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Non-energy use and related carbon dioxide emissions in Germany: A carbon flow analysis with the NEAT model for the period of 1990–2003

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ABSTRACT

Non-energy use of fossil fuels accounts for 7% of the Total Primary Energy Supply (TPES) of Germany and represents an important potential source of CO_2 (carbon dioxide) emissions. To gain a better understanding of emissions associated with non-energy use in Germany, we conduct a *bottom-up* carbon flow analysis with the Non-energy use Emission Accounting Tables (NEAT) model for the period of 1990–2003. We calculate average yearly non-energy use emissions to be 25 ± 2 megatonnes (Mt) CO_2, of which 77% are related to industrial processes, 17% to solvent and other product use, 2% to fertilizer use in agriculture, and 4% to wastewater treatment. The comparison of NEAT estimates and official data reveals gaps and errors in the German greenhouse gas (GHG) inventory. This research highlights the difficulties associated with non-energy use emissions accounting not only in Germany but in other countries as well. To ensure correct calculation of non-energy use emissions, we recommend that inventory experts (i) obtain detailed insight into the system boundaries of non-energy use data as stated in national energy statistics, (ii) allocate non-energy use emissions accordingly to the relevant emission source categories (i.e., energy, industrial processes, solvent and other product use, agriculture, or waste), (iii) ensure completeness of emission estimates, and (iv) be cautious with the use of default emission factors as given by the Intergovernmental Panel on Climate Change (IPCC).

1. Introduction

In the greenhouse gas (GHG) inventory of Germany (UNFCCC, 2005a,c), most attention has been paid to CO_2 emissions originating from fossil fuel combustion. In Germany, approximately 7% of all fossil fuels are, however, not used for energy but for non-energy purposes, e.g., as feedstock in the chemical industry or for the production of lubricants and bitumen in refineries (IEA, 2005). Non-energy use is therefore an important potential source of CO_2 (carbon dioxide) emissions. Moreover, the importance of non-energy use in Germany has increased substantially and is expected to grow further due to the expansion of mainly polymer production (more than 75% growth between 1990 and 2003).

In this paper, we define non-energy use as the sum of two components[1]:

(i) The consumption of fossil fuels as feedstock in the chemical industry (e.g., the use of naphtha for olefins and aromatics production in steam crackers or the consumption of natural gas for the production of ammonia).
(ii) The consumption of refinery and coke oven products as well as other solid carbon for non-energy purposes (e.g., the use of lubricants for transportation, the use of bitumen in the building sector, or the consumption of electrodes for aluminium production).

The non-energy use of fossil fuels leads to *non-energy use emissions* (mainly in the form of CO_2) in various ways: (i) due to partial or complete oxidation of feedstock, electrodes, and other solid carbon during production processes in the chemical and non-ferrous metal industry, (ii) due to product use of, e.g., solvents or lubricants, (iii) due to the application of urea fertilizers in agriculture, and (iv) due to the oxidation of surfactants in the course of wastewater treatment.[2] Estimating non-energy use emissions is not straight-

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[1] The consumption of coal and cokes in blast furnaces for pig iron production is part of the energy conversion sector in German energy statistics. We follow this practice and exclude these items from the non-energy use of fossil fuels.

[2] Potential sources of non-energy use emissions from waste treatment also include landfilling and waste incineration (with and without energy recovery). In line with UBA (2004), we regard the oxidation of fossil-based carbon in landfills

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forward because only parts of the carbon initially contained in non-energy use are emitted during production, consumption, and disposal of materials, whereas a remainder is stored in products with lifetimes ranging from years to decades and longer. Various parallel and subsequent conversion steps in the chemical industry as well as multiple forms of chemicals' use and product life cycles further complicate the accurate accounting of non-energy use emissions.

According to the inventory guidelines issued by the Intergovernmental Panel on Climate Change (IPCC) in 1997, non-energy use emissions are calculated by two methods, i.e., the relatively simple *top-down* Reference Approach (IPCC-RA) and the more detailed *bottom-up* Sectoral Approach (IPCC-SA) (IPCC, 1997).[3] In 2006, the IPCC issued new guidelines for national GHG inventories in which (i) non-energy use emissions accounting in the IPCC-RA was practically abolished and (ii) the IPCC-SA has been refined (IPCC, 2006). Nevertheless, many countries, among them Germany, make use of their right to report their GHG emissions according to the 1997 IPCC guidelines until the end of the first Kyoto period in 2008–2012. The 1997 IPCC guidelines are therefore relevant for the discussion of non-energy use emissions in this paper.[4]

For monitoring GHG emissions in Germany (and in all other Annex I countries), the IPCC-SA is the standard approach, whereas the IPCC-RA plays an important role as crosscheck. By comparing non-energy use emissions as calculated according to IPCC-RA and IPCC-SA, inventory makers discovered substantial inconsistencies within the German GHG inventory (Fig. 1). The results according to the IPCC-RA exceeded the ones calculated with the IPCC-SA by a factor 3–5 (UNFCCC, 2004, 2005a). This raised questions about the real level of non-energy use emissions in Germany. An international review team appointed by the United Nations Framework Convention on Climate Change (UNFCCC) also recognized inconsistencies in the German GHG inventory and pinpointed incomplete emission estimates for various source categories in the IPCC-SA, among them for chemical processes (UNFCCC, 2005b).

Given these problems, the Federal Environmental Agency (Umweltbundesamt, UBA) commissioned Utrecht University to apply its Non-energy use Emission Accounting Tables (NEAT) model to arrive at independent estimates of yearly non-energy use emissions for Germany in the period of 1990–2003 (UBA, 2003).[5] This gave us the interesting though challenging opportunity to analyze in detail the strengths and weaknesses of the IPCC-RA and IPCC-SA as used in the German GHG inventory. The objective of this paper is to apply an improved version of the NEAT model (NEAT 3.0, see below) for calculating non-energy use and related emissions

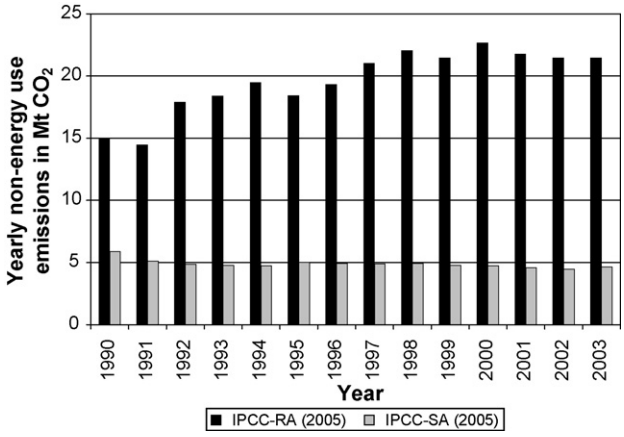

Fig. 1. Yearly non-energy use emissions as calculated according to IPCC-RA and IPCC-SA of the German GHG inventory for the period of 1990–2003 (UNFCCC, 2005a). We include here solvent and other product use emissions. For this, we multiply emission estimates given according to the IPCC-SA in NMVOC (non-methane volatile organic compound) equivalents with a conversion factor of 2.31 kilogrammes (kg) CO_2/kg NMVOC equivalents (Schmidt-Stejskal et al., 2004).

and to compare our results with emission estimates according to the German GHG inventory. Based on our results, we give detailed recommendations on how to improve data consistency between the IPCC-RA and the IPCC-SA. Our research is not only valuable for improving the quality of the German GHG inventory but it also provides critical knowledge for assuring consistent emissions reporting in the GHG inventories of any other Annex-I country.

The paper is structured as follows: In the next chapter, we explain methodology and data sources of our NEAT 3.0 model (Section 2). In Section 3, we present our model results and compare them with official emission data according to IPCC-RA and IPCC-SA of the German GHG inventory. In Section 4, we discuss our findings, address model uncertainties, and give advice on critical aspects of non-energy use emissions accounting. The paper ends with conclusions and general recommendations for inventory experts.

2. Methodology

NEAT is a spreadsheet-based model, for estimating non-energy use and related CO_2 emissions based on a carbon flow and mass balance approach. The NEAT model calculations are based mainly on official production and trade statistics and are, to a large extent, independent of data published in national energy statistics. The non-energy use emissions calculated with NEAT can be allocated to four principle IPCC-SA source categories, i.e., (i) industrial processes, (ii) solvent and other product use, (iii) agriculture, and (iv) waste. A detailed description of the NEAT model (NEAT 2.0) can be found in Neelis et al. (2005b). Here, we only explain key features and model adaptations made in the new model version (NEAT 3.0) that is used for our analysis. In comparison to NEAT 2.0, we track in NEAT 3.0 non-energy use emissions closer to their actual source[6] thereby calculating more reliable emission estimates. We account for uncertainties attached to (i) production and trade data, (ii) emission factors, (iii) feedstock distribution, (iv) the carbon content of chemicals, and (v) the fractions of carbon that become oxidized during product use and wastewater treatment. We assume that the implemented uncertainty intervals represent the 95% confidence interval

as negligible. Waste incineration without energy recovery does not take place in Germany. Emissions from waste incineration with energy recovery are reported as secondary fuel use emissions under the source category of *energy* in the German GHG inventory (UNFCCC, 2005a,c). We therefore exclude these emissions from our non-energy use emission estimates.

