



## Modelling CO<sub>2</sub> emissions from non-energy use with the non-energy use emission accounting tables (NEAT) model

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### Abstract

To contribute to a more accurate accounting of CO<sub>2</sub> emissions originating from the non-energy use of fossil fuels, the non-energy use emission accounting tables (NEAT) model has been developed. The model tracks the final fate of the carbon embodied in this non-energy use by means of a carbon flow analysis for the relevant sectors. The model generates estimates for total non-energy use, carbon storage in synthetic organic chemicals and CO<sub>2</sub> emissions resulting from non-energy use that are independent from energy statistics. This paper describes the basic methodology of the NEAT model. It is shown that the results obtained with the model can be used as an important addition to and crosscheck for the non-energy use emission accounting in official greenhouse gas (GHG) emission inventories prepared according to the guidelines of the Intergovernmental Panel on Climate Change (IPCC). The model can help to identify which definitions of non-energy use are applied in the energy statistics employed in national emission inventories and can help to improve national inventory methodologies based on this insight.

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## 1. Introduction

In the context of greenhouse gas (GHG) emission inventories, so far most attention has been paid to CO<sub>2</sub> emissions resulting from the combustion of fossil fuels. A significant fraction of fossil fuels is not directly used in combustion processes, however, but is consumed for non-energy use purposes. The non-energy use of fossil fuels consists of two parts:

- The consumption of fossil fuels as feedstock in the chemical industry. Examples are the use of naphtha for the production of olefins and the use of natural gas for the production of ammonia.<sup>1</sup>
- A limited number of non-energy refinery and coke oven products that are consumed in various economic sectors and the use of solid carbon for the production of metals and inorganic chemicals. Examples are the use of bitumen in the building industry, lubricants for transportation and the use of cokes for the production of metals.<sup>2</sup>

Worldwide, the non-energy use of fossil fuels represented 5.3% of the total primary energy supply (TPES) in 2000. This share differs from country to country, depending on the relative importance of refineries and basic chemical industries. In the Netherlands for example, with its large petrochemical industry, the non-energy use share was 13.5% in 2000 and in Korea, the share was 14.1% in 2000 (IEA, 2002). Estimating CO<sub>2</sub> emissions resulting from the non-energy use of fossil fuels is not straightforward, because part of the carbon embodied in these fossil fuels is first stored in chemicals that have lifetimes ranging from days to decades. These chemicals lead to emissions during the use phase (e.g. solvents) or in the waste treatment phase. In other cases (e.g. asphalt and land filled plastics), these chemicals do not lead to emissions at all within a time span relevant for emission accounting. Apart from the emissions originating from the carbon embodied in synthetic organic chemicals, non-energy use may lead to industrial process emissions during the production of certain chemicals such as ammonia. In some processes, the hydrocarbon input is used both as fuel and as feedstock. Depending on the definition of non-energy use applied in the energy statistics, part of the carbon embodied in the non-energy use might therefore also lead to CO<sub>2</sub> emissions from fuel combustion. In Section 2 of this paper, the various emission source categories will further be defined and discussed.

In their emission inventory guidelines (IPCC/IEA/OECD/UNEP, 1997), the Intergovernmental Panel on Climate Change (IPCC) recommends two principal methods of calculating national GHG emissions, the reference approach (IPCC-RA) and sectoral approach (IPCC-SA). The IPCC-RA only calculates fossil CO<sub>2</sub> emissions and is supposed to be applied as a crosscheck for the IPCC-SA and for countries with limited data availability. The principal idea behind the IPCC-RA is to subtract the amount of fossil carbon stored from the total CO<sub>2</sub> emissions calculated on basis of the total primary energy supply of a country. The carbon storage is calculated by multiplying the non-energy use of a certain fuel with a storage

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<sup>1</sup> In energy statistics published by the International Energy Agency (IEA) this feedstock use is reported as a memo item under the final energy consumption of the chemical industry.

<sup>2</sup> In energy statistics published by the International Energy Agency (IEA) the use of these refinery, coal and coke oven products is reported as non-energy use in (i) industry/transformation/energy, (ii) transport and (iii) other sectors.

fraction for this fuel:

$$\begin{aligned} \text{carbon storage (t carbon)} &= \text{non-energy use (J)} \times \text{emission factor (t carbon/J)} \\ &\times \text{storage fraction (\%)} \end{aligned} \quad (1)$$

The IPCC provides default values for the storage fractions (100% for bitumen; 80% for naphtha, LPG and ethane; 75% for coal oils and tars from coking oil; 50% for lubricants and gas/diesel oil and 33% for natural gas; IPCC/IEA/OECD/UNEP, 1997, vol. 2, pp. 1–37). The resulting emission estimate (TPES in carbon equivalents minus the carbon storage) is nowadays generally regarded as an estimate for national fossil CO<sub>2</sub> emissions from ‘Fuel combustion’ only (see Section 6 for a further discussion on the scope of the IPCC-RA). In the more detailed IPCC-SA, instead of taking the national fossil fuel supply as the basis for the calculations, data on energy use by sector are used to calculate fossil CO<sub>2</sub> emissions from fuel combustion per sector. In the tiers 1 and 2 methods described in the guidelines, the carbon storage is still calculated using formula 1. Only in more complex ‘Tier 3’ methods, which are not explicitly described in the guidelines, CO<sub>2</sub> emissions from fuel combustion are estimated using data other than those from the energy statistics<sup>3</sup>. In addition to CO<sub>2</sub> emissions from fuel combustion, GHG emissions in the IPCC-SA are also reported in other emission source categories. These include ‘Industrial process emissions’, ‘Solvent and other product use’ and ‘Waste’. Various disadvantages exist with regard to the current IPCC methods for non-energy use CO<sub>2</sub> emission accounting such as:

- The failure of methods based on only the energy statistics to take into account the variety of downstream non-energy carbon flows through the economy (e.g. trade in synthetic organic chemicals). These flows might differ substantially between countries.
- The unclear scope of the IPCC-RA, either as a method to calculate CO<sub>2</sub> emissions from fuel combustion only or as a tool to calculate total fossil CO<sub>2</sub> emissions (further discussed in Section 6).
- The lack of proper definitions of non-energy use in the energy statistics for important processes such as steam cracking, leading to possible overestimation or underestimation of emissions in both the IPCC-RA and IPCC-SA (further discussed in Sections 4 and 6).

For these reasons, emissions resulting from the non-energy use of fossil fuels contribute considerably to the overall uncertainty in many national GHG emission inventories, especially in countries with a large share of non-energy use relative to the TPES. In the Netherlands, emissions from oil feedstocks are, for example, among the top 10 of *key sources* contributing to both *level* and *trend* uncertainty according to Olivier and Peters (2005)<sup>4</sup>.

To contribute to a more accurate accounting of GHG emissions resulting from the non-energy use of fossil fuels, we developed the non-energy use emission accounting

<sup>3</sup> An example of a country applying such a method is the Netherlands in which emissions reported by individual firms are combined with emission estimates based on the energy statistics. For more details, we refer to Neelis et al., 2005.

<sup>4</sup> Definitions of the terms ‘key source’, ‘level uncertainty’ and ‘trend uncertainty’ can be found in the IPCC Good Practice Guidance (IPCC, 2000).

tables (NEAT) model. The model, developed as an Excel spreadsheet tool, is based on a bottom-up carbon flow analysis. The model tracks the final fate of the carbon embodied in the fuels used for non-energy use purposes using primarily production and trade statistics. The first version of the model has been described by Gielen and Patel (1999) and was with minor adaptations used by Gielen and Yagita (2002) to study Japanese carbon storage in 1996. The main focus of the first model version was on the correct calculation of the carbon storage in the economy. Since the first version, the model has further been refined and extended by a module to calculate direct industrial process emissions resulting from non-energy use (e.g. from ammonia production). The extended model now systematically deals with all carbon flows related to the non-energy use of fossil fuels and can be used to generate estimates for total non-energy use, carbon storage and non-energy use emissions that are independent from the energy statistics. The aim of this paper is to investigate whether the results obtained with the extended NEAT model (version 2.0) can be used as a crosscheck for the non-energy use emission accounting in official GHG emission inventories. We start with an overall overview of the NEAT methodology (Section 2), followed by three sections in which the various model calculations are described. In Section 6, the comparison with the official GHG inventory is discussed. We end with a discussion and some main conclusions and recommendations for future work. The application of the model for country studies of Korea, Italy and the Netherlands is described elsewhere in this special issue (Park, 2005; La Motta et al., 2005; Neelis et al., 2005).

