

DRAFT VERSION (SEPTEMBER 2003)

Modelling non-energy use CO₂ emissions and carbon storage with the Non-energy use Emission Accounting Tables (NEAT)

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Abstract

To contribute to a more accurate accounting of CO₂ emissions originating from the non-energy use of fossil fuels, the NEAT (Non-energy Emission Accounting Tables) model has been developed. In this paper, the NEAT model methodology is explained. The model is based on a carbon flow analysis of the petrochemical sector. The NEAT model calculates CO₂ emissions resulting from the non-energy use of fossil fuels and allows comparison with official sources dealing with the non-energy use of fossil fuels like energy balances and official CO₂ emission inventories prepared according to the guidelines of the Intergovernmental Panel on Climate Change (IPCC). Apart from its use for estimating CO₂ emissions, the NEAT model can also be used to calculate the non-energy use of fossil fuels according to different definitions. This information is valuable in the context of international harmonization of the definitions of non-energy use in energy balances. The model works independently from official sources (energy balances, emission inventories) and can therefore be used as a valuable crosscheck of the official data.

1 Introduction

The system shown in Figure 1 covers all activities, which add up to the country's Total Primary Energy Supply (TPES) according to energy balances. The trade of all commodities included in the energy balance is accounted for in the TPES. Primary energy commodities (crude oil, natural gas) are converted to secondary energy commodities. These conversions result in CO₂ emissions from (primary) fuel combustion (E1 in Figure 1). The resulting secondary energy commodities (fuels, electricity) are available for final consumption. The majority of the energy commodities is consumed for energy purposes (final energy use) in all economic sectors, leading to CO₂ from fuel combustion (E2 in Figure 1). In the context of greenhouse gas emissions so far most attention has been paid to these CO₂ emissions from the combustion of fossil fuels.

A considerable fraction of the secondary energy commodities is, however, consumed for non-energy purposes. The share of non-energy use relative to the TPES differs from country to country, depending on the relative importance of refineries and basic chemical industries in the country. The non-energy use of fossil fuels represented 6.5% of the total primary energy supply in the European Union in 2000. Within Western Europe, the share of non-energy use relative to the total primary energy supply is highest in the Netherlands and Belgium with 13.5 and 10.1% respectively. The share relative to the energy available for final consumption is 9.0% (European Union), 17.0 % (the Netherlands) and 14.2% (Belgium) respectively (IEA, 2002). From Figure 1 it becomes clear that this final non-energy use consists of two parts:

- In the first place, non-energy use consists of several non-energy refinery products that are consumed in various economic sectors. Examples are the use of bitumen in the building industry and lubricants for transportation. This final non-energy use of these refinery products is in international energy statistics (e.g. IEA, 2002) reported as non-energy use in the respective end-use sectors.
- The second part of non-energy use consists of feedstock use in the (petro-) chemical industry.

Part of the carbon embodied in the fossil fuels used for non-energy purposes is stored in chemical products that have lifetimes ranging from months to centuries. Depending on the type of product, oxidation of the embodied carbon will take place in the use phase of the chemical product (E4 in Figure 1) and/or only during the waste treatment phase. When waste is incinerated with energy recovery, the emissions are part of the emissions from fuel combustion (E1 in Figure 1), otherwise they are reported as emissions from waste treatment (E5 in Figure 1). Another part of the carbon embodied in the fossil fuels that are used for non-energy purposes is already oxidised to CO₂ during the production phase of chemical products (industrial process emissions E3 in Figure 1). The production of ammonia is the most important source of industrial process CO₂ emissions. Undesirable carbonaceous by-products (“non-specs”) in the chemical industry can also be incinerated and used for energy recovery. The position of the incineration of these “non-specs” in energy balances is rather unclear. Ideally, they should re-enter the energy balances as indicated in Figure 1 (together with waste that is used for energy recovery), leading to CO₂ emissions from fuel combustion (E1 in Figure 1). It is however unclear if and to which extent this is common practice.