[3] As a *top-down* method, the IPCC-RA calculates fuel-specific non-energy use emissions by multiplying non-energy use data from energy statistics and fuel-specific carbon storage fractions. The more detailed IPCC-SA, in turn, is a *bottom-up* method for calculating non-energy use emissions based on three methodologies (Tier 1 to Tier 3) differing in their level of detail and accuracy. In the simplest case (Tier 1), emissions are calculated, e.g., by multiplying activity data with average default emission factors. Non-energy use emissions are reported in the IPCC-SA according to various different source categories (i.e., industrial processes, solvent and other product use, agriculture, and waste).

[4] We make exemptions from this general rule by calculating emissions that result from (i) industrial processes, (ii) solvent and other product use, (iii) the application of urea fertilizers in agriculture, and (iv) wastewater treatment at a greater level of detail than required by IPCC (1997).

[5] Earlier model versions were applied to Italy, Korea, and the Netherlands and provided the necessary insight to substantially improve the quality of national GHG inventories in these countries (La Motta et al., 2005; Park, 2005; Neelis et al., 2005a).

[6] This refers to the calculation of emissions that result from chemical conversion processes (i.e., chemical conversion losses), product use, the application of urea fertilizers in agriculture, and wastewater treatment.

of possible values. We calculate uncertainty intervals for total non-energy use, carbon storage, total non-energy use emissions, as well as for each source category of non-energy use emissions individually by uniformly applying standard error propagation rules.

2.1. Estimating emissions from industrial processes

Both components of non-energy use (i.e., feedstock use and the consumption of non-energy use refinery products, coke oven products, and other solid carbon) lead to *industrial process emissions*. NEAT 3.0 calculates industrial process emissions for the following processes: (i) steam cracking, (ii) the production of ammonia, methanol, and carbon black,[7] (iii) chemical conversions[8] (including 36 chemical conversion processes; see Appendix A), and (iv) electrodes and other solid carbon use in the manufacturing of 19 non-ferrous metals, ferroalloys, and other inorganic chemicals.[9] We calculate total industrial process emissions as the sum of emissions from individual processes based on process-specific emission factors and production data as

$$E_{\mathrm{IP}(k)} = \sum_i (P_{(i,k)} \times \mathrm{EF}_{(i,k)}) \quad (1)$$

where $E_{\mathrm{IP}(k)}$ [megatonnes (Mt) CO_2 equivalents] represents the total yearly emissions from industrial processes, $P_{(i,k)}$ [Mt] the physical production (e.g., ammonia or methanol) in process i, $\mathrm{EF}_{(i,k)}$ the process-specific emission factor [tonnes (t) CO_2 equivalents/t product], and k the index for the year of study.

We derive (i) production data from Destatis (1990–2003a), Consultic (1990–2003), and GDA (2007)[10] and (ii) process- and feedstock-specific emission factors from a variety of different sources as described in detail by Neelis et al. (2005b). We estimate feedstock composition for steam cracking, ammonia, and methanol production based on VCI (2004a) and interviews with several industry experts.

In the earlier versions of NEAT, Neelis et al. (2005a,b) assume all chemical conversion processes to be 100% carbon efficient, i.e., they model the total amount of carbon initially contained in basic and intermediate chemicals as being incorporated in final products (e.g., polymers). This simplification, however, neglects carbon losses that occur in the various chemical conversion processes due to partial feedstock oxidation, leakages, and the generation of non-specified by-products. In this research, we extend NEAT by a module that allows us to estimate CO_2 emissions resulting from conversion processes of 36 basic and intermediate chemicals (e.g., production of ethylene dichloride, acrylonitrile, polyvinylchloride).[11] We identify chemical conversion processes for Germany based on Neelis et al. (2007), Patel et al. (1999), Ullmann (1997), Weissermel and Arpe (2004) and miscellaneous expert interviews. We multiply production data of the various chemicals with process-specific carbon losses as determined by Neelis et al. (2007) (see Appendix A).[12]

The accounting of industrial process emissions is complicated by the fact that for many processes (the most prominent being ammonia production and steam cracking), parts of the hydrocarbon input are strictly speaking not used as feedstock but as fuel to sustain chemical reactions. This situation makes the exact allocation of fossil fuels (e.g., naphtha, natural gas) to either non-energy use or to energy use very difficult. Detailed investigations revealed that German energy statistics (DIW, 2005; MWV, 2005) do not possess uniform system boundaries for the non-energy use of the various types of fossil fuels:

(i) For coal- and oil-based hydrocarbons (e.g., coke, hard coal, lignite, coal oils and tars, fuel oils, naphtha) a *gross* definition of non-energy use is applied. Here, the total fossil hydrocarbon input into industrial processes (including hydrocarbons used as fuel) is regarded as non-energy use.
(ii) For natural gas, a *net* definition of non-energy use is applied, i.e., the parts of natural gas that are consumed for fuel purposes are excluded from non-energy use and reported as fuel.

With NEAT, we calculate non-energy use and related industrial process emissions according to the system boundaries as applied in German energy statistics to ensure comparability with data from the official German GHG inventory (which are largely based on German energy statistics).[13]

2.2. Estimating emissions from solvent and other product use

In contrast to previous NEAT studies, we apply a simple *bottom-up* approach to estimate *emissions from solvent and other product use* separately for four relevant *key* sources, i.e., the consumption of (i) solvents, (ii) lubricants, (iii) pesticides, and (iv) waxes and paraffins. We refer to this method as the *key sources approach*. We calculate total solvent and other product use emissions as

$$E_{\mathrm{SPU}(k)} = \sum_i (C_{(i,k)} \times \mathrm{FC}_{(i)} \times \mathrm{SC}_{(i)}) \quad (2)$$

where $E_{\mathrm{SPU}(k)}$ [Mt CO_2 equivalents] represents the total yearly emissions from solvent and other product use, $C_{(i,k)}$ [Mt] the consumption of product i,k $\mathrm{FC}_{(i)}$ the product-specific fossil carbon content [kg CO_2 equivalents/kg product], and $\mathrm{SC}_{(i)}$ [%] the product-specific shares of fossil carbon that become oxidized during product use.[14] The principal data sources for our calculations are Destatis

[7] We account for the various types of feedstock used (i) in steam cracking (i.e., naphtha, gas oil, ethane, butane, propane) and (ii) in the production of ammonia and methanol (i.e., natural gas, lignite, heavy fuel oils).

[8] We define chemical conversion processes as conversions of basic and intermediate chemicals within the chemical industry (e.g., production of styrene from ethylbenzene). The use of energy carriers as feedstock and their subsequent conversion to basic chemicals (e.g., ethylene, propylene, methanol, or carbon black) is, therefore, excluded from the category of chemical conversions.

[9] We include emissions from the production of: primary aluminium, electric arc furnace steel, white phosphorus, titanium dioxide, ferrosilicon, calcium carbide, silicon carbide, silicon, ferromanganese, silicon manganese, ferrochromium, ferrochromium-silicon, chromium, primary and secondary lead, magnesium, nickel, tin, and zinc.

[10] Data for polymer and aluminium production are taken from Consultic (1990–2003) and GDA (2007), respectively because we identified inconsistencies in the data sets as stated by the official German production statistics (i.e., Destatis, 1990–2003a).

[11] Our estimates of emissions from chemical conversion processes in principle exclude emissions from the combustion of fuel-grade by-products. There is, however, a small risk of double counting emissions, if NEAT results are used directly in the IPCC-SA because emissions can potentially be reported twice, once under *industrial processes* and again under the category of *energy*. Detailed insight into both the German energy statistics and the GHG inventory gives strong indication that this is, however, not the case (Weiss et al., 2007).

[12] The calculation of carbon losses for 36 chemical conversion processes with NEAT 3.0 exceeds the degree of detail as specified by both IPCC (1997) and IPCC (2006). The 1997 guidelines (that are followed by the German GHG inventory) do not specify any of the chemical conversion processes that are included in NEAT 3.0 as potential sources for CO_2 emissions. The 2006 IPPC guidelines point out only the production of ethylene dichloride, ethylene oxide, and acrylonitrile as potential emission sources.

[13] Ensuring consistency of system boundaries is critical for calculating industrial process emissions because depending on the definition chosen for non-energy use in energy statistics, emissions are reported according to the IPCC-SA either under the source categories *energy* or *industrial processes*.

[14] For calculating emissions from solvent use, we make use of detailed *bottom-up* emission studies as conducted by Theloke et al. (2000) and Jepsen et al. (2004). Both studies are used as principal data sources for *solvent and other product use* emission estimates in the German GHG inventory (UNFCCC, 2007a).