## 2. Overview of emission source categories and system boundaries in the NEAT model approach

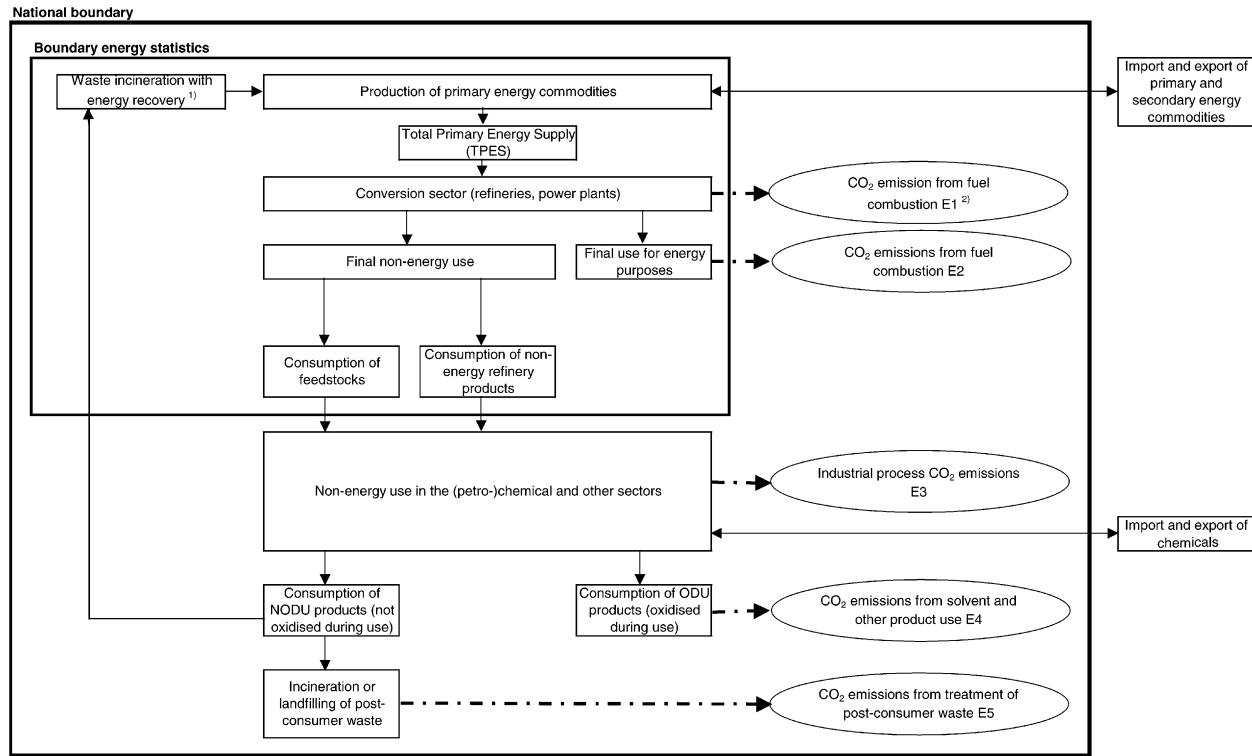
As mentioned in the introduction, the four IPCC emission source categories that are relevant for non-energy use emission accounting are:

1. Fuel combustion,
2. Industrial processes,
3. Solvent and other product use,
4. Waste.

In the NEAT model, we also distinguish these source categories. We convert all flows into CO<sub>2</sub> equivalents based on the carbon content of the flows under consideration. We then calculate the CO<sub>2</sub> emissions in the various source categories<sup>5</sup>. Fig. 1 shows how the NEAT emission categories relate to the overall national energy and carbon flows. The figure shows all activities, which add up to a country's TPES as it can be found in energy statistics. Primary energy commodities (crude oil, natural gas) are converted to secondary commodities. The conversions result in CO<sub>2</sub> emissions from 'Fuel combustion' in the conversion sector (E1). The secondary energy commodities produced in the conversion sector (fuels, electricity) are available for final consumption. The majority of the energy

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<sup>5</sup> For fuel combustion, incomplete combustion is neglected.



<sup>1)</sup> In line with the international energy balance (IEA, 2002), it is assumed that the waste used for energy recovery is in the energy balance reported as a produced energy commodity. The energy recovery (to e.g. electricity) is subsequently covered in the conversion sector and the CO<sub>2</sub> emissions are part of the emissions from fuel combustion (E1).

<sup>2)</sup> Including emissions from waste incineration with energy recovery.

Fig. 1. Overview of national energy flows and fossil CO<sub>2</sub> emissions in the NEAT model approach (the solid lines indicate energy and/or material flows, the dotted lines indicate emissions flows, the ovals are the relevant IPCC emission source categories).

commodities are consumed for energy purposes in all economic sectors, leading to CO<sub>2</sub> emissions from ‘Fuel combustion’ (E2). The remainder is used for the two types of non-energy use described in the introduction. Part of the carbon embodied in this non-energy use is already oxidised to CO<sub>2</sub> during the production phase of certain chemicals of which ammonia is the most important example in terms of total worldwide CO<sub>2</sub> emissions. These emissions have been defined by the IPCC as CO<sub>2</sub> emissions from ‘Industrial processes’ (E3). As we will show in Section 4, various possible definitions can be applied to divide the total hydrocarbon input over final energy use and final non-energy use for a number of these processes and the allocation between emissions from ‘Fuel combustion’ (E2) and emissions from ‘Industrial processes’ (E3) is therefore not always straightforward. The remainder of carbon embodied in the fossil fuels used for non-energy use purposes is first stored in chemicals. Some of these products only lead to GHG emissions during incineration of post-consumer waste. In the NEAT model, we refer to these products as products that are not oxidised during use (NODU). According to the emission inventory guidelines (IPCC/IEA/OECD/UNEP, 1997), waste that is incinerated with energy recovery is considered as fuel and is hence defined to lead to emissions from ‘Fuel combustion’ (E1). Emissions from incineration without energy recovery are assigned to the emission category ‘Waste’ (E5). Another group of chemicals (e.g. detergents and solvents) is already released into the atmosphere during or directly after use (fully or at least partially). In NEAT, these products are referred to as products that are oxidised during use (ODU). The emissions from the use of these ODU products are assigned to the IPCC emission source category of ‘Solvent and other product use’ (E4).<sup>6</sup> In the NEAT model, we count these emissions as CO<sub>2</sub> emissions. In the official emission inventories according to the IPCC-SA, these emissions might also be reported as non-methane volatile organic compounds (NMVOC) emissions from ‘Solvent and other product use’ or as methane emissions in the category ‘Waste’.

We discuss the NEAT model calculation of CO<sub>2</sub> emissions from ‘Solvent and other product use’ (E4) in Section 3 and of CO<sub>2</sub> emissions from ‘Industrial processes’ (E3) in Section 4. In Section 4, we also discuss possible definitions for non-energy use applied in the energy statistics for a number of processes and the resulting difficulties in allocating emissions to either ‘Industrial processes’ (E2) and ‘Fuel combustion’ (E3). Emissions from waste incineration of NODU products (E1 and E5) are not calculated in the NEAT model. We assume that these emissions are correctly calculated in the official emission inventories. The model can be used to generate independent estimates for the total non-energy use in CO<sub>2</sub> equivalents and for the carbon storage. Based on this, storage fractions for use in the IPCC-RA can be calculated and the total fossil CO<sub>2</sub> emissions can be estimated. These elements are discussed in Section 5. The compari-

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<sup>6</sup> In the current IPCC Guidelines (IPCC/IEA/OECD/UNEP, 1997, vol. 3, pp. 1.25) and in previous descriptions of the NEAT model (Gielen and Patel, 1999; Gielen and Yagita, 2002), a distinction was made between ‘long-life’ and ‘short-life’ products. We consider this nomenclature to be confusing, because certain products called long-life (e.g. polyethylene bags) are consumed and oxidised (during waste incineration) very shortly after their production. The current nomenclature (ODU versus NODU) better reflects the type of oxidation in line with CO<sub>2</sub> emission categories (‘Solvent and product use’ versus ‘Waste’ or ‘Fuel combustion’). For a more detailed discussion, reference is made to Patel et al. (2005).