In its emission inventory guidelines (IPCC/IEA/OECD/UNEP, 1997), the International Panel on Climate Change (IPCC) recommends two principal methods of calculating national CO₂ emissions, the Reference Approach and the Sectoral Approach. The principal idea behind the simpler IPCC Reference Approach (IPCC-RA) is to subtract the carbon stored from the national total apparent carbon consumption to obtain a value for national CO₂ emissions. The carbon stored is calculated by multiplying the non-energy use of a certain fuel with a storage fraction for this fuel:

carbon stored (t carbon) =

$$\text{non-energy use (J)} * \text{emission factor (t carbon / J)} * \text{storage fraction (\%)} \quad 1)$$

In the more detailed IPCC Sectoral Approaches (IPCC-SA), CO₂ emissions are reported in various source categories. The CO₂ emissions resulting from the non-energy use of fuels may be allocated to the source categories ‘Industrial Process Emissions’, ‘Solvent and other product use’ or ‘Waste’. However, the guidelines allows a large degree of freedom concerning the allocation of emissions to the three source categories as long as double counting is avoided. The various difficulties, weak points and disadvantages of the current IPCC methods with respect to non-energy use CO₂ emission accounting are discussed by **Patel et al. (2004)**.

To contribute to a more accurate accounting of non-energy use related CO₂ emissions, the NEAT model (Non-Energy use Emission Accounting Tables) has been developed within the International Network on Non-energy Use and CO₂ Emissions (NEU-CO₂). The model is based on a carbon flow analysis of the petrochemical sector. Earlier model versions have been described by Gielen et al. (1999) and Gielen et al. (2002). Since then, the NEAT model has been extended with:

- A module to calculate industrial process emissions (e.g. from ammonia production)
- A module to compare the results with other available sources
- A module to obtain carbon storage fractions for use in the IPCC-RA.

The model, which will be described in detail in this article, now consists of three stages:

1. In stage 1 of the model, the national CO₂ emissions resulting from the non-energy use of fossil fuels are calculated.
2. In stage 2 of the model, the results are linked to and compared with other available sources.
3. In stage 3 of the model, country specific storage fractions are determined for use in the IPCC-RA. These are recommended for use instead of the IPCC default values (IPCC/IEA/OECD/UNEP, 1997).

In the remainder of this article, the three stages of the model will be described in more detail.

2 Stage 1 of the NEAT model, calculating national non-energy use CO₂ emissions

In stage 1 of the NEAT model, CO₂ emissions from the non-energy use of fossil fuels are calculated. In analogy with the IPCC-SA, the emissions are determined by source categories. Two types of emissions are distinguished in the model. These are emissions from solvent and other product use (E4 in Figure 1) and industrial process emissions (E3 in Figure 1). CO₂ emissions from the incineration of “non-specs” (part of E1 in Figure 1) and CO₂ emissions from waste incineration either with (part of E1) or without energy recovery (E5 in Figure 1) are not separately calculated in the current version of the NEAT model. However, their position relative to the NEAT model will be explained in this article. In order to have a complete overview, some emissions falling under the source category fuel combustion are also calculated in the model as will be explained later on.

2.1 Emissions from solvent and other product use

Emissions from solvent and other product use are emissions that are released during the consumption phase of carbon containing chemical products like solvents. To come to an estimate of these emissions, the downstream structure of the (petro-)chemical industry is modelled by means of a national carbon balance covering the 77 most important chemical commodities. The carbon balance contains the conversion routes from 22 basic chemicals to 55 intermediate and final products (compare Table 1). The method will be explained by use of the simplified example of the downstream structure of ethylene derivatives shown in Figure 2. In this simplified example, ethylene is used for the production of polyethylene. The remaining ethylene consumption is used for the production of other ethylene derivatives, which are not explicitly modelled in NEAT¹. The purpose of the carbon balance is to allocate the consumption of ethylene derivatives to one of the categories ‘Oxidised During Use (further referred to as ODU) and ‘Not Oxidised During Use’ (further referred to as NODU)². For some products, the allocation to one of the two source categories is clear-cut. For the remaining products, the fraction of ODU versus NODU applications has been estimated based on consumption patterns found in literature (e.g. Weissermel et. al., 1998 and Chauvel et. al., 1989). In the example shown in Figure 2, polyethylene is assumed to be a 100% NODU product. For the other ethylene derivatives, a division of 95% ODU products and 5% NODU products has been estimated. The fractions of ODU versus NODU applications for all 77 core products included in NEAT are given in Table 1. The second column from the left in Table 1 indicates whether the chemical compound is used for the production of other compounds modelled in NEAT (e.g. ethylene in the example of Figure 2) or whether it represents the total *final* consumption of the compound in the country of study, because it is not used for the production of other NEAT core products (e.g. polyethylene in the example of Figure 2). In the first case, the consumption value is calculated by means of a carbon balance incorporated in NEAT, whereas in the second case the consumption directly results from production and trade statistics.