Table 1
Emission factors as applied in the *key sources approach* for calculating emissions from solvent and other product use

Product[a]	Fossil carbon content in kg CO_2 equivalents/kg product	Carbon oxidation rate in %	Emission factor in kg CO_2 equivalents/kg product
Solvents (1)	2.31 ± 0.23	100	2.31 ± 0.23[b]
Lubricants (2)	3.15	30 ± 20	0.95 ± 0.18
Pesticides (3,4,5)	1.28 ± 0.37	80 ± 20	1.03 ± 0.23
Waxes and paraffins (6,7,8)	3.15	43 ± 14	1.36 ± 0.19

[a] The indices stated in the table refer to the following sources: (1) Schmidt-Stejskal et al. (2004); (2) Trischler (1997); (3) Theloke et al. (2000); (4) UBA (2007); (5) Sonnenberg and Sietz (2007); (6) Patel et al. (1999); (7) Ullmann (1997); (8) Weissermel and Arpe (2004).
[b] Conversion factor for re-calculating solvent use emissions from NMVOC equivalents into CO_2 equivalents.

(1990–2003a,b), UBA (2007), FAO (2007), Theloke et al. (2000), and Jepsen et al. (2004). For calculating emissions, we multiply consumption data with specific emission factors as given in Table 1.

It is rather straightforward to calculate the fossil carbon content of (i) lubricants and (ii) waxes and paraffins because their chemical composition is relatively homogenous. Solvents and pesticides, however, comprise a relatively large group of substances, making our estimates for the fossil carbon content of these substances more uncertain (see first column in Table 1). Depending on the application, solvent use leads to emissions of the entire carbon initially contained in products within rather short time periods. This is not the case for the other three *key sources* where substances serve as intermediate chemicals (i.e., waxes and paraffins), are recycled or eventually combusted with energy recovery (i.e., lubricants), or oxidize over longer time periods (i.e., pesticides) (see second column in Table 1). We neglect other emission sources such as the use of chemical auxiliaries in the textile, paper, and leather industry because of their minor share on total solvent and other product use emissions.

2.3. Estimating emissions from agriculture

Non-energy use emissions in *agriculture* ($E_{AC(k)}$) result from the application of urea fertilizers. We estimate yearly CO_2 emissions from this source based on consumption data for urea containing fertilizers as provided by Yara (2008). We assume (i) that 50% of the nitrogen contained in ammonia–nitrate–urea solutions is derived from urea and (ii) that sulphur fertilizers account for 5% of the total urea consumption in agriculture. We assume a carbon oxidation rate of 100% and a carbon content of 0.73 kg CO_2/kg urea.

2.4. Estimating emissions from waste

Non-energy use emission in the source category *waste* result from the oxidation of surfactants and other fossil carbon containing substances during wastewater treatment. We estimate fossil CO_2 emissions from wastewater treatment ($E_{W(k)}$) based on domestic surfactant consumption (i.e., roughly 670 kt per year in Germany or approximately 8 kg per capita and year). We assume the fossil carbon content in surfactants to be 1.32 kg CO_2/kg surfactant and a carbon oxidation rate of 100% (Patel, 1999; Patel et al., 1999).

2.5. Estimating non-energy use and carbon storage

As stated in the introduction, the non-energy use of fossil fuels consists of two components, (i) the consumption of feedstock in the chemical industry and (ii) the consumption of refinery products, coke oven products, and other solid carbon for non-energy purposes. We account for the carbon that is contained (i) in the physical production of 15 basic chemicals (including urea),[15] (ii) in emissions that result from the production processes of basic chemicals as well as from electrode and other solid carbon use in the production of non-ferrous metals, ferroalloys, and inorganic chemicals, and (iii) in the consumption of refinery products for non-energy purposes.[16] Non-energy use is then calculated as

$$\mathrm{NEU}_{(k)} = \left[\left(\sum_{i=1}^{15} P_{(i,k)}\right) + (E_{S(k)} + E_{A(k)} + E_{M(k)} + E_{C(k)} + E_{\mathrm{NF}(k)})\right] + \left[\left(\sum_{i=1}^{4} \mathrm{CR}_{(i,k)}\right)\right] \quad (3)$$

where $\mathrm{NEU}_{(k)}$ [Mt CO_2 equivalents] represents non-energy use in year k, $P_{(i,k)}$ [Mt CO_2 equivalents] the production of chemical i, $E_{S(k)}$, $E_{A(k)}$, $E_{M(k)}$, $E_{C(k)}$, $E_{\mathrm{NF}(k)}$ [Mt CO_2 equivalents] emissions from steam cracking, the production of ammonia, methanol, carbon black, and the manufacturing of non-ferrous metals, ferroalloys, and inorganic chemicals, respectively, and $\mathrm{CR}_{(i,k)}$ the domestic consumption of refinery and coke oven products for non-energy use applications.

Carbon storage is calculated in NEAT as the carbon that is initially contained in the non-energy use of fossil fuels minus all further downstream emissions:

$$\mathrm{CS}_{(k)} = \mathrm{NEU}_{(k)} - (E_{\mathrm{IP}(k)} + E_{\mathrm{SPU}(k)} + E_{\mathrm{AC}(k)} + E_{W(k)}) \quad (4)$$

where $\mathrm{CS}_{(k)}$ [Mt CO_2 equivalents] represents the total carbon storage in year k. For further details on the NEAT methodology, we refer the reader to Neelis et al. (2005b).

3. Results

In this section, we present the results of our NEAT calculations and we compare our findings with emission estimates from the German GHG inventory as submitted to the UNFCCC in the years 2005, 2006, and 2007. It is surprising that NEAT estimates on total non-energy use emissions substantially exceed the values as calculated according to both IPCC-RA and IPCC-SA of the German GHG inventory (Fig. 2). Emission estimates according to the IPCC-RA are essentially identical in the GHG inventory submissions of 2006 and 2007 and denoted as "IPCC-RA (2006, 2007)" in the legend of Fig. 2. The same is true for emission estimates as stated according to the IPCC-SA (denoted as "IPCC-SA (2006, 2007)" in Fig. 2). The GHG inventory submission of 2005, however, differs from the submissions for 2006 and 2007 because in later years, important adaptations were made that also include the use of parts of our NEAT results.

We first present and discuss our NEAT results in comparison to inventory estimates according to the IPCC-SA at the level of individual source categories. Later, we focus on total non-energy use

[15] We include the following basic chemicals: acetylene, benzene, butadiene, butylene, carbon black, carbon monoxide, ethylene, methanol, naphthalene, propylene, toluene, *ortho*-, *meta*-, *para*-xylene, and urea.

[16] We include the following refinery and coke oven products: creosote oil, bitumen, lubricants, and waxes and paraffins.

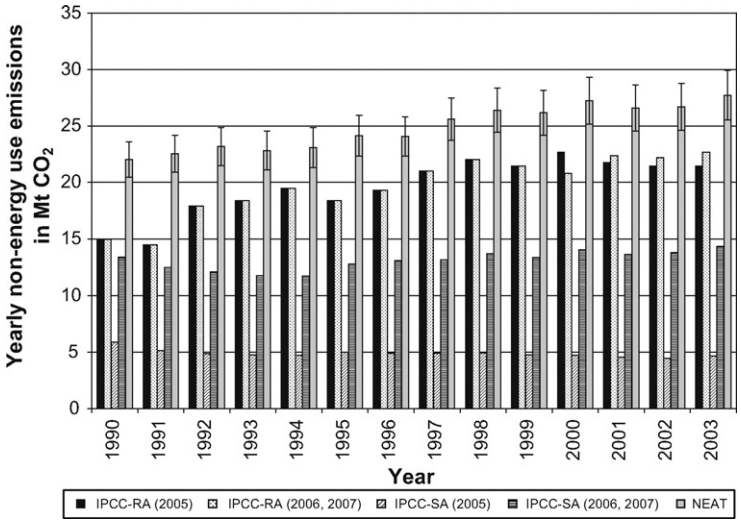

Fig. 2. Yearly non-energy use emissions as estimated by NEAT and as calculated according to IPCC-RA and IPCC-SA of the German GHG inventory (submissions to the UNFCCC in the years 2005, 2006, and 2007; UNFCCC, 2005a, 2006, 2007a).

emissions, total non-energy use, and carbon storage and we compare our results to estimates from the IPCC-RA.

3.1. Emissions from industrial processes

Total yearly industrial process emissions as calculated with NEAT range from 16.0 ± 1.4 Mt CO_2 to 22.6 ± 2.1 Mt CO_2 and show an increasing trend (on average 2.7% per year) in the period of 1990–2003 (Fig. 3). NEAT results exceed the values calculated according to IPCC-SA on average by 640% when compared to data from the 2005 inventory submission and by 77% when compared to the submissions of the years 2006 and 2007 (Fig. 3).[17]

We explain the differences between NEAT and the IPCC-SA as follows[18]:

(i) CO_2 emissions from steam cracking are not reported according to the IPCC-SA, whereas we calculate yearly emissions of 5.8 ± 1.2 Mt CO_2 to 8.6 ± 1.7 Mt CO_2 for the period of 1990–2003. This fact explains 43% and even 87% of the difference between NEAT and the IPCC-SA of the inventory submission 2005 and the inventory submissions 2006 and 2007, respectively.