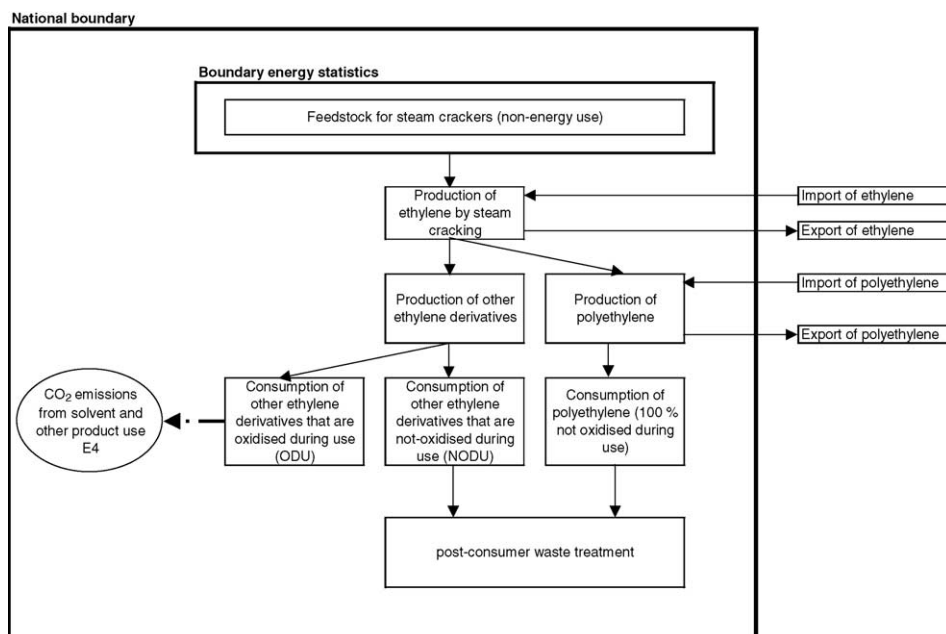


Fig. 2. Calculation of emissions from solvent and other product use in NEAT, simplified example for ethylene (the solid lines indicate energy and/or material flows, the dotted line indicate an emissions flow, the oval is the relevant IPCC emission source categories).

son with the energy statistics and the official GHG emission inventory is discussion in Section 6.

### 3. Emissions from solvent and other product use

To develop an estimate of the emissions from the use of ODU products ('solvent and other product use'), the (petro-)chemical industry is modelled by means of a national carbon balance, covering (in the current model version), 77 of the most important organic chemical commodities in terms of production volume.<sup>7</sup> The carbon balance contains the conversion routes from 22 basic chemicals to 55 intermediate and final products (Table 1). The method will be explained by use of the simplified example of ethylene use as shown in Fig. 2. In this simplified example, ethylene is used for the production of polyethylene and for the production of other ethylene derivatives, which are not individually modelled.<sup>8</sup> Both the total consumption of polyethylene and the remaining ethylene consumption, which is

<sup>7</sup> The selection has been made based on own insight. The list contains all organic chemicals listed in the top 50 of chemicals produced in the US (DOE/OIT, 2000) with the exception of methylchloride.

<sup>8</sup> In the simplified example polyethylene is the only ethylene derivative individually modelled. In the actual NEAT model, synthetic ethanol, ethylene oxide, ethylbenzene, ethylene dichloride, ethylene-propylene-diene-monomer (EPDM), epoxy resin and polyvinyl acetate are also modelled.

Table 1  
Assumed fractions of ODU vs. NODU products for the 77 NEAT core products (the datasets ‘MIN release’ and ‘MAX release’ are used for a sensitivity analysis)

Chemicals	Total consumption or ‘other use’ <sup>a</sup>	Mean (%)		MIN release ODU <sup>b</sup> (%)	MAX release ODU <sup>b</sup> (%)
		NODU <sup>b</sup> (%)	ODU <sup>b</sup> (%)		
<b>Basic chemicals</b>					
Acetylene	Other	50	50	10	70
Benzene	Other	50	50	20	70
Bitumen	Total	100	0	0	0
Butadiene	Other	100	0	0	20
Other C4	Other	37	63	45	100
Carbon black	Total	100	0	0	0
CO-source	Other	50	50	0	0
Ethylene	Other	5	95	85	100
Lubricants	Total	67	33	9	50
Methanol	Other	50	50	30	70
Petroleum coke	Total	0	100	100	100
Pitch	Total	0	100	100	100
Creosote oil	Total	100	0	0	0
Naphthalene	Total	50	50	20	70
Other tar products	Total	100	0	0	0
Propylene	Other	37	63	50	75
Toluene	Other	17	83	70	97
Waxes, paraffins	Total	0	100	40	100
Xylenes ( <i>o</i> -, <i>m</i> -, <i>p</i> -, mixed xylene)	Total	0	100	30	100
<i>ortho</i> -Xylene	Other	0	100	30	100
<i>meta</i> -Xylene	Total	0	100	30	100
<i>para</i> -Xylene	Other	0	100	30	100
<b>Intermediates</b>					
Acetic acid	Other	35	65	35	75
Acetone	Other	60	40	40	65
Acrylic acid	Other	100	0	0	5
Acrylonitrile	Other	100	0	0	10
Adipic acid	Other	100	0	0	5
Aniline	Other	80	20	5	25
Bisphenol A	Other	100	0	0	0
Butanol	Total	19	81	70	90
Caprolactam	Other	100	0	0	0
Cumene	Total	100	0	0	5
Cyclohexane	Total	20	80	60	100
Cyclohexanone	Other	5	95	90	100
Dimethylterephthalate	Other	100	0	0	0
Ethanol	Total	0	100	70	100
Ethylbenzene	Other	100	0	0	70
Ethylendichloride	Other	0	100	100	100
Ethylene glycol	Other	0	100	70	100
Ethylene oxide	Other	29	71	65	95
Formaldehyde	Other	0	100	70	100
Methyl- <i>tert</i> -butyl-ether (MTBE) <sup>c</sup>	Total	0	0	0	0



Table 1 (Continued)

Chemicals	Total consumption or 'other use' <sup>a</sup>	Mean (%)		MIN release ODU <sup>b</sup> (%)	MAX release ODU <sup>b</sup> (%)
		NODU <sup>b</sup> (%)	ODU <sup>b</sup> (%)		
Higher alcohols	Other	50	50	10	90
Orthophtalates	Other	100	0	0	50
Phenol	Other	0	100	70	100
Phthalic anhydride	Other	0	100	30	100
Polyether-polyols	Other	100	0	0	50
<i>i</i> -Propanol	Other	7	93	80	100
Propylene oxide	Other	0	100	100	100
Styrene	Other	100	0	0	0
Terephthalic acid	Other	100	0	0	0
Isocyanates	Other	100	0	0	0
Urea	Other	0	100	0	100
Vinylchloride monomer	Other	20	80	30	100
Products					
Acrylonitrile–butadiene–styrene	Total	100	0	0	0
Butadiene rubber	Total	100	0	0	0
Ethylene–propylene–diene–monomer	Total	100	0	0	0
Epoxy resin	Total	100	0	0	0
Melamineformaldehyde resin	Total	100	0	0	0
Phenolic resin	Total	100	0	0	0
Polyacetates	Total	100	0	0	0
Polyacrylates	Total	100	0	0	0
Polyacrylonitrile	Total	100	0	0	0
Polyamide	Total	100	0	0	0
Polycarbonate	Total	100	0	0	0
Polyethylene	Total	100	0	0	0
Polyethyleneterephthalate	Total	100	0	0	0
Polypropylene	Total	100	0	0	0
Polystyrene	Total	100	0	0	0
Polyurethane	Total	100	0	0	0
Polyvinylacetate	Total	100	0	0	0
Polyvinylchloride	Total	100	0	0	0
Styrene–acrylonitrile	Total	100	0	0	0
Saturated polyester	Total	100	0	0	0
Styrene–butadiene rubber	Total	100	0	0	0
Unsaturated polyester/alkyd resin	Total	100	0	0	0
Urea formaldehyde resin	Total	100	0	0	0

<sup>a</sup> Chemicals labelled 'other' are used for the production of other chemicals included in NEAT. Chemicals labelled 'total' are not used for the production of other chemicals included in NEAT. See text for further explanation.