The NEAT a carbon balance just mentioned covers 77 chemical products or product groups. The final consumption figures used in the estimate for emissions from product related emissions³ are therefore limited to these core products. The restriction to the 77 key chemicals results in the omission of imports and exports of many downstream derivatives. For countries with large net trade streams this could to an underestimation for net importing

¹ In the real model, ethylene is not only used for the production of polyethylene, but also for the production of ethanol, ethylene oxide, ethylbenzene, ethylenedichloride, ethylene-propylene-diene-monomer (EPDM), epoxy resin and polyvinylacetate.

² In the current IPCC Guidelines (IPCC/IEA/OECD/UNEP, 1997, Vol 3, pp. 1.25) and in previous descriptions of the NEAT model (Gielen et. al., 1999 and Gielen et. al., 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) already very shortly after their production. The current nomenclature (ODU versus NODU) better reflects the type of oxidation in line with CO₂ emission categories (solvent and product use versus waste). For a more detailed discussion, reference is made to **Patel et. al. (2004)**.

³ Product related emissions are emissions resulting from the use of ODU products.

countries or an overestimation for net exporting countries of the consumption of carbon containing chemicals 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 calculations, referred to as the additional trade module.

The key assumptions and the uncertainties inherent to the NEAT model carbon balance are:

- All chemical conversions are assumed to be 100% carbon efficient. As a result, CO₂ emissions from the incineration of “non-specs” (part of E1 in Figure 1) are not explicitly modelled in NEAT and can therefore not be calculated. As a result of this simplifying assumption, the consumption of basic chemicals and intermediates for the production of other derivatives is overestimated and includes carbon losses from incomplete conversions. The consumption of basic chemicals and intermediates for other derivatives is in the model divided into an ODU and a NODU fraction with the fractions indicated in Table 1. As a consequence, the carbon losses, which are part of the consumption value, are also divided into an ODU and a NODU fraction. This could only be avoided if relevant survey data were available for carbon losses from incomplete conversions, which is currently not the case.
- The NEAT assumptions about the ODU and NODU fractions are subject to uncertainty. These uncertainties are relatively high for some products for which the exact use structure of the *other* derivatives is unknown. For this reason, a sensitivity analysis has been implemented in NEAT (Table 1).
- In general, 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 both from benzene 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 these cases, the actual production routes applied in the country of study must be identified and should be implemented in the model based on an in-depth study of the production routes for the respective country.
- Since all calculation in NEAT are conducted in terms of CO₂ equivalents, the carbon content of all products must be known. While exact values are available for pure components (e.g. ethylene), approximations must be made for mixed product groups.

Besides model inherent uncertainties there are uncertainties related to the 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. This data may not be available for all NEAT core products or the available data are 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 basis of capacity data, on basis of mass balance calculations or by contacting producers. Apart from non-existing data, 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.

2.2 Industrial process emissions

Part of the carbon embodied in the fossil fuels that are used for non-energy purposes is directly oxidised to CO₂ during the production phase of (chemical) products, leading to industrial process emissions (E4 in Figure 1). Important examples in the chemical industry are the production of ammonia, methanol and carbon black. In the basic metals production industry, carbon sources are also used as for example anodes in aluminium production. The carbon embodied in the feedstock is either not (ammonia, metals) or only partly (methanol, carbon black) embodied in the final product, while the remainder is emitted as industrial process CO₂ emissions during production. The NEAT model contains a module to calculate these industrial process emissions by multiplying the production values of the products with an emission factor representing the CO₂ release from the feedstock used. The production and use of coal cokes in pig iron production is excluded from the NEAT model, because these processes are normally completely addressed and covered in the energy conversion section

of energy balances and are therefore not part of the non-energy use. In this section, the raw material structure will be discussed in more detail for the processes mentioned.

Ammonia

Ammonia is most frequently produced from natural gas, but lower grade fuel oils or coal are sometimes also used. The hydrocarbon feedstock serves to produce hydrogen, which is then converted with hydrogen to produce ammonia. Depending on the fuel, steam reforming or partial oxidation is applied to produce hydrogen. In 1990, 77% of the global ammonia capacity was produced by steam reforming of natural gas, 6% by steam reforming of naphtha, LPG and refinery gas, 3% by partial oxidation of heavy hydrocarbons, 13.5% from the partial oxidation of coal and 0.5% by electrolysis of water. Excluding Asia (and most particularly China), 90% of the global ammonia capacity is operated on natural gas (IPTS, 2003). In all processes, part of the feedstock is burned to provide heat for the endothermic formation of synthesis gas. It is therefore unclear from the outset which part of the hydrocarbon input should be regarded as final energy use of the hydrocarbon input and which part should be regarded as non-energy use of the hydrocarbon input. In conventional natural gas steam reforming process configurations the division is relatively easy to make, because combustion and reforming take place in separate reactors. In these processes, approximately 30% of the feedstock 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), the division cannot easily be determined in a straightforward way.