(ii) The IPCC-SA of the 2005 inventory submission excludes emissions from the production of methanol and carbon black (together representing 14% of the difference) as well as losses from chemical conversion processes (accounting for 19% of the difference between NEAT and IPCC-SA). In the inventory submissions of 2006 and 2007, NEAT results are used to fill these data gaps in the IPCC-SA.

(iii) NEAT and IPCC-SA differ with respect to emission estimates for ammonia production due to incompatible emission factors (discussed below). The observed deviations account on average for 12% and −10% of the total differences between NEAT and IPCC-SA of the inventory submissions in 2005 and 2006, 2007, respectively.

(iv) The IPCC-SA accounts only incompletely for emissions from electrodes and other solid carbon use in the production of non-ferrous metals, ferroalloys, and inorganic chemicals (deviations explain 12% and 23% of the total differences between NEAT results and the IPCC-SA of the inventory submissions in 2005 and 2006, 2007, respectively).

As indicated above, NEAT results were used to improve the completeness of the IPCC-SA (in the inventory submissions of 2006 and 2007) with respect to emissions resulting from the production of methanol, carbon black, as well as losses of chemical conversion processes (Fig. 4). Gaps, however, still remain in the IPCC-SA (UNFCCC, 2006, 2007a). This refers in first instance to emissions from steam cracking. According to our investigations, these are part of non-energy use emissions as stated according to the IPCC-RA of the German GHG inventory and should therefore be reported as industrial process emissions in the IPCC-SA. Omitting this emission source in the IPCC-SA probably results in substantial underreporting of emissions (Fig. 4).[19]

NEAT emission estimates for ammonia production differ from IPCC-SA data as stated in the German GHG inventories submitted to the UNFCCC in the period of 2005–2007. According to the IPCC-SA (inventory submission 2005) emissions are 33–58% lower than our NEAT results. This deviation is entirely caused by the IPCC-SA emission factor (i.e., 0.84 kg CO_2/kg nitrogen contained in ammonia). This emission factor substantially underestimates actual ammonia production emissions. This shortcoming was also addressed by an external review team (UNFCCC, 2005b)[20] and has been corrected in the inventory submissions of the years 2006 and 2007. In these sub-

[17] Electrodes and other solid carbon are used for the production of non-ferrous metals, ferroalloys, and inorganic chemicals. The IPCC-SA reports emissions from these processes under the following source categories: (i) aluminium production, (ii) carbide production, and (iii) ferroalloy production.

[18] The differences specified for the following source categories explain 100% of the total deviations between NEAT and IPCC-SA with respect to industrial process emissions. In the case of the inventory submissions of 2006 and 2007, we determine negative deviations of roughly 10% for ammonia production because estimates according to IPCC-SA exceed NEAT results.

[19] Given the insight obtained in the course of our research, we consider it unlikely that parts of these emissions are reported according to the IPCC-SA under the source category of *energy*. Indication is given, e.g., by the fact that the entry for ethylene production (in steam crackers) in the IPCC-SA is labelled as NO (not occurring) instead of IE (included elsewhere). However, further research is recommended to entirely clarify this point.

[20] The external review team states: "Emissions from ammonia production are estimated using an EF [emission factor] that is lower than the IPCC default and the lowest of all reporting parties, and is not well documented. The ERT [external review team] noted that Germany has planned to begin using the IPCC default value, which is recommended in the future" (UNFCCC, 2005b).

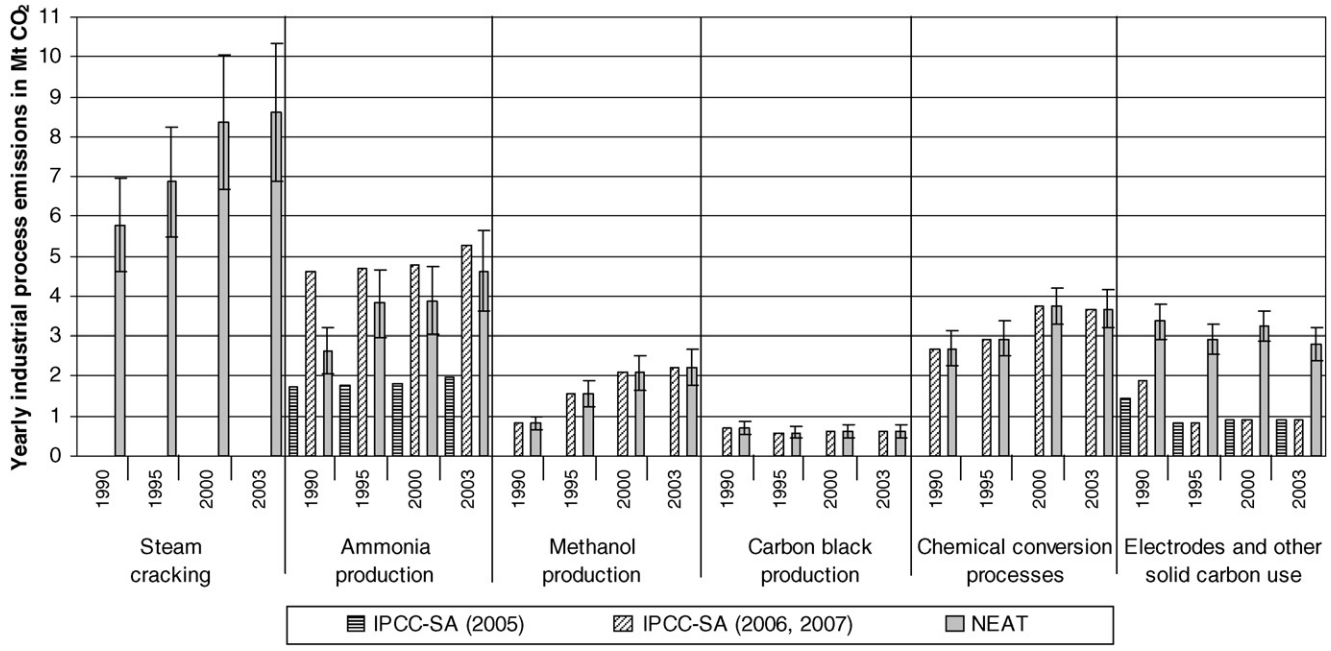

Fig. 3. Yearly industrial process emissions as estimated with NEAT and as calculated according to the IPCC-SA (UNFCCC, 2005a, 2006, 2007a).

missions, the IPCC default emission factor of 1.5 kg CO_2/kg ammonia is applied (IPCC, 1997). This results in emission estimates that are higher than our NEAT results. We argue that the use of the IPCC-SA default emission factor does not correctly account for emissions from ammonia production in Germany because it neglects several country-specific features:

(i) The IPCC default emission factor assumes natural gas to be used as only feedstock for ammonia production and neglects that roughly 30% of ammonia is produced from oil-based feedstock in Germany.
(ii) The IPCC default emission factor does not account for the fractions of CO_2 sequestered for the production of urea (i.e., 13–26% of process emissions from ammonia production in the various years). This leads to double counting of emissions, once under the source category of industrial processes and again under the source category of agriculture.
(iii) The IPCC default emission factor does not account for the system boundaries of the non-energy use of natural gas and oil-based feedstock as applied in the German energy statistics. Consequently, emissions from the fuel use of oil-based feedstock are erroneously excluded from the emission estimates for ammonia production in the IPCC-SA.

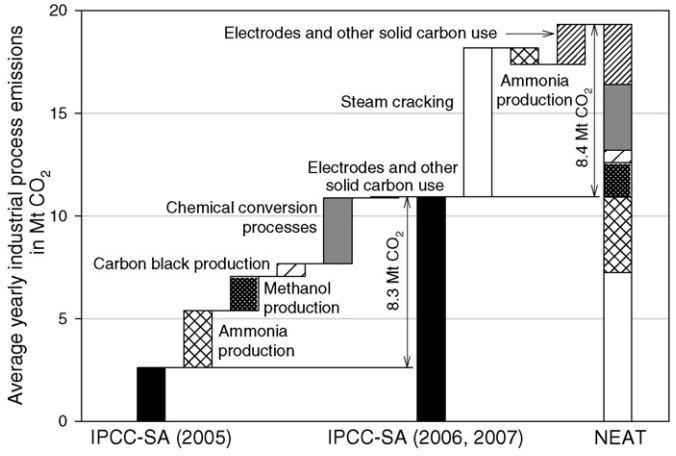

Fig. 4. Average yearly industrial process emissions as estimated with NEAT and as calculated according to the IPCC-SA (UNFCCC, 2005a, 2006, 2007a) for the period of 1990–2003.

Combining these three points, we argue that the IPCC default emission factor of 1.5 kg CO_2/kg ammonia overestimates actual emissions from ammonia production in Germany. The emission factors as implemented in NEAT (1.2–1.4 kg CO_2/kg ammonia) assume efficient ammonia plants and account for both (i) the sequestration of process CO_2 for urea production[21] and (ii) the system boundaries for the non-energy use of natural gas and heavy oil in the German energy statistics (see Section 2.1).

According to the IPCC-SA, CO_2 emissions from the use of electrodes and other solid carbon comprise three principle source categories, i.e., production of aluminium, carbides, and ferroalloys. NEAT, furthermore, covers the manufacturing of other non-ferrous metals and inorganic chemicals (e.g., silicon, lead, zinc). Both NEAT and the IPCC-SA use the same production data and emission factors to estimate emissions from aluminium production. For the production of other non-ferrous metals, ferroalloys, and inorganic chemicals, NEAT arrives at clearly higher estimates than the IPCC-SA (the difference is on average 1 Mt CO_2). This deviation is partly explained by the NEAT results, which exceed IPCC-SA emission estimates for the production of carbides by, on average, 0.5 Mt CO_2. Emissions from ferroalloy production are only calculated in the IPCC-SA of the inventory submissions for the years 2006 and 2007.

[21] The fast majority of urea is used for fertilizer production, whereas a small share becomes incorporated into urea resins. The carbon that is initially contained in urea is thereby either stored in urea resins or it becomes emitted after the application of fertilizers in agriculture. The resulting emissions are accounted for under the source category *agriculture* in the IPCC-SA (IPCC, 1997).

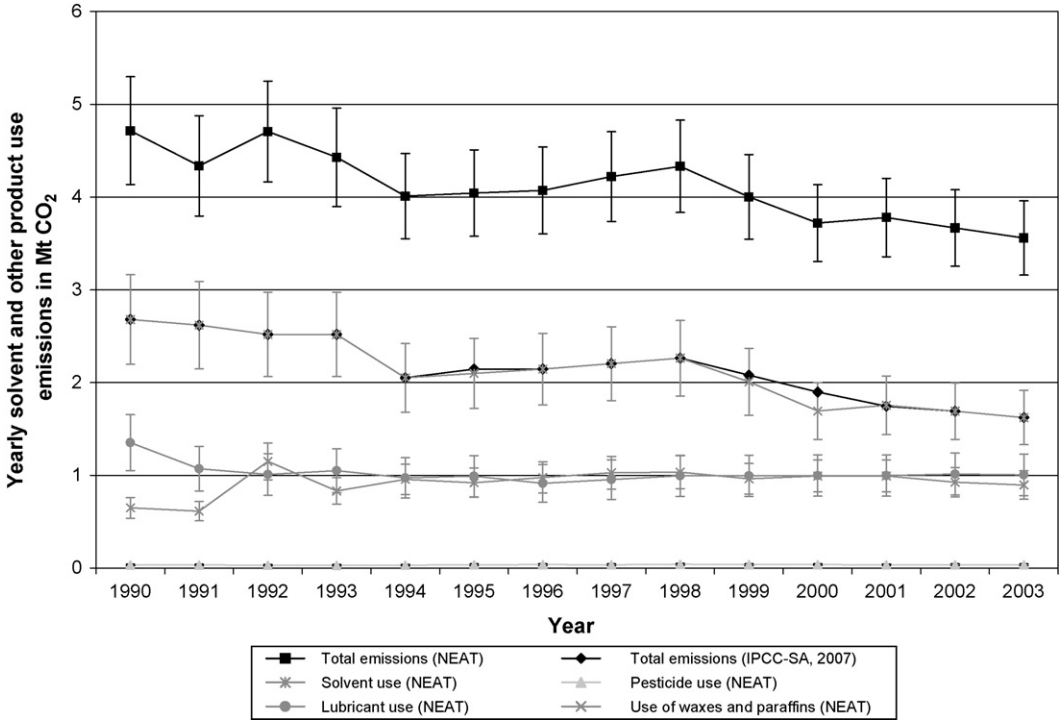

Fig. 5. Yearly solvent and other product use emissions as estimated based on our *key sources approach* and as calculated according to the IPCC-SA (UNFCCC, 2007a).

Here, emission estimates are substantially lower than our NEAT results. For both emission sources (i.e., production of carbides and ferroalloys) activity data and emission factors are not stated in the German GHG inventory. However, based on (i) the emission quantities calculated according to the IPCC-SA and (ii) the information provided by the German inventory report (UNFCCC, 2007b), we argue that total IPCC-SA emission estimates for electrodes and other solid carbon use in the production of non-ferrous metals, ferroalloys, and inorganic chemicals are incomplete because relevant emission sources (e.g., production of lead, magnesium, or zinc) are neglected.

3.2. Emissions from solvent and other product use

With our *key sources approach*, we identify a decrease in yearly solvent and other product use emissions from 4.7 ± 0.6 Mt CO_2 in 1990 to 3.6 ± 0.4 Mt CO_2 in 2003 (Fig. 5). The German GHG inventory reports emissions from solvent and other product use in kt NMVOC equivalents.[22] To make IPCC-SA results comparable with our estimates, we apply a conversion factor of 2.31 kg CO_2/kg NMVOC (Schmidt-Stejskal et al., 2004).[23]

The IPCC-SA estimates regarding total solvent and other product use emissions are only about half of our NEAT values. The differences are explained by the fact that emissions as calculated according to the IPCC-SA include only solvents use[24] but exclude emissions from the consumption of other relevant products. Whereas the omission of pesticides consumption is negligible, disregarding lubricant use and the consumption of waxes and paraffins leads to considerable underestimation of yearly solvent and other product use emissions in the IPCC-SA by roughly 2 Mt CO_2 equivalents.

3.3. Emissions from agriculture

Yearly fossil CO_2 emissions from the application of urea fertilizers in agriculture increase from 0.44 ± 0.07 Mt CO_2 in 1990 to 0.71 ± 0.11 Mt CO_2 in 2003. The IPCC-SA of the German GHG inventory accounts for the first time in the submission of 2007 for emissions from this source category. The estimates of the 2007 inventory submission are within the uncertainty ranges of our results.

3.4. Emissions from waste

We quantify yearly fossil CO_2 emissions from the oxidation of surfactants during wastewater treatment to be 0.89 ± 0.27 Mt CO_2. The IPCC-SA of the German GHG inventory does not calculate fossil-based CO_2 emissions from wastewater treatment. We regard our results as a very rough first estimate that might serve as a benchmark for a more detailed calculation of emissions from this source category.

[22] Note that solvent and other product use emissions are covered in the German GHG inventory according to IPCC (1997). These emissions are typically NMVOCs that quickly become oxidized to CO_2 once released to the atmosphere. Solvent and other product use emissions are nevertheless not converted to CO_2 equivalents in the German GHG inventory. They remain excluded from the estimate of total national GHG emissions that is relevant as reference for the Kyoto target (UNFCCC, 2005c, 2007b).

[23] We show here only results based on the IPCC-SA of the German GHG inventory submitted in the year 2007. Data of earlier inventory submissions (i.e., for the years 2005 and 2006) differ only marginally from the ones presented in Fig. 5.

[24] Both our estimates on solvent use emissions and the results of the IPCC-SA on emissions from total solvent and other product use are based on detailed *bottom-up* analyses of solvent consumption in Germany as conducted by Theloke et al. (2000) and Jepsen et al. (2004). The minor differences depicted in Fig. 5 for solvent use emissions in the year 2000 might be attributed to data adaptations in the German GHG inventory that are not communicated in the *bottom-up* analyses.

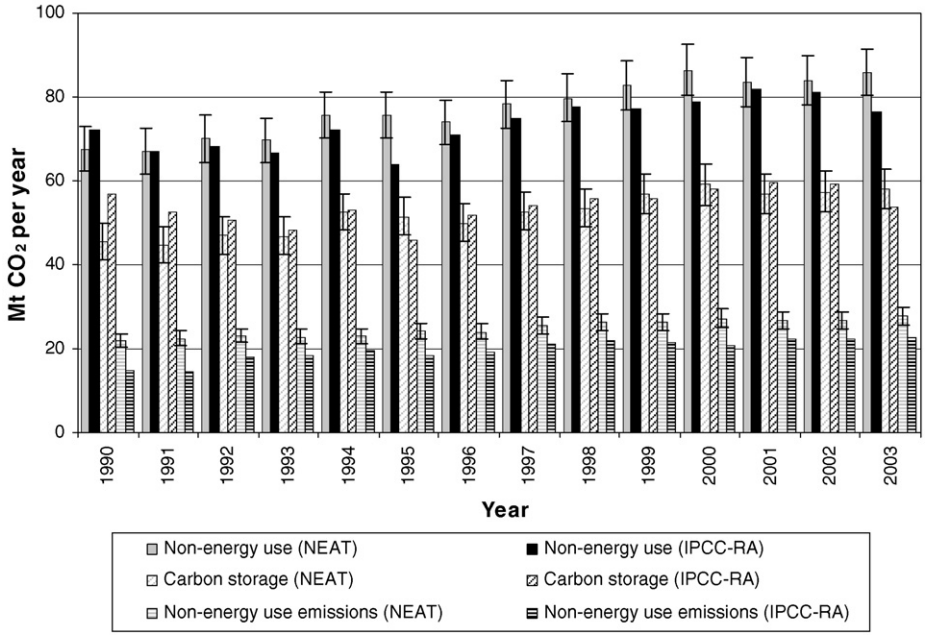

Fig. 6. Total yearly non-energy use, carbon storage, and non-energy use emissions as estimated with NEAT and as calculated according to the IPCC-RA (inventory submission 2007, UNFCCC (2007a)).

3.5. Total non-energy use emissions, carbon storage, and non-energy use of fossil fuels

In this section, we compare total yearly non-energy use emissions as calculated by NEAT with data from the IPCC-RA. Our NEAT estimates range from 22 ± 2 Mt CO_2 (1990) to 28 ± 2 Mt CO_2 (2003). This is 4–8 Mt CO_2/a higher than the non-energy use emissions as calculated with the IPCC-RA of the German GHG inventory (submission 2007) (Fig. 6). The observed differences are caused per definition by deviations in either total non-energy use ($NEU_{(k)}$) or carbon storage ($CS_{(k)}$) as calculated with NEAT and IPCC-RA.

Addressing the first parameter, total yearly non-energy use as calculated with NEAT ranges between 67 ± 5 Mt CO_2 (1991) and 86 ± 6 Mt CO_2 (2000) and shows an overall increasing trend in the period of 1990–2003. With the exception of the years 1990[25] and 1991, non-energy use as calculated with NEAT exceeds the values reported according to the IPCC-RA (inventory submission 2007), which originate from German energy statistics (AGE, 2007) by 2–18%.[26] The differences are mainly caused by the following factors:

(i) The estimates for non-energy use of coal products according to the IPCC-RA are incomplete (by roughly 1 Mt CO_2), as they do not cover all feedstock requirements for the domestic production of coal-derived tars and crude benzene.
(ii) In addition to electrodes, NEAT estimates also include the amounts of other solid carbon such as coal and cokes that are used as reducing agents for metallurgical processes (i.e., the manufacturing of non-ferrous metals, ferroalloys, and inorganic chemicals). Within the IPCC-RA, this carbon (1.1–1.8 Mt CO_2) might be accounted for under the source category *energy* and could have therefore been excluded from non-energy use.
(iii) Chemical grade refinery propylene (roughly 1.8 Mt CO_2 equivalents) is excluded and refinery butadiene and aromatics are likely to be excluded from non-energy use according to the IPCC-RA. All three chemicals are, however, included in NEAT because they are consumed for non-energy purposes by the chemical industry.
(iv) Butene produced in steam crackers (0.7–1.2 Mt CO_2) can be used for both the production of polymers and as a gasoline additive. It remains, however, unclear if and to what extent the fractions of butene consumed for fuel additives enter both the German energy statistics (and subsequently the IPCC-RA) and official production statistics (see also Section 4.1).
(v) The non-energy use of natural gas for carbon black production is included in NEAT (0.15–0.18 Mt CO_2) but excluded from the IPCC-RA (VCI, 2004b).

Combining these factors and leaving the uncertain position of butene aside, we estimate that average yearly non-energy use is potentially underestimated within the IPCC-RA by roughly 4 Mt CO_2. If we apply these corrections, the differences between NEAT and the values calculated according to the IPCC-RA (inventory submission 2007) are substantially reduced.[27]

[25] Due to the reunification of Germany in 1990, official production data (Destatis, 1990–2003a) are particularly uncertain for this year as they might account for production in the former western part of Germany only. It was beyond the scope of this research to entirely clarify this uncertainty. The problem we encounter here is, however, also acknowledged as a major source of uncertainty within the German GHG inventory (UNFCCC, 2005c).

[26] The deviation of 18% in the year 1995 is exceptionally high. It is caused by the comparatively low non-energy use as reported by the German energy statistics. Unlike for all other years, the energy statistics do not report non-energy use of residual fuel oils, leading to roughly 10% lower non-energy use than reported for the years 1994 and 1996. This might be an error in the energy statistics that should be corrected in the future.

[27] An exception is the year 1990 for which the uncorrected IPCC-RA value already exceeds the NEAT estimate. After correction, the values according to IPCC-RA are outside the NEAT uncertainty ranges for the years 1990, 1995, and 2003. If the data correction is applied, deviations between IPCC-RA and NEAT for the two latter years reduce considerably.

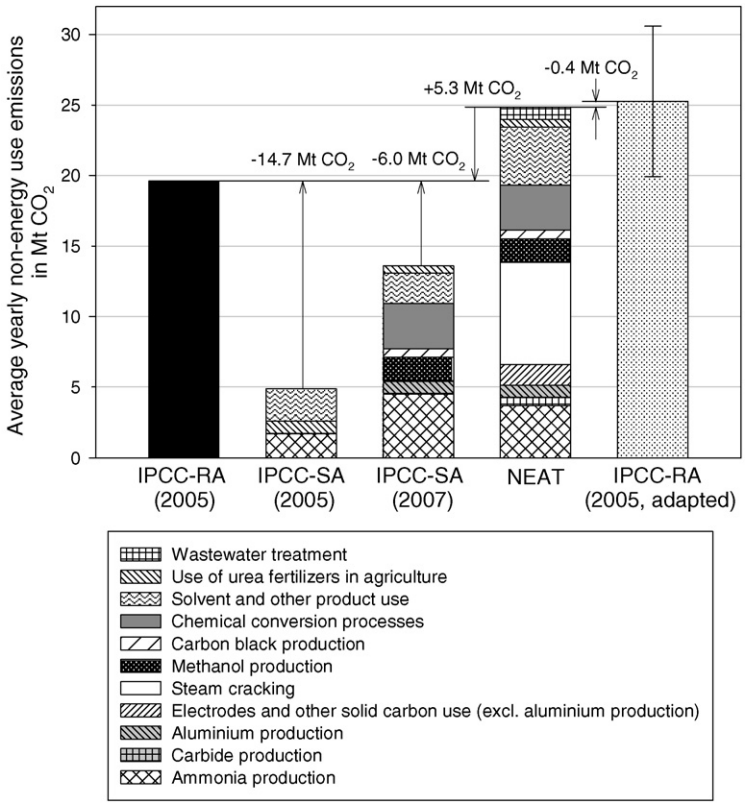

Fig. 7. Overview: closing the gap between IPCC-RA and IPCC-SA by applying NEAT emission estimates (UNFCCC, 2005a, 2006, 2007a).

We now address the second parameter that is relevant for explaining the differences between NEAT results and the IPCC-RA with respect to non-energy use emissions, i.e., carbon storage. NEAT carbon storage is generally in line with official values from the IPCC-RA (inventory submission 2007). However, the good correspondence is an artefact that results from deviations in both non-energy use and carbon storage fractions. Carbon storage is calculated in the IPCC-RA by multiplying the non-energy use of fossil fuels with fuel-specific carbon storage fractions. The average carbon storage fractions according to the IPCC-RA were determined by Prognos (2000) and vary between 70 and 79%. They are higher than our NEAT carbon storage fractions ($66 \pm 10\%$ to $69 \pm 8\%$). The differences are caused by deviations in the system boundaries of the applied carbon storage fractions. The carbon storage fractions as applied in the IPCC-RA are neither entirely consistent with the system boundaries of non-energy use data nor with the aim of the IPCC-RA as outlined by IPCC (1997). The IPCC-RA carbon storage fractions only account for (i) emissions resulting from the combustion of feedstock and (ii) *direct* CO_2 emissions from solvent and other product use (Prognos, 2000). They hence treat parts of the industrial process emissions (e.g., emissions resulting from ammonia production) as well as NMVOC emissions from solvent and other product use as storage.[28] We argue that this methodological flaw alone leads to an underestimation of actual non-energy use emissions in the IPCC-RA (inventory submission 2007) by on average 2 Mt CO_2. In line with the system boundaries of non-energy use data in German energy statistics (AGE, 2007), NEAT carbon storage fractions account for the entire amount of non-energy use emissions resulting from the various source categories as presented previously (Sections 3.1–3.4).

Despite the fact that both NEAT and the IPCC-RA (based on carbon storage fractions as calculated by Prognos, 2000) result in similar estimates for carbon storage, the IPCC-RA underestimates non-energy use emissions. This finding indicates that the identified gap between the IPCC-RA and IPCC-SA methods (i.e., 9–18 Mt CO_2 per year; see Fig. 1) is even larger due to (i) incomplete non-energy use data and (ii) the application of carbon storage fractions that only insufficiently account for non-energy use emissions in the IPCC-RA. In the following section, we show at the example of average yearly non-energy use emissions in the period of 1990–2003 how NEAT results can help removing this inconsistency from the German GHG inventory.

3.6. Comparison between IPCC-RA and IPCC-SA emission estimates

One core objective of this research is to improve data consistency between IPCC-RA (i.e., average yearly non-energy use emissions of 19.6 Mt CO_2 in the period of 1990–2003) and IPCC-SA (i.e., average yearly non-energy use emissions of 4.9 Mt CO_2) (inventory submission 2005) (Fig. 7). We have already discussed in Section 3.1 that NEAT emission estimates for methanol and carbon black production as well as for losses from chemical conversion processes have been used within the IPCC-SA of the German GHG inventory submissions in the years 2006 and 2007 to correct for data gaps in the IPCC-SA of the 2005 inventory submission. Furthermore, the emission factor for ammonia production has been adapted and emissions from urea application in agriculture were estimated for the first time in the inventory submission of 2007. Combining these adaptations

[28] For a more detailed discussion on assumptions, system boundaries, and methodology applied to calculate NEAT and IPCC-RA storage fractions, we refer to Weiss et al. (2007).

reduces the differences between IPCC-RA (submission 2005) and IPCC-SA results (submission 2007) by almost 60% (Fig. 7).

If we furthermore include emission sources that are currently not covered by the IPCC-SA method (i.e., steam cracking, additional non-ferrous metals, ferroalloy, and inorganic chemicals production, product use, wastewater treatment) and if we correct the IPCC (1997) default emission factor currently applied for ammonia production, the resulting non-energy use emissions exceed the estimates according to the IPCC-RA by 5.3 Mt CO_2. The gap between IPCC-RA, IPCC-SA, and NEAT can, however, be closed up to a difference of 0.4 Mt CO_2, if two adaptations are made. First, we add 4 Mt CO_2 to the results of the IPCC-RA to account for the underestimation of non-energy use in the German energy statistics (see Section 3.5). For the second adaptation, we recall our discussion regarding the system boundaries of the Prognos (2000) carbon storage fractions as applied in the IPCC-RA. These were designed to account for emissions from the combustion of feedstock and therefore neglect a large part of emissions from, e.g., industrial processes and solvent and other product use. To correct for this, we can calculate *adapted* IPCC-RA non-energy use emissions by deducting NEAT carbon storage from the *adapted* non-energy use as stated according to the IPCC-RA.[29] The average difference between NEAT and the *adapted* IPCC-RA emission estimates is within the uncertainty range of our results (see Fig. 7). The difference can however be higher than shown in Fig. 7 for individual years (e.g., 1990, 1991, or 2003) for which deviations between NEAT and official non-energy use data in the German energy statistics are not fully explained by the factors described in Section 3.5.

4. Discussion

We first provide a critical discussion of the NEAT approach that has been used for calculating non-energy use and related emissions. In the second part, we give recommendations for both German and international inventory experts and we highlight general aspects, being critical for the correct reporting of non-energy use emissions in the national GHG inventories of Annex I countries.

4.1. Discussion of NEAT methodology

Total non-energy use emissions as calculated with NEAT are attached with uncertainties in the range of 10% of the final result. Given both the scope of this research and the general difficulties attached to the complete and reliable accounting of non-energy use emission, we regard our model uncertainties as acceptable. We nevertheless see potentials for reducing uncertainties by future research. This refers in the first instance to the calculation of industrial process emissions that account for 70% of all uncertainties related to total non-energy use emissions as calculated with NEAT.

We estimate industrial process emissions in NEAT by assuming efficient to very efficient plants for steam cracking as well as for the production of ammonia, methanol, and carbon black. This results in CO_2 emission factors, which are at the lower end of their possible value range.[30] The uncertainty intervals of NEAT results (i.e., ranging from 10 to 25% for individual processes) may be reduced by applying country-specific emission factors based on detailed company surveys. The uncertainty intervals of industrial process emissions can be further reduced by applying more detailed estimation approaches according to Tier III methodology as outlined by IPCC (1997).

Model uncertainties are also attached to emissions from chemical conversion processes that are based in NEAT on process-specific emission factors from open literature (Neelis et al., 2007). Our results represent average estimates for the most important conversion processes in the chemical industry but they do not, however, account for specific settings on the level of individual plants. The estimates of CO_2 emissions from chemical conversion processes refer to reaction losses and exclude both the generation of fuel-grade by-products as well as energy use of feedstock in conversion processes. However, uncertainties result because only some parts of the losses are directly emitted as CO_2, whereas other parts might be either flared with or without additional fuel input and with or without energy recovery (Neelis et al., 2007). Within the scope of this research project, it was not possible to elaborate in greater detail on the exact fate of carbon losses from the various chemical conversion processes. Further research is recommended to reduce uncertainties of our NEAT estimates (which we quantify with 12–16%) for this emission source category. A source of uncertainty, which is excluded from the uncertainty intervals, refers to the assumed chemical conversion routes. Identifying chemical conversion routes is by no means straightforward and requires detailed insight into the structure of the chemical industry in Germany. Various alternative production routes for individual chemicals exist (e.g., phenol is produced from cumene in Germany, whereas it is produced entirely from toluene in the Netherlands). Companies tend to give only vague information due to confidentiality reasons. Further research is recommended to improve the reliability of information on chemical conversion routes that are operated in Germany.

With regard to emissions from solvent and other product use, we highly recommend more detailed *bottom-up* analyses on the fate and oxidation of lubricants and waxes and paraffins. Such research could substantially reduce the uncertainty intervals (i.e., around 20%) that are currently attached to our results.

Our estimates for yearly non-energy use (and therefore also the ones for yearly carbon storage) are associated with additional uncertainties that are linked to the reliability of production and trade data used as model input. We argue that trade data for basic chemicals and refinery products as published by Destatis (1990–2003b) can generally be considered reliable (because they are used for taxation purposes). This is, however, not necessarily the case for production data. We identified major inconsistencies in the production data as stated by the Federal Statistical Office of Germany (Destatis, 1990–2003a) (e.g., for bitumen, lubricants, basic chemicals like butadiene and toluene).

Further uncertainties attached to non-energy use and carbon storage as calculated with NEAT relate to (i) the unclear position of butene in German production and energy statistics and (ii) the system boundaries for coal- and lignite-based non-energy use in German energy statistics. Intensive discussions with experts preparing the energy statistics for Germany did not allow clarification of the exact definition of system boundaries for coal-, lignite-, and coke-based non-energy use beyond any doubts. The non-energy use of these energy carriers, which accounts on average for 7% of total non-energy use, is therefore particularly uncertain.

4.2. Recommendations for inventory experts and energy statisticians

Our NEAT model results provide important insight into non-energy use and related CO_2 emissions and allow us to derive

[29] Note that carbon storage is independent from the system boundaries of non-energy use and therefore does not depend on choices regarding a *net* versus *gross* definition of feedstock use.

[30] For a detailed comparison of NEAT emission factors with data from literature, we refer to Neelis et al. (2003).

recommendations for energy statisticians as well as GHG inventory experts. One outcome of this research is the identification of system boundaries applied to non-energy use in German energy statistics. The system boundaries for non-energy use in energy statistics are not uniform for the various types of fuels (i.e., a *gross* definition for coal-, lignite-, and oil-derived feedstock and a *net* definition for natural gas is applied, see Section 2.1). We explain this inconsistency with different levels of insight obtained by data suppliers into the consumption structure of non-energy use.[31] We recommend harmonizing the system boundaries of non-energy use. Ideally, a uniform approach should be agreed upon *internationally*. This would not only simplify the calculation of non-energy use emissions for the various relevant source categories, it would also allow international comparisons. From this research, we therefore recommend to link the processes of preparing both GHG inventories and national energy statistics more closely to each other.

Insight into energy statistics is also important for the application of IPCC default carbon storage fractions in the IPCC-RA (IPCC, 1997) because these storage fractions are often inconsistent with the system boundaries of non-energy use data. To simplify the calculation of emissions in the IPCC-RA, the improved 2006 IPCC inventory guidelines generally recommend applying storage fractions of 100%, thereby completely removing non-energy use emissions from the IPCC-RA and only considering them in the relevant source categories of the IPCC-SA.

Although solving the difficulties regarding the IPCC-RA storage fractions, the 2006 inventory guidelines no longer allow for crosschecking non-energy use emissions within GHG inventories (IPCC, 2006). Such data comparison can, however, be extremely useful for reliable and complete emissions accounting based on the IPCC-SA method, as the data gaps in the German GHG inventory have demonstrated (see Fig. 1). We therefore recommend inventory experts to apply independent model tools such as NEAT or NEAT-SIMP (Weiss et al., submitted for publication) to check the completeness of IPCC-SA emission estimates. NEAT-SIMP is a simplified version of the NEAT model that avoids the detailed mass balance calculations of NEAT. NEAT-SIMP requires considerably less input data but still generates reliable emission estimates for the various source categories. NEAT-SIMP can, however, not be used for estimating process-specific emissions resulting from conversion processes in the chemical industry.

Due to their high level of detail, NEAT results allow us to identify and reduce gaps regarding industrial process emissions in the IPCC-SA of the German GHG inventory. The accounting of CO_2 emissions from chemical conversion processes in the current German IPCC-SA goes beyond the reporting requirements of both IPCC (1997) and IPCC (2006). We acknowledge this fact but point to remaining gaps and uncertainties within the German GHG inventory. Emissions from steam cracking are still not included under industrial processes in the 2007 inventory submission. The comparison between NEAT and IPCC-SA furthermore revealed that the applied IPCC default emission factor for ammonia production is incorrect for Germany given feedstock distribution, system boundaries of non-energy use, and CO_2 sequestration for urea production. Moreover, emission estimates for the production of non-ferrous metals, ferroalloys, and inorganic chemicals are incomplete in the IPCC-SA (2007 inventory submission). For these cases, we recommend adapting the emission factors and completing the IPCC-SA calculations by using our NEAT model results.

Although the current reporting of solvent and other product use emissions in the German GHG inventory is consistent with the requirements stated by IPCC (1997), the improved IPCC (2006) guidelines request more detailed calculations. We therefore recommend complementing emission estimates from solvent use (Theloke, 2000, Jepsen, 2004) by emission data for the most prominent sources of product use emissions, i.e., the consumption of lubricants and waxes and paraffins. We furthermore suggest using our estimates on emissions from wastewater treatment as a benchmark for further, more detailed IPCC-SA analysis of emissions from this source category.

5. Conclusions

In this paper, we apply the NEAT 3.0 model to estimate non-energy use and related CO_2 emissions for Germany in the period of 1990–2003. NEAT 3.0 calculates both parameters independently from energy statistics and national GHG inventories, providing hence an important consistency check for official data. We regard our estimates to be reliable and useful for filling data gaps in the respective source categories of the IPCC-SA. A drawback with respect to the applicability of NEAT is the requirement for large numbers of production and trade data as well as detailed insight into the German chemical industry for calculating in particular emissions from chemical conversion processes, carbon storage, and total non-energy use. To avoid extensive data collection, a simplified version of NEAT (i.e., NEAT-SIMP) can be used for estimating non-energy use and related emissions for the most important source categories.

NEAT helped to identify and reduce inconsistencies in the German GHG inventory to a large extent. By implementing the recommendations given in the section above, most of the shortcomings that remain in the German GHG inventory submission of 2007 can be addressed in a satisfactory manner. Uncertainties that deserve special attention in the future are firstly related to non-energy use data as applied within the IPCC-RA (i.e., definition of system boundaries and data completeness) and secondly to emission estimates for (i) the use of electrodes and other solid carbon for non-ferrous metals, ferroalloy, and inorganic chemicals production and (ii) the consumption of lubricants and waxes and paraffins.

We finally conclude that applying the NEAT model to Germany has made an important contribution to a more accurate and reliable accounting of GHG emissions. The insight gained by this research is not only relevant for Germany but more generally for the accounting of non-energy use and related emissions in any other country. We summarize our conclusions with the following recommendations for inventory experts:

- Identify the system boundaries of non-energy use data as applied in national energy statistics and allocate emissions accordingly

[31] For example, non-energy use data for oil-based feedstock and refinery products are provided in Germany by individual refineries. They lack the detailed insight in to the final consumption of their deliveries within the chemical sector and can, therefore, only report less detailed *gross* deliveries. The non-energy use data of natural gas, on the other hand, are provided by the Association of the German Chemical Industry (VCI—Verband der Chemischen Industrie e.V.). This association has relatively good insight into the consumption of natural gas by the various chemical companies and can thus distinguish the fractions consumed either as feedstock or as fuel. The VCI delivers, hence, *net* data for non-energy use, excluding the fractions of natural gas used for combustion purposes in chemical processes. Another factor that explains the current non-energy use reporting in Germany (and possibly also in other countries) is that natural gas is used *directly* as fuel for, e.g., ammonia production, whereas naphtha and other oil products are only *indirectly* consumed as fuel via the production of, e.g., hydrogen and other waste gases.

to the various relevant source categories outlined by the IPCC-SA (i.e., either energy or industrial processes, solvent and other product use, agriculture, and waste).
- Ensure completeness of source categories relevant for non-energy use emissions.
- Be cautious with the use of default emission factors. Ensure that the applied emission factors account for country specifics such as (i) system boundaries of non-energy use, (ii) feedstock composition, and (iii) plant efficiencies.
- Aim at reducing uncertainties of emission estimates by applying more detailed approaches according to Tier II and Tier III methodology (IPCC, 1997).

Acknowledgements

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Appendix A

See Table A1.

Table A1
Chemical conversion processes and process-specific emission factors as implemented in NEAT

Production of	Feedstock	Feedstock consumption in t/t product	By-products	Generation of by-products in t/t product	Emission factor in t CO_2 equivalents/t product
Phenol	Cumene	1.35	Acetone	0.61	–
	Toluene	1.20	Benzene	0.01	1.17
Propylene oxide	Propylene	0.88	Dichloro-propane	0.11	0.33
			Dichloro-ethylether	0.03	
	Propylene	0.90	Misc. Acetone	0.25	–
	Isobutene	2.35	Butanol	2.45	0.97
	Propylene	0.74	Styrene	2.29	0.06
	Ethylbenzene	2.52			0.62
Caprolactam	Cyclohexane	1.03	–	–	0.88
	Phenol	0.92	–	–	0.25
Phthalic anhydride	*o*-Xylol	0.92	Maleic acid	0.05	0.60
	Naphthalene	0.92	–	–	0.78
Adiponitrile	Acrylonitrile	1.13	–	–	0.54
	Adipic acid	1.48	–	–	0.40
	Butadiene	0.63	–	–	0.76
	Hydrogencyanide	0.60	–	–	–
Acrylonitrile	Propylene	1.06	Hydrogen cyanide	0.08	0.71
Adipic acid	Cyclohexane	0.75	–	–	0.55
Ethylene oxide	Ethylene	0.78	–	–	0.45
Toluene diisocyanate (TDI)	Toluene	0.67	–	–	–
	Carbon monoxide	0.43	Heavy products	0.08	0.44
Bisphenol-A	Phenol	0.88	–	–	–
	Acetone	0.29	–	–	0.37
	Toluene	0.04	–	–	–
Dimethyl-terephthalate	*p*-Xylene	0.63	–	–	0.27
	Methanol	0.38	–	–	0.07
Polyamide-6	Caprolactam	1.11	–	–	0.26
Isopropanol	Propylene	0.78	–	–	0.25
Polycarbonate	Bisphenol-A	0.90	–	–	–
	Carbon monoxide	0.23	–	–	0.19
Diocthylphthalate	2-Ethylhexanol	0.73	–	–	–
	Phthalic anhydride	0.38	–	–	0.17

Table A1 (*Continued*)

Production of	Feedstock	Feedstock consumption in t/t product	By-products	Generation of by-products in t/t product	Emission factor in t CO_2 equivalents/t product
Terephthalic acid	*p*-Xylene	0.66	–	–	0.07
	Acetic acid	0.05	–	–	0.07
Methylene di-*para*-phenylene-isocyanate (MDI)	Aniline	0.76	–	–	–
	Formaldehyde	0.14	–	–	0.07
	Carbon monoxide	0.26	–	–	0.07
Formaldehyde	Methanol	1.15	–	–	0.12
Acetaldehyde	Ethylene	0.67	–	–	0.11
Acetic acid	Acetaldehyde	0.76	–	–	0.06
	Methanol	0.54	–	–	0.05
	Carbon monoxide	0.53	–	–	0.05
n-Butanol	Propylene	0.66	*i*-Buteraldehyde	0.09	0.07
	Carbon monoxide	0.44	–	–	0.02
Vinylchloride	Ethylene	0.47	–	–	0.07
Aniline	Benzene	1.35	–	–	0.06
Ethylene glycol	Ethylene oxide	0.83	Diethylene glycol	0.1	0.05
			Triethylene glycol	0.01	
Styrene	Ethylbenzene	1.07	Benzene	0.01	0.05
			Toluene	0.02	
Polyvinylchloride	Vinylchloride	1.03	–	–	0.04
Polyethylene terephthalate (PET)	Ethylene glycol	0.33	–	–	0.03
	Terephthalic acid	0.87	–	–	–
Cumene	Propylene	0.35	–	–	0.02
	Benzene	0.66	–	–	0.01
Polystyrene	Styrene	1.01	–	–	0.03
Acetone	Isopropanol	1.05	–	–	0.03
Polyethylene	Ethylene	1.01	–	–	0.03
Polyetherpolyols	Glycerol	0.03	–	–	–
	Propylene oxide	1	–	–	0.02
Urea	Ammonia	0.57	–	–	–
	Carbon dioxide	0.75	–	–	0.02
Cyclohexane	Benzene	0.93	–	–	0.02
Polypropylene	Propylene	1.01	–	–	0.02
Ethylbenzene	Benzene	0.74	–	–	–
	Ethylene	0.27	–	–	0.01

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