<sup>b</sup> ODU: oxidised during use, NODU: not-oxidised during use.

<sup>c</sup> MTBE ends up as a antiknocking agent in the fuel pool and the emissions are thus taken into account in the CO<sub>2</sub> emissions from fossil fuel combustion.

used for the production of other ethylene derivatives, are divided into ODU and NODU applications. For some of the products, this division is clear-cut. All polymers, including the polyethylene of the example, are for example NODU products. For other products (like the total of other ethylene derivatives in the example), the fraction of ODU versus NODU products has been estimated based on the use pattern of these products found in literature (e.g. Weissermel and Arpe, 2003; Chauvel and Lefebvre, 1989). Solvents and surfactants are regarded completely ODU. An uncertainty range between ODU and NODU was determined for products for which the exact use was unknown. The fractions of ODU versus NODU applications for all 77 core commodities as well as the uncertainty ranges are given in Table 1. The calculation of emissions from ‘solvent and other product use’ can be summarised with the following formula:

Emissions from solvent and other product use

$$= \sum_{i=1}^{77} (P_i + I_i - E_i - C_{\text{NEAT},i}) \times \% \text{ODU}_i \quad (2)$$

With  $P_i$ ,  $I_i$  and  $E_i$  representing production, import and export of chemical  $i$  in CO<sub>2</sub> equivalents and  $C_{\text{NEAT},i}$  representing the consumption of chemical  $i$  for the production of other NEAT core chemicals, also in CO<sub>2</sub> equivalents. For chemicals that are not used as intermediate for the production of other NEAT chemicals ( $C_{\text{NEAT},i} = 0$ ), the total consumption is divided into an ODU and NODU fraction. For those commodities used for the production of other NEAT commodities ( $C_{\text{NEAT},i} \neq 0$ ), the consumption for remaining derivatives is divided into an ODU and NODU fraction. These two cases are marked by the entries ‘total’ or ‘other’ in Table 1. The key simplifications in the current NEAT model carbon balance are:

- We restrict ourselves to 77 key chemicals and do not take into account imports and exports of all more downstream derivatives, which are covered as consumption for other derivatives. For countries with large net trade streams this could lead to an underestimation (net importing countries) or an overestimation (net exporting countries) of the consumption of both ODU and NODU products in the country of study. To be able to study this effect in more detail, the trade of about 450 product groups in addition to the NEAT core products is included in NEAT as an optional refinement of the model and is referred to as the additional trade module.
- We assume that all chemical conversions from basic chemicals to intermediates and end products are 100% carbon efficient. In practice, this is not the case and carbon is lost either in the form of direct CO<sub>2</sub> emissions or in the form of non-valuable by-products or off-specification products (non-specs), which can be burned either with or without energy recovery. As a result of the model assumption of 100% carbon efficiency, these carbon losses from incomplete conversions end up in the consumption for other derivatives. This consumption is divided into an ODU and a NODU fraction and hence might lead to an overestimation of both the consumption of NODU and ODU products. This could only be avoided if relevant survey data or other estimates were available for carbon losses from incomplete conversions, which is currently not the case. There are however indications that the magnitude of these emissions might be substantial (Tonkovich and Gerber,

1995; Freed et al., 2005) and further research is therefore warranted (see discussion in Section 7).

- We assume that the structure of the chemical industry is very similar worldwide and bulk chemicals are made via the same production routes and similar production processes everywhere. However, some intermediates and final products can be made in more than one way. An example is phenol, which can be made from benzene, cumene and toluene. Other examples are the mixed product groups like polyamides where the various representatives (e.g. polyamide 6 and polyamide 6,6) are manufactured from different raw materials. In the NEAT model, default assumptions are made about the production routes in these cases. Model users can identify the actual production routes applied in the country based on an in-depth study for the respective country and can introduce these routes in the NEAT model.

The NEAT model has extensive data requirements. For a correct application of the model, production and trade data are needed for all 77 core products in the NEAT model. These data may not be available for all NEAT core products or the available data may be too aggregated due to inclusion of different types of products in one single product category in production statistics. In such cases, the data has to be estimated on the basis of capacity data, on the basis of mass balance calculations, or by contacting producers. Apart from data availability problems, data reported in statistics can also be erroneous. One typical reason is that intermediates that are converted further on the same site (e.g. ethyl benzene to styrene) may not always be reported as production in production statistics.

The carbon balance in the NEAT model can be used to estimate, in CO<sub>2</sub> equivalents, the fraction of carbon associated with non-energy use in a country that is embodied in chemical products. It is important to realise that for this estimate, we express this fraction as a proportion of an “upstream carbon flow”; – i.e., we study carbon flows at a different level than so far. To make this clear, we refer to Figs. 1 and 2. For the calculation of emissions from solvent and other product use, the aim was to estimate the emissions related to the final consumption downstream (E4 in Figs. 1 and 2). We are now interested in the non-energy use as it is reported in the energy statistics; this is a feedstock value, thus representing an upstream flow. In the example of Fig. 2, an estimate for non-energy use can be obtained by using the feedstock required for ethylene production. It is hence not necessary to study all the downstream material flows indicated in Fig. 2. It is, in this case, sufficient to know the amount of ethylene produced in the country of study. In more general terms, the estimate for feedstock use can be obtained by adding the CO<sub>2</sub> equivalents of all (not only ethylene) basic chemicals produced from the hydrocarbon feedstocks.<sup>9</sup> The consumption of non-energy use refinery and coke oven products (the second element of non-energy use mentioned in the introduction) in CO<sub>2</sub> equivalents can directly be estimated

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<sup>9</sup> The definition of basic chemicals is less straightforward as it may seem. In the Netherlands, for example, aromatics like benzene and even styrene are reported as energy commodities in energy statistics and only the conversion of these basic aromatics to more downstream chemicals (e.g. polystyrene) is reported as non-energy use. As a consequence, the production values of these more downstream products should be added to obtain an estimate for non-energy use that is comparable to the definition applied in the Dutch energy statistics (see Neelis et al., 2004; Neelis et al., 2005).

by taking the consumption values of these products.<sup>10</sup> Summation of the two (production of basic chemicals from feedstocks and consumption of non-energy refinery and coke oven products) yields the carbon associated with non-energy use in a country that is embodied in chemical products.

#### 4. Industrial process emissions

Part of the carbon embodied in the fossil fuels that are used for non-energy purposes is directly oxidised to CO<sub>2</sub> during the production of chemical products, leading to industrial process emissions (E3 in Fig. 1). In certain processes (e.g. production processes for ammonia, methanol, carbon black and the steam cracking process), part of the fossil fuel input is used as fuel (either directly or via the intermediate production of residual gases and other fuels). In energy statistics, there may be two ways to report non-energy use for these industrial processes. Using a gross definition of non-energy use, the total fossil fuel input is allocated to non-energy use. Using a net definition of non-energy use, the part that is used as fuel is subtracted from the non-energy use and is reported as final energy use. It is evident that the storage fractions used in Eq. (1) in the IPCC-RA calculation should reflect the allocation method used between energy and non-energy use in order to yield the correct carbon storage and CO<sub>2</sub> emissions. In the IPCC-SA, there is also a risk of double counting or omission of emissions. If Eq. (1) is used in the IPCC-SA to calculate emissions from fuel combustion, the emissions from non-energy use are already accounted for via Eq. (1) (the part of non-energy use not stored). In that case, these emissions should not again be counted as emissions in one of the other source categories. On the other hand, if the non-energy use is excluded from the emissions from fuel combustion (by setting storage fractions to 100% or by simply excluding non-energy use from the calculation), the emissions resulting from the non-energy use should be accounted for in one of the other source categories. In that case, the allocation method between energy and non-energy use used in the energy statistics determines the correct amount of emissions, since it can be assumed that emission from the part allocated to energy use are already accounted for under fuel combustion. In calculating emissions for these processes for national inventories, one should therefore always keep in mind the applied non-energy use definition in the energy statistics. In the current IPCC guidelines, the risk of double counting is acknowledged for ammonia production (IPCC/IEA/OECD/UNEP, 1997, vol. 1, pp. 2.1 and 2.13), but some of the important processes for which double counting or omission of emissions is likely to happen (methanol, carbon black and steam cracking) are not separately discussed. The NEAT model contains a module to calculate the total CO<sub>2</sub> emissions from the relevant industrial processes. The processes are discussed in detail below. In Fig. 3, we give a schematic general energy balance of a process in which a hydrocarbon feedstock is converted to chemicals. We will use this figure to explain possible definitions of non-energy use for the relevant processes. The results of the NEAT model can be compared with the non-energy use figures in energy

<sup>10</sup> Of the NEAT basic chemicals, bitumen, lubricants, petroleum coke, pitch, creosote oil, naphthalene and waxes and paraffins are non-energy use refinery and coke oven products. The trade in these products is already accounted for in the energy statistics and these products therefore enter the calculation with their production values.

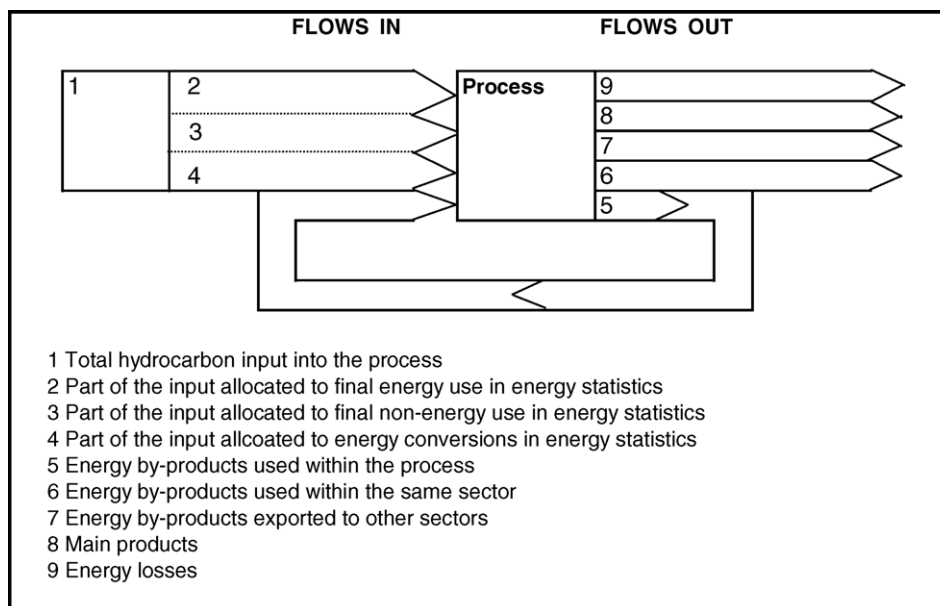


Fig. 3. General energy balance of industrial processes producing chemicals from feedstocks (size of flows arbitrarily chosen).

statistics and with the GHG inventory. This comparison is discussed in Section 6. It should be noted that the production and use of cokes in pig iron production is excluded from the NEAT model, because these processes are normally covered in the energy conversion section of energy statistics and are therefore not part of the non-energy use.

#### 4.1. Ammonia

Ammonia is most frequently produced from natural gas, but lower grade fuel oils or coal are also used. The hydrocarbon feedstock serves to produce hydrogen, which is then converted with nitrogen to produce ammonia. Depending on the fuel, steam reforming or partial oxidation is applied to produce hydrogen. In 1994, 77% of global ammonia capacity was based on steam reforming of natural gas, 13.5% on the partial oxidation of coal, 6% on steam reforming of naphtha, LPG and refinery gas, 3% on partial oxidation of heavy hydrocarbons, and 0.5% on the electrolysis of water. Excluding Asia, 90% of global ammonia capacity is operated on natural gas (IPTTS, 2004). The default total CO<sub>2</sub> emissions factors from ammonia production chosen for the NEAT model are given in Table 2 and represent low (i.e. based on efficient plants) estimates based on a literature survey (Neelis et al., 2003). The model user has the opportunity to insert specific (higher) emission factors based on the situation in the country of study. In all processes applied, part of the hydrocarbon input is directly burned to provide heat for the endothermic formation of synthesis gas. Countries might allocate the total input into the process to non-energy use (flow 1 equals flow 3, and flows 2 and 4 are zero in Fig. 3) or might allocate part of the hydrocarbon input

Table 2  
Overview of default NEAT CO<sub>2</sub> emission factors for ammonia production

Process	kg CO <sub>2</sub> /kg NH <sub>3</sub>	Comment
Steam reforming of natural gas	1.6	Based on a natural gas consumption of 28.5 GJ/t NH <sub>3</sub> and an emission factor of 56 kg CO <sub>2</sub> /GJ natural gas
Partial oxidation of coal	3.9	Based on a total coal consumption of 42 GJ/t NH <sub>3</sub> and an emission factor of 93 kg CO <sub>2</sub> /GJ coal
Partial oxidation of oil	2.5	Based on a total oil consumption of 34.5 GJ/t NH <sub>3</sub> and an emission factor of 74 kg CO <sub>2</sub> /GJ oil

to final energy use of the input (flow 2). In cases where the process exports energy (e.g. steam) to other processes (flow 6) or to other industries (flow 7), part of the input might also be allocated to energy conversions (flow 4).<sup>11</sup> For conventional steam reforming of natural gas, the part of the input used as fuel can easily be distinguished, because combustion and reforming take place in separate reactors. In these processes, approximately 30% of the input is burned and 70% is reformed to produce synthesis gas (e.g. Hinderink et al., 1996). In newer process configurations (e.g. auto thermal reforming) and for partial oxidation processes, the part used as fuel is less straightforward to determine. In the NEAT model, the use of CO<sub>2</sub> for the production of urea is accounted by subtraction from the overall CO<sub>2</sub> emissions. The subsequent use of urea is taken into account in the calculation of emissions from 'solvent and other product use'.<sup>12</sup>

#### 4.2. Methanol

Similar to ammonia, methanol is mainly produced from natural gas but depending on the raw material availability and prices in the country studied oil products and coal may also be used. Depending on the feedstock, steam reforming or partial oxidation is applied. The feedstock serves to produce synthesis gas (a mixture of hydrogen and carbon monoxide), which is then converted to methanol. Per tonne of methanol, an amount of carbon equivalent to 1.38 tonnes of CO<sub>2</sub> is embodied in the product. Some carbon is also emitted during methanol production; the CO<sub>2</sub> emission factors chosen for the NEAT model are given in Table 3. They again represent low estimates with the model user having the opportunity to insert country-specific (higher) emission factors. Worldwide, almost 80% of the methanol is produced by steam reforming of natural gas (Appl, 1997). Contrary to ammonia production, the final objective in the production of synthesis gas is not to obtain a maximal hydrogen yield, but to obtain a hydrogen to carbon ratio between 2 and 3, based on the stoichiometry of methanol synthesis.<sup>13</sup> In partial oxidation, the ideal H<sub>2</sub>/CO ratio can be obtained by adjusting the oxygen content. In the steam reforming of natural gas, the hydrogen to carbon ratio in the synthesis gas mixture is adjusted by purging part of the excess hydrogen or

<sup>11</sup> This would require a statistical system that monitors the heat recovery within the chemical sector as energy conversions.