The CO₂ emissions factors from ammonia production chosen for the NEAT model are given in Table 2 and represent conservative estimates based on a literature survey (Neelis et. al., 2003). With respect to the allocation between energy and non-energy use of the hydrocarbon input, two alternative approaches are implemented. In the 'NEAT, standard' approach, the total hydrocarbon input is allocated to non-energy use and the resulting CO₂ emissions are considered industrial process emissions (E3 in Figure 1). In the 'NEAT, allocated' approach, 70% of the input is allocated to non-energy use, again resulting in industrial process emissions. The remaining 30% is allocated to final energy use of the input and the resulting CO₂ emissions are regarded as CO₂ emissions from fuel combustion (E2 in Figure 1). Although the allocation to one of the two source categories 'industrial process emissions' or 'fuel combustion' obviously does not have an influence on the *total* emissions from ammonia production, the allocation method has consequences on the emissions by source category. Moreover, the allocation to either energy or non-energy use has an influence on the non-energy use reported in the energy balances and, as a consequence, on the correct storage fractions that should be applied in the IPCC-RA calculation (compare Equation 1).

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, 1.38 tonnes of CO₂ equivalents are embodied in the molecule while the remainder is released during production. Worldwide, almost 80% of the methanol capacity is produced by steam reforming of natural gas (Chauvel et. al., 1989). 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 reactions during methanol synthesis⁴. In partial oxidation, the ideal H₂/CO ratio can be obtained by adjusting the oxygen content during the partial oxidation. In the steam reforming of natural gas, the hydrogen to carbon ratio in the synthesis gas mixture is too high and is adjusted by purging part of the excess hydrogen or by the addition of CO₂ to the synthesis gas mixture (Chauvel et. al., 1989). As a result, the division between input used as feedstock and input used as fuel cannot easily be determined in an easy straightforward way for methanol based on natural gas.

⁴ In methanol synthesis, 2 reactions take place: $\text{CO} + 2\text{H}_2 \rightarrow \text{CH}_3\text{OH}$ and $\text{CO}_2 + 3\text{H}_2 \rightarrow \text{CH}_3\text{OH} + \text{H}_2\text{O}$

The CO₂ emission factors for methanol production chosen for the NEAT model are given in Table 3. They represent conservative estimates based on a literature survey (Neelis et. al., 2003). With respect to the allocation between energy and non-energy use of the hydrocarbon input, two approaches have been implemented in NEAT, as is the case for ammonia. In the 'NEAT-standard' approach, the feedstock as a whole is regarded as non-energy use and all CO₂ emissions are considered industrial process emissions (E3 in Figure 1). The approach 'NEAT-allocated' is based on the assumption that the non-energy use of the raw materials for methanol production is identical to the carbon equivalent that is finally embodied in the methanol molecule. In this approach, the industrial process emissions from methanol production are zero, because it is assumed that the carbon content of the process input that is used for non-energy purposes is fully embodied in the methanol product. The remainder of the process input is assumed to be used for energy purposes, leading to CO₂ emissions from fuel combustion (E2 in Figure 1). Contrary to ammonia, there is not other easy and straightforward division between non-energy and energy use of the input as explained above. As is the case for ammonia, the allocation method applied in the country of study does not have an influence on the *total* CO₂ emissions from methanol production, but it certainly has an effect on the emissions by source category and on the total non-energy use applied in the IPCC-RA (Equation 1).

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 et. al., 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, which is achieved by burning a fuel with air. The oxygen is not sufficient for the 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 et. al., 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 et. al., 1997). As a result of the process configuration (oil and natural gas are fed into one single reactor) and as a result of the use of the tail gas energy, there are again different ways for dividing between non-energy use and energy use of the process input.

The CO₂ emission factors for carbon black production chosen for the NEAT model are given in Table 4 and are based on literature (Voll et. al., 1997). Similarly to methanol production, two approaches are modelled in NEAT. In the 'NEAT, standard' approach, all input is regarded to be used for non-energy purposes and the CO₂ emