doi.org/10.1007/978-3-8349-8447-0. (in German).

Raffinerie Heide GmbH (2012): Mit Hightech und Leistungskraft – die Zukunft im Blick. Voller Energie für den Norden. (engl.: With high tech and performance - the future in sight. Full of energy for the north). (in German).

Raffinerie Heide GmbH (2016): Zahlen und Statistiken der Raffinerie Heide. Alle wichtigen Daten und Fakten der Raffinerie auf einen Blick. (engl.: Figures and statistics of the Heide refinery. All important facts and figures of the refinery at a glance). Available online at http://www.heiderefinery.com/de/ueber-uns/daten-fakten/, checked on 11/20/2018. (in German).

Rebitzer, Gerald (2002): Integrating Life Cycle Costing and Life Cycle Assessment for Managing Costs and Environmental Impacts in Supply Chains. In Stefan Seuring, Maria Goldbach (Eds.): Cost Management in Supply Chains. Heidelberg: Physica-Verlag HD, pp. 127–146.

Reliance Industries Ltd. (2009): Nelson´s Complexity Factor. Available online at http://pakpas.org/0.REFINERY%20LIBRARY/2.EDC-business_petroleum_refiningmktg_lc_ncf.pdf), checked on 11/20/2018.

Ren, Tao (2009): Petrochemocals from oil, natural gas, coal and biomass. Energy use, economics and innovation. [S.l.]: [s.n.].

Ren, Tao; Patel M.; BLOK, K. (2006): Olefins from conventional and heavy feedstocks. Energy use in steam cracking and alternative processes. In Energy 31 (4), pp. 425–451. DOI: 10.1016/j.energy.2005.04.001.

Ren, Tao; Patel M.; BLOK, K. (2008): Steam cracking and methane to olefins. Energy use, CO2 emissions and production costs. In Energy. DOI: 10.1016/j.energy.2008.01.002.

Rieckhof, Ramona; Guenther, Edeltraud (2018): Integrating life cycle assessment and material flow cost accounting to account for resource productivity and economic-environmental performance. In Int J Life Cycle Assess 23 (7), pp. 1491–1506. DOI: 10.1007/s11367-018-1447-7.

Rosneft (2016): Rosneft and BP Conclude Dissolution of the Refining Joint Venture Ruhr Oel GmbH in Germany. Available online at https://www.rosneft.com/press/releases/item/185259/, checked on 11/20/2018.

Roy, Poritosh; Nei, Daisuke; Orikasa, Takahiro; Xu, Qingyi; Okadome, Hiroshi; Nakamura, Nobutaka; Shiina, Takeo (2009): A review of life cycle assessment (LCA) on some food products. In Journal of Food Engineering 90 (1), pp. 1–10. DOI: 10.1016/j.jfoodeng.2008.06.016.

Saygin, Değer (2012): Assessing industrial energy use and CO2 emissions. Opportunities for energy efficiency, biomass and CCS.

Schiessl, Andreas; Müller, Richard; Volk, Rebekka; Zimmer, Konrad; Breun, Patrick; Schultmann, Frank (2020): Integrating site-specific environmental impact assessment in supplier selection. Exemplary application to steel procurement. In J Bus Econ 27, p. 93. DOI: 10.1007/s11573-020-00967-1.

Schönbucher, Axel (2002): Thermische Verfahrenstechnik. Grundlagen und Berechnungsmethoden für Ausrüstungen und Prozesse. (engl.: Thermal process engineering. Fundamentals and calculation methods for equipment and processes). Berlin, Heidelberg: Springer. Available online at http://dx.doi.org/10.1007/978-3-642-56308-9. (in German).

Schrack, Daniela (2016): Nachhaltigkeitsorientierte Materialflusskostenrechnung. Anwendung in Lieferketten, der Abfallwirtschaft und Integration externer Effekte. (engl.: Sustainability oriented material flow cost accounting. Application in supply chains, waste management and integration of external effects). (in german)

Shell Rheinland Raffinerie (2018): Imagebroschüre. (engl.: Image brochure). Available online at www.shell.de/rheinlandraffinerie, checked on 11/20/2018. (in German).

Sonnemann, Guido; Castells, Francesc; Schuhmacher, Marta (2004): Integrated life-cycle and risk assessment for industrial processes. Boca Raton: Lewis. Available online at http://www.loc.gov/catdir/enhancements/fy0646/2003054632-d.html.

Statista (2018): Weltweite und europäische Produktionsmenge von Kunststoff in den Jahren von 1950 bis 2016 (in Millionen Tonnen). (engl.: World and European production volume of plastics in the years from 1950 to 2016 (in million tonnes)). Available online at https://de.statista.com/statistik/daten/studie/167099/umfrage/weltproduktion-von-kunststoff-seit-1950/. (in German).

GFSO (2018a): Statistisches Bundesamt. Produzierendes Gewerbe 2017. Produktion des Verarbeitenden Gewerbes sowie des Bergbaus und der Gewinnung von Steinen und Erden. (engl.: German Federal Statistical Office. Manufacturing industry 2017. production of manufacturing industry and mining and quarrying). In Erden - Fachserie 4 Reihe 3.1. (in German).

GFSO. (2018b): Statistisches Bundesamt. Umweltnutzung und Wirtschaft - Tabellen zu den UGR, Teil 3: Luftemissionen - Ausgabe 2018. Umweltökonomische Gesamtrechnung. (engl.: Federal Statistical Office. Environmental use and economy - Tables on UGR, Part 3: Air emissions - 2018 edition. Environmental-economic accounts). (in German).

Saevarsdottir, Gudrun; Kvande, Halvor; Welch, Barry J. (2020): Aluminum Production in the Times of Climate Change. The Global Challenge to Reduce the Carbon Footprint and Prevent Carbon Leakage. In: JOM 72 (1), S. 296–308. DOI: 10.1007/s11837-019-03918-6.

Suh, Sangwon; Lenzen, Manfred; Treloar, Graham J.; Hondo, Hiroki; Horvath, Arpad; Huppes, Gjalt et al. (2004): System boundary selection in life-cycle inventories using hybrid approaches. In Environmental science & technology 38 (3), pp. 657–664. DOI: 10.1021/es0263745.

SWR (2018): Für TDI-Anlage Schwertransport mit Reaktor erreicht BASF. (engl.: For TDI plant heavy transport with reactor arrives at BASF). 02.03.2018. Available online at https://www.swr.de/swraktuell/rp/fuer-tdi-anlage-schwertransport-mit-reaktor-erreicht-basf/-/id=1682/did=21264170/nid=1682/jv8ejg/index.html. (in German).

Thinkstep (2019): Ökobilanzen erstellen mit GaBi Software. (engl.: Creating life cycle assessments with GaBi software). Available online at https://www.thinkstep.com/de/software/gabi-software. (in German).

Total Raffinierie Mitteldeutschland (2018): Kraftstoffe aus Leuna. (engl.: Fuels from Leuna). Available online at https://www.total.de/ueber-total/profil-in-deutschland/raffinerie-mitteldeutschland.html#oben, checked on 11/20/2018. (in German).

Trippe, Frederik (2013): Techno-ökonomische Bewertung alternativer Verfahrenskonfigurationen zur Herstellung von Biomass-to-Liquid (BtL) Kraftstoffen und Chemikalien. (engl.: Techno-economic evaluation of alternative process configurations for the production of Biomass-to-Liquid (BtL) fuels and chemicals). Zugl.: Karlsruhe, KIT, Diss., 2013. Print on demand. Hannover, Karlsruhe: Technische Informationsbibliothek u. Universitätsbibliothek; KIT Scientific Publishing (Produktion und Energie, 3). Available online at https://edocs.tib.eu/files/e01fn13/750499583.pdf. (in German).

UBA (2009): Nachhaltige Chemie. Positionen und Kriterien des Umweltbundesamtes. (engl.: Sustainable chemistry. Positions and criteria of the Federal Environment Agency in Germany). (in German).

UBA (2016): Federal Environment Agency Germany. CO2-Emissionsfaktoren für fossile Brennstoffe (engl.: CO2 emission factors for fossil fuels). (27/2016). (in German).

UBA (2018a): Federal Environment Agency Germany. Nationale Inventarberichte zum Deutschen Treibhausgasinventar 1990 bis 2016. Emission der von der UN-Klimarahmenkonvention abgedeckten Treibhausgase. (engl.: National inventory reports on the German greenhouse gas inventory 1990 to 2016. emission of the greenhouse gases covered by the UN Framework Convention on Climate Change). (in German).

UBA (2018b): Federal Environment Agency Germany. Strom- und Wärmeversorgung in Zahlen. Entwicklung der spezifischen Kohlendioxid-Emissionen des deutschen Strommix 1990-2016 und erste Schätzungen 2017 im Vergleich zu CO2-Emissionen der Stromerzeugung. (engl.: Electricity and heat supply in figures. Development of the specific carbon dioxide emissions of the German electricity mix 1990-2016 and first estimates 2017 compared to CO2 emissions from electricity generation). Edited by Umweltbundesamt Deutschland. Available online at https://www.umweltbundesamt.de/themen/klima-energie/energieversorgung/strom-waermeversorgung-in-zahlen#Strommix, checked on 11/23/2018. (in German).

VCI (2018): Verband der chemischen Industrie: Chemiewirtschaft in Zahlen 2018. (engl.: Association of the Chemical Industry: Chemical industry in figures 2018). (in German).

VCI (2019a): Verband der chemischen Industrie: Produktionsvolumen ausgewählter petrochemischer Primärprodukte in Deutschland im Jahr 2017 (in 1.000 Tonnen). (engl.: Association of the Chemical Industry: Production volume of selected petrochemical primary products in Germany in 2017 (in 1,000 tons)). Edited by Statista. Available online at https://de.statista.com/statistik/daten/studie/868074/umfrage/produktion-von-petrochemikalien-in-deutschland/, checked on 2/21/2019. (in German).

Vogt, E. T. C.; Weckhuysen, B. M. (2015): Fluid catalytic cracking: recent developments on the grand old lady of zeolite catalysis. In Chemical Society reviews 44 (20), pp. 7342–7370. DOI: 10.1039/c5cs00376h.

Wang, Z. (2014): Optimization of technological process of reducing energy consumption of ethylene plant. In Public Commun. Sci. Technol. (9 (18)), 136-137 (in Chinese).

Weber, Eva (2014): Prozessbedingte CO2-Emissionen in Bayern. Beiträge aus der Statistik. In Bayern in Zahlen 5. (engl.: Process-related CO2 emissions in Bavaria. Contributions from the statistics. In Bavaria in figures 5). Available online at https://www.destatis.de/GPStatistik/servlets/MCRFileNodeServlet/BYMonografie_derivate_00000079/201405A3.pdf;jsessionid=BE4A7020B7ABC76C295FC1EE3FE355FB. (in German)

Weitz, K. A.; Todd, J. A.; Curran, M. A.; Malkin, M. J. (1996): Streamlining Life Cycle Assessment: considerations and report on the state of practice. In International Journal of Life Cycle Assessment (2), pp. 79–85.

Wirtschaftsregion Lausitz GmbH (2018): Chemiestandort Schwarzheide. (engl.: Schwarzheide chemical site). Available online at http://wirtschaftsregion-lausitz.de/de/wirtschaft/industrie-und-technologieparks/chemiestandort-basf-schwarzheide-gmbh.html, checked on 11/22/2018. (in German).

World Steel Association (2014): Steel's contribution to a low carbon future. worldsteel position paper. Available online at https://www.worldsteel.org/en/dam/jcr:cd2258b7-728e-4042-a865-1bf3cb20a61c/Steel%2527s+contribution+to+a+Low+Carbon+Future+2014.pdf, checked on 09.07.2020.

Worrell, E.; Price, L.; Neelis, M.; Galitsky, C.; Nan, Z. (2008): World Best Practice Energy Intensity Values for Selected Industrial Sectors.

Worrell, E.; van Heijningen, R.J.J.; Castro, J.F.M. de; Hazewinkel, J.H.O.; Beer, J. G. de; Faaij, A.P.C.; Vringer, K. (1994): New gross energy-requirement figures for materials production. In Energy 19 (6), pp. 627–640. DOI: 10.1016/0360-5442(94)90003-5.

Xiang, Dong; Qian, Yu; Man, Yi; Yang, Siyu (2014a): Techno-economic analysis of the coal-to-olefins process in comparison with the oil-to-olefins process. In Applied Energy 113, pp. 639–647. DOI: 10.1016/j.apenergy.2013.08.013.

Xiang, Dong; Yang, Siyu; Li, Xiuxi; Qian, Yu (2015): Life cycle assessment of energy consumption and GHG emissions of olefins production from alternative resources in China. In Energy Conversion and Management 90, pp. 12–20. DOI: 10.1016/j.enconman.2014.11.007.

Xiang, Dong; Yang, Siyu; Liu, Xia; Mai, Zihao; Qian, Yu (2014b): Techno-economic performance of the coal-to-olefins process with CCS. In Chemical Engineering Journal 240, pp. 45–54. DOI: 10.1016/j.cej.2013.11.051.

Yao, Yuan; Graziano, Diane J.; Riddle, Matthew; Cresko, Joe; Masanet, Eric (2015): Understanding Variability To Reduce the Energy and GHG Footprints of U.S. Ethylene Production. In Environmental science & technology 49 (24), pp. 14704–14716. DOI: 10.1021/acs.est.5b03851.

Yao, Yuan; Graziano, Diane J.; Riddle, Matthew; Cresko, Joe; Masanet, Eric (2016): Prospective Energy Analysis of Emerging Technology Options for the United States Ethylene Industry. In Ind. Eng. Chem. Res. 55 (12), pp. 3493–3505. DOI: 10.1021/acs.iecr.5b03413.

Yellishetty, Mohan; Mudd, Gavin M.; Ranjith, P. G.; Tharumarajah, A. (2011): Environmental life-cycle comparisons of steel production and recycling. Sustainability issues, problems and prospects. In Environmental Science & Policy 14 (6), pp. 650–663. DOI: 10.1016/j.envsci.2011.04.008.

Zhao, Zhitong; Liu, Yong; Wang, Feng; Li, Xuekuan; Deng, Shuping; Xu, Jie; Wei, Wei (2017): Life cycle assessment of primary energy demand and greenhouse gas (GHG) emissions of four propylene production pathways in China. In Journal of Cleaner Production 163, pp. 285–292. DOI: 10.1016/j.jclepro.2015.12.099.

Zimmer, Konrad (2016): Entscheidungsunterstützung zur Auswahl und Steuerung von Lieferanten und Lieferketten unter Berücksichtigung von Nachhaltigkeitsaspekten. Dissertation. Karlsruher Institut für Technologie. (engl.: Decision support for the selection and management of suppliers and supply chains considering sustainability aspects. dissertation. Karlsruhe Institute of Technology). (in German).

Zimmer, Konrad; Fröhling, Magnus; Breun, Patrick; Schultmann, Frank (2017): Assessing social risks of global supply chains. A quantitative analytical approach and its application to supplier selection in the German automotive industry. In Journal of Cleaner Production 149, pp. 96–109. DOI: 10.1016/j.jclepro.2017.02.041.

Zimmer, Konrad; Fröhling, Magnus; Schultmann, Frank (2015): Sustainable supplier management – a review of models supporting sustainable supplier selection, monitoring and development. In International Journal of Production Research 54 (5), pp. 1412–1442. DOI: 10.1080/00207543.2015.1079340.