<sup>12</sup> We do not correct for other use of CO<sub>2</sub> in for example beverages. This carbon is finally released as CO<sub>2</sub> during use of these beverages. Since it is hard to track the trade in these beverages (and the carbon content), we decided to account for those emissions as emissions from ammonia production.

<sup>13</sup> In methanol synthesis, two reactions take place:  $\text{CO} + 2\text{H}_2 \rightarrow \text{CH}_3\text{OH}$  and  $\text{CO}_2 + 3\text{H}_2 \rightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}$ .

Table 3  
Overview of default NEAT CO<sub>2</sub> emission factors for methanol production

Process	kg CO <sub>2</sub> /kg methanol <sup>a</sup>	Comment
Steam reforming of natural gas	0.4	Based on a natural gas consumption of 31.6 GJ/t methanol and an emission factor of 56 kg CO <sub>2</sub> /GJ natural gas
Partial oxidation of coal	2.2	Based on a total coal consumption of 38.6 GJ/t methanol and an emission factor of 93 kg CO <sub>2</sub> /GJ coal
Partial oxidation of oil	1.4	Based on a total oil consumption of 38.4 GJ oil/t methanol and an emission factor of 74 kg CO <sub>2</sub> /GJ oil

<sup>a</sup> In all cases, the carbon content of methanol (1.4 t CO<sub>2</sub>/t methanol) is deducted from the total hydrocarbon input.

by the addition of CO<sub>2</sub> to the synthesis gas mixture (Chauvel and Lefebvre, 1989). For methanol production it is therefore not straightforward to determine, which part of the process input should be allocated to feedstock use and which part to fuel use. Similar to ammonia, countries will allocate the total input to non-energy use (flow 1 equals flow 3 in Fig. 3) or might allocate part of the input to energy use (flow 2) or to energy conversions (flow 4).

#### 4.3. Carbon black

Carbon black is primarily produced from oils, which originate from coal or crude oil. Another type of raw material used in much smaller quantities for special grades of carbon black is acetylene. More than 95% of the world production of carbon black is produced in the furnace black process. The advantage of the furnace black process is its great flexibility in manufacturing various grades of carbon black. For small amounts of special grade carbon black other processes are used (Voll and Kleinschmit, 1997). The heart of the furnace black process is the furnace in which the carbon black is formed. The oil feedstock is injected in a high-temperature zone. The temperature is maintained by burning a fuel with air. The oxygen is not sufficient for complete combustion of the feedstock, which is therefore pyrolysed to form carbon black. Natural gas is normally the fuel of choice, but other gasses, e.g. coke oven gas are also occasionally used (Voll and Kleinschmit, 1997). The tail gas from the carbon black process is available at high temperature and contains a certain amount of combustible gasses, the amount of which depends on the feedstock and the processing conditions. The gas must be burned off for environmental reasons and the energy is generally used to produce steam or electricity (Voll and Kleinschmit, 1997). The CO<sub>2</sub> emission factors for carbon black production chosen for the NEAT model are given in Table 4 and are based on one literature source (Voll and Kleinschmit, 1997). The model user has the opportunity to insert specific emission factors for the country of study. As a result of the process configuration (oil and natural gas are fed into one single reactor and the tail gas contains energy that is recovered), there are again various ways of allocating the hydrocarbon input (flow 1 in Fig. 3) to non-energy use (flow 3), energy use (flow 2) and energy conversions (flow 4).

Table 4  
Overview of default NEAT CO<sub>2</sub> emission factors for carbon black production

Process	kg CO <sub>2</sub> /kg carbon black	Comment
Furnace black process	1.9	Based on a total oil input of 69.6 GJ/t carbon black and a total natural gas input of 7.7 GJ/t carbon black and emission factors of 56 kg CO <sub>2</sub> /GJ for natural gas and 74 kg CO <sub>2</sub> /GJ for oil. The carbon content of carbon black (assumed to be 3.7 t CO <sub>2</sub> /t carbon black) is deducted from the total hydrocarbon input.

#### 4.4. Steam cracking

Steam cracking is by far the most important petrochemical process with respect to energy use. It leads to the key building blocks of the petrochemical industry, namely ethylene, propylene, butadiene and aromatics. A variety of feedstocks are used for steam cracking. In Western Europe, naphtha accounts for three quarters of the total steam cracker input (IPTS, 2003), while plants operating on natural gas liquids dominate in the USA (Weissermel and Arpe, 2003). In NEAT, the ultimate yields are modelled, which have been estimated based on a best available technique reference document (IPTS, 2003), enquiries among industry experts and information from literature (Table 5). In addition to the high value basis chemical petrochemicals (flow 8 in Fig. 3), low value by-products are generated. These products are partly used to fuel the endothermic cracker reactions (flow 5) and are partly recycled back to refineries (flow 7) or used elsewhere within the petrochemical sector (flow 6). The NEAT model calculates absolute values for the process energy and the backflows to refineries in CO<sub>2</sub> equivalents with the ethylene production and the feedstock mix as model inputs. The

Table 5  
Ultimate yields of steam crackers with various feedstocks (in kg for 1000 kg of feedstock)

	Naphtha	Gas oil	Ethane	Propane	Butane
High value chemicals	645	569	842	638	635
Ethylene (E)	324	250	803	465	441
Propylene (P)	168	144	16	125	151
Butadiene	50	50	23	48	44
Aromatics	104	124	0	0	0
Fuel grade products and backflows	355	431	157	362	365
Hydrogen	11	8	60	15	14
Methane	139	114	61	267	204
Ethane and propane after recycle cracking	0	0	0	0	0
Other C4	62	40	6	12	33
C5/C6	40	21	26	63	108
C7 + non-aromatics	12	21	0	0	0
<430C	52	26	0	0	0
>430C	34	196	0	0	0
Losses	5	5	5	5	5
Total	1000	1000	1000	1000	1000



Table 6

Overview of default CO<sub>2</sub> emissions from fuel use in steam crackers and carbon equivalents of backflows to refineries

	Naphtha	Gas oil	Ethane	Propane	Butane
Specific CO <sub>2</sub> emissions from fuel use steam crackers (Mt CO <sub>2</sub> /Mt ethylene)	1.7	2.2	0.8	1.0	1.1
Specific CO <sub>2</sub> equivalents of backflows steam crackers (Mt CO <sub>2</sub> /Mt ethylene)	0.9	2.1	0.0	0.8	0.9

emission factors are given in Table 6. The remainder of the carbon is stored in chemicals. For steam cracking, the allocation to final energy and non-energy use is particularly problematic and can easily lead to substantial errors in national CO<sub>2</sub> emissions accounting (see Park, 2005 and Neelis et al., 2005 for examples). In some countries, the hydrocarbon input as a whole is regarded as non-energy use (flow 1 equals flow 3) and the backflows to the refineries might be double-counted in energy statistics, both as non-energy use and once more as energy use in refineries. For such countries, the fuel use in steam crackers (flow 5 in Fig. 3) might not be covered under emissions from fuel combustion and the emissions should be regarded as industrial process emissions from non-energy use to avoid omission of these emissions in the national totals. In the Netherlands, the conversion of the hydrocarbon input to the fuel by-products (flows 5–7) is separately monitored, but this also results in difficulties for emission accounting since the emission factors of the fuels produced differ from the feedstock used (see Neelis et al., 2005).

#### 4.5. Carbon use in metals and inorganics production

The NEAT model also contains a module on the use of solid carbon for the production of various metals (except for pig iron production in blast furnaces) and inorganic products. The solid carbon is either used as reducing agent (e.g. silicon carbide) or in the form of electrodes used for electrolysis (e.g. aluminium) or in electric arc furnaces (e.g. electric steel). Sometimes a combination of electrodes and other solid carbon input is used (e.g. white phosphorus). Whether or not these emissions are regarded as industrial process emissions or as emissions from fossil fuel combustion depends on how the non-energy use of fossil carbon for metallurgical purposes is treated in the energy statistics of the country studied. The emission factors for all processes currently implemented in NEAT are given in Table 7 based on a report by Sjardin (2003). The primary data sources for this report are IPTS (2001) and Ullman (1997).

### 5. Total non-energy use, carbon storage, storage fractions and total fossil CO<sub>2</sub> emissions

We have now systematically dealt with all carbon flows related to the non-energy use of fossil fuels. We can use the results to obtain estimates for total non-energy use and carbon storage, which are independent from the energy statistics. Using the total primary energy supply as additional input, we can also estimate the total fossil CO<sub>2</sub> emissions.

Table 7  
Overview of default CO<sub>2</sub> emission factors from the production of metals and inorganics (Sjardin, 2003)

	Input raw materials (wt.%)			Specific CO <sub>2</sub> emissions (t CO <sub>2</sub> /t product)
	Pet coke	Pitch	Coke/coal	
Use of carbon electrodes				
Primary aluminium	84	16		1.55
Electric steel	70	30		0.01
White phosphorus	72	28		0.18
Ferrosilicon	72	28		0.17
Silicon metal	85	15		0.36
Calcium silicon	85	15		0.32
Ferromanganese	72	28		0.04
Silicomanganese	72	28		0.09
Ferrochromium	72	28		0.06
Ferrochromiumsilicon	72	28		0.11
Magnesium	85	15		0.05
Ferronickel	72	28		0.01
Tin	85	15		0.04
Use of other solid carbon				
White phosphorus	6		94	4.18
Titanium dioxide	100			0.49
Ferrosilicon			100	2.75
Silicon metal	100			4.49
Calcium silicon			100	2.39
Ferromanganese			100	1.75
Silicomanganese			100	1.57
Ferrochromium			100	1.57
Ferrochromiumsilicon			100	2.71
Lead			100	0.64
Ferronickel			100	1.35
Tin			100	1.08
Zinc			100	0.43
Calcium carbide	15	5	80	1.10
Silicon carbide	100			2.30

### 5.1. Total non-energy use in CO<sub>2</sub> equivalents

As said in the introduction, the non-energy use of fossil fuel consists of two parts: the consumption of fossil fuels as feedstock and the consumption of non-energy use refinery and coke oven products. The first part can be estimated by taking:

- 1a. The CO<sub>2</sub> equivalents of *all* basic chemicals produced from non-energy use feedstocks. The calculation method has been explained in Section 3.
- 1b. The industrial process emissions resulting from the feedstock use. The calculation is discussed in Section 4.

The second part of non-energy use can be estimated by taking:

- 2a. The consumption of non-energy use refinery and coke oven products in CO<sub>2</sub> equivalents.

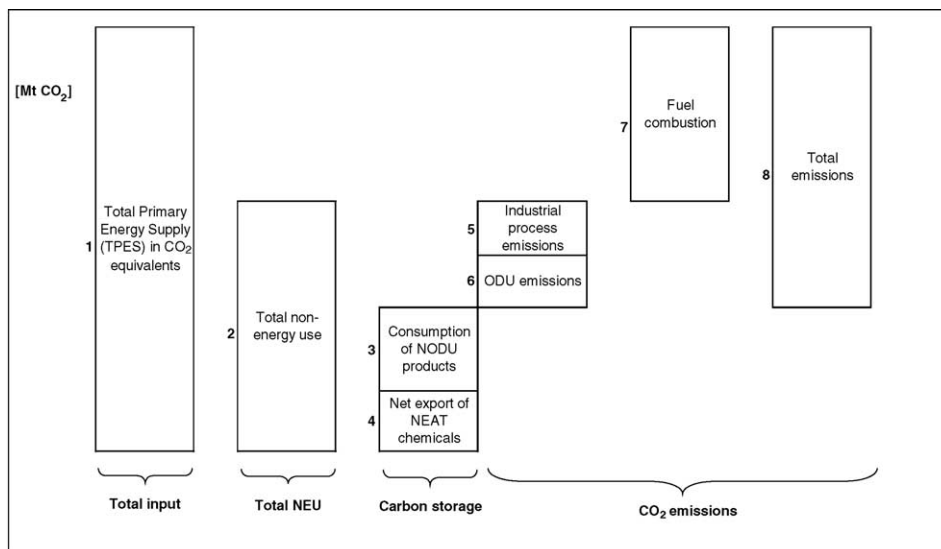


Fig. 4. NEAT methodology for calculating CO<sub>2</sub> emissions and carbon storage.

2b. The industrial process emissions resulting from the use of solid carbon in the production of metals and inorganic chemicals discussed in Section 4.

It should be emphasised that the total non-energy use in CO<sub>2</sub> equivalents very much depends on the definition of non-energy use applied for the industrial processes discussed in Section 4.

### 5.2. Carbon storage, storage fractions and total fossil CO<sub>2</sub> emissions

An overview of the calculation procedure for carbon storage, storage fraction and total fossil CO<sub>2</sub> emissions is given in Fig. 4. The total primary energy supply multiplied with CO<sub>2</sub> emission factors for the various fuels yields a value for the total fossil CO<sub>2</sub> emission potential of the country (1 in Fig. 4). Part of this total CO<sub>2</sub> emission potential is used for 'non-energy use purposes' (2, calculation explained above). The CO<sub>2</sub> equivalents of non-energy use are partly emitted as industrial process emissions (5, Section 3) and partly as emissions from solvent and other product use (6, Section 4). The remainder of the non-energy use is stored (i.e. not emitted, 3+4). In Fig. 4, we show that the carbon storage consists of two elements:

- the consumption of NODU products in the country of study and
- the net export of all basic chemicals<sup>14</sup>, intermediates and final products included in the NEAT model.

<sup>14</sup> Excluding the non-energy use refinery and coke oven products (footnote 9) for which the trade is already accounted for in the energy statistics.

The first element has been estimated in the calculation of emissions from the use of ODU products (Section 3), where we divided the consumption of end-products and the consumption for other derivatives into a part used for ODU and a part used for NODU applications. The second element can be estimated by deducting the total consumption of carbon (ODU emissions and NODU products) and the industrial process emissions from the non-energy use or directly from the trade data used. This net export is positive for countries that are net exporters of carbon-containing chemicals and negative for net importers of these chemicals.

Deducting the carbon storage from the total CO<sub>2</sub> potential of the country yields and estimate for total fossil CO<sub>2</sub> emissions (8). Based on the carbon storage (3 + 4 in Fig. 4) and the total non-energy use (2), the NEAT model also calculates carbon storage fractions for use in the IPCC-RA (3 + 4 divided by 2). These storage fractions will of course depend on the non-energy use definition chosen for the industrial processes discussed in Section 4.

### 5.3. Allocation to individual fuels

In the NEAT model, both the CO<sub>2</sub> emissions from non-energy use and the carbon storage are allocated to the various feedstocks used for non-energy use purposes. For the industrial process emissions, this allocation is straightforward. Emissions from ammonia are, for example, allocated to the respective feedstock ammonia is made from. For ODU emissions and for carbon storage, the allocation is more complex, because downstream emissions have to be allocated back to upstream fuels with the help of the carbon balance used to calculate the emissions from solvent and other product use. For example, all the carbon storage and emissions from derivatives of steam cracking products are allocated to the steam cracker inputs. The allocation to individual fuels enables the model user to conduct analyses and comparisons on the level of individual fuels.

## 6. Comparisons with the official GHG inventory

The calculation procedure for total fossil CO<sub>2</sub> emissions obtained with the NEAT model is mathematical equivalent to the estimate for total fossil CO<sub>2</sub> emissions according to the IPCC-RA (Eq. (1)). The two can therefore directly be compared. Since the starting point of both calculations is the same (the total primary energy supply of the country), differences between the two estimates are by definition caused by differences in either:

1. The total non-energy use in CO<sub>2</sub> equivalents determined by NEAT and the total non-energy use in CO<sub>2</sub> equivalents used in the IPCC-RA calculation. The latter is obtained by multiplying the non-energy use according to the energy statistics with appropriate emission factors.
2. The proportion of ‘carbon storage’ (3 + 4 in Fig. 4) versus ‘CO<sub>2</sub> emissions’ (5 + 6 in Fig. 4). In NEAT the division is calculated on basis on a material flow analysis, while in the IPCC-RA the division is usually based on the IPCC default storage fractions.

The comparison of the total non-energy use in CO<sub>2</sub> equivalents between NEAT and the IPCC-RA (difference 1) can be used to clarify which definitions for non-energy use are

used in the energy statistics for the various industrial processes discussed in Section 4. This is an iterative process in which the model user should use both the NEAT model results and the non-energy use in CO<sub>2</sub> equivalents, which is used in the IPCC-RA calculation. If for example, a country produces methanol from natural gas, but does not report non-energy use of natural gas in the energy statistics, this is an indication that this process is not properly accounted for in the energy statistics and that emissions are overestimated in the national GHG inventory. Another example is the steam cracking process. Based on the NEAT model, one can judge whether a country is likely to use a gross (including backflows and fuel use) or net definition of non-energy use (excluding these flows) in the energy statistics. For the other industrial processes in the NEAT model, comparable comparisons can be made. The use of the NEAT model for clarification of non-energy use accounting practices can be found in the country studies for Korea (Park, 2005), Italy (La Motta et al., 2005) and the Netherlands (Neelis et al., 2005). A summary is given in Patel et al., 2005.

Regarding the second difference (storage versus CO<sub>2</sub> emissions), it should in the first place be emphasised that the NEAT estimate for total fossil CO<sub>2</sub> includes all fossil CO<sub>2</sub> emissions, including fuel combustion, solvent and other product use and industrial processes. Only emissions from incineration without energy recovery are excluded. The IPCC-RA, however, is nowadays generally regarded as a method to calculate CO<sub>2</sub> emissions from fuel combustion only. This is also emphasised in recent versions of the Common Reporting Format used to report GHG emissions (SBSTA, 1999). Certain section of the IPCC guidelines also stress the role of the IPCC-RA as a tool for estimating CO<sub>2</sub> emissions from fuel combustion only (e.g. IPCC/IEA/OECD/UNEP, 1997, vol. 3, p. 1.1). On the other hand, in other sections of the guidelines, industrial process emissions and emissions from solvent and other product use are also stated to be included in the IPCC-RA emissions estimate (e.g. IPCC/IEA/OECD/UNEP, 1997, vol. 3, pp. 1.25–27). The default carbon storage fractions provided in the IPCC guidelines were determined by Marland and Rotty (1984). They also aimed to calculate total CO<sub>2</sub> emissions rather than only emissions from fuel combustion. Recently, Marland and Marland (2003) follow the same approach. The use of the Marland and Rotty fractions is therefore inconsistent with the use of the IPCC-RA as a tool to estimate emissions from fuel combustion only. In the second place, it is by definition impossible that the use of default IPCC fractions will yield the correct emissions for all countries as long as there are no uniform definitions of non-energy use in the energy statistics, even if there would be consensus on the scope of the IPCC-RA.

As explained in Section 4, emissions from non-energy use can be omitted or double counted in the IPCC-SA. Whether or not this is likely to happen depends on the allocation between energy and non-energy use in the energy statistics and the use of these statistics in the IPCC-SA. Based on the comparison of the NEAT results with the IPCC-RA, one can therefore explore whether non-energy use emissions are consistently dealt with in the IPCC-SA calculation. This involves comparison of the NEAT model results with the emissions according to the IPCC-SA in the various source categories. This comparison is however by no means straightforward and requires detailed insight into the reporting practices of the country of study. However, it can be a very worthwhile exercise as the country analyses in this special issue show.

## 7. Discussion

To our knowledge, the NEAT model is the only tool that systematically deals with all carbon flows related to the non-energy use of fossil fuels. The model calculates both CO<sub>2</sub> emissions and carbon storage resulting from the non-energy use of fossil fuels independent from the energy statistics<sup>15</sup> and the national GHG inventory. The lack of proper and consistent definitions for non-energy use is the most important problem of the current methods to calculate carbon storage and emissions from non-energy use. The NEAT model can help to identify which definitions are used in the energy statistics. Its application can guide people preparing national GHG inventories in treating GHG emissions from non-energy use in a consistent way.

To run the full NEAT model, production and international trade data for 77 organic chemicals is required, supplemented with production data for 18 inorganic chemicals and metals and with data on feedstock types and specific energy consumption (SEC) figures for some industrial processes.<sup>16</sup> The extensive data requirement is one of the main drawbacks of the model. However, the country studies for Korea (Park, 2005), Italy (La Motta et al., 2005) and the Netherlands (Neelis et al., 2005) show that it is in principle possible to collect the required data, either via close cooperation with national statistical offices (the Netherlands) or via consultancy companies collecting these data for business purposes (Italy, Korea).

By far the most time-consuming and data-intensive part of the NEAT model is the bottom-up carbon balance, resulting in an estimate for emissions from solvent and other product use (ODU products). As a result of the limited reliability of production data for chemical intermediates and as a result of the uncertain split between ODU and NODU products for some products, the largest uncertainty is present in this part (see e.g. Neelis et al., 2005). To reduce this uncertainty, it is planned to further study the final fate (ODU versus NODU) of some complex products like lubricants.

An alternative would be to make detailed comparisons between the NEAT model estimates for solvent and other product use and other available emissions inventories based on comprehensive surveys of these emissions (e.g. Freed et al., 2005). These surveys have the advantage of directly surveying emissions rather than estimating them based on the consumption patterns of the intermediate precursor chemicals as it is done in the NEAT model. However, the surveys are not always complete and are not available for all countries. Based on the comparisons between NEAT and available studies, it might be possible to derive generic values (e.g. solvent emissions per capita) for implementation in NEAT, thereby reducing the need for the data-intensive carbon balance in the current NEAT model. This would make the model easier to apply also for countries with limited data availability. Such a simplified model could focus on the upstream carbon flows related to the reported non-energy use in energy statistics (industrial process emissions and initial carbon storage in petrochemicals) and could rely on more detailed downstream emission estimates for the estimation of emissions from solvent and other product use.

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<sup>15</sup> There may be exceptions based on the general data availability in the country of study. Sometimes, production and trade data for refinery products are not collected separately from the energy statistics and the energy statistics therefore become the only available source (e.g. in the Netherlands, Neelis et al., 2005).

<sup>16</sup> When SEC values are not available, the model user can use the default values included in the model.

An area requiring further research is the position of CO<sub>2</sub> emissions from incineration of “non-specs”, which result from incomplete conversions in the chemical industry and are used for energy purposes. In the NEAT methodology, these emissions are so far not explicitly modelled and are partly included in the emissions from solvent and other product use (ODU products). There are indications that the magnitude of these emissions might be substantial. For the US, they were estimated to be 9.5 Mt CO<sub>2</sub> in 1992 (Tonkovich and Gerber, 1995), which is more than 2% of the total non-energy use (379 Mt CO<sub>2</sub> in 2002 according to US-EPA, 2004).

The NEAT model can be extended in order to include the emissions from waste incineration. This requires substantial additional data analyses, which is strongly recommended for future research. By doing so, all CO<sub>2</sub> emissions from fossil fuel origin would be covered by the model. With such an extended model it would be possible to estimate the fraction of non-energy use that is finally incinerated, and to investigate the relative amount of waste emissions versus the non-energy use as a function of time.

## 8. Conclusions

The non-energy use emission accounting tables model is a tool that systematically deals with the carbon flows related to the non-energy use of fossil fuels, based on a carbon flow analysis of the relevant sectors. Earlier model versions (Gielen and Patel, 1999) focussed on the correct calculation of carbon storage in petrochemical products and on the calculation of emissions from solvent and other product use. The current model version also calculates direct industrial process emissions (from e.g. ammonia) related to the non-energy of fossil fuels and calculates total non-energy use, carbon storage and non-energy use emissions independent from energy statistics. We have shown that the results obtained with the extended model can be used as a valuable crosscheck for the non-energy use emission accounting in official GHG emission inventories. The model can help to identify which definitions for non-energy use are used in the energy statistics that are employed in the emission inventory. Based on this information, the NEAT model results can be used to improve national emission inventory methodologies in order to avoid double counting or omission of emissions.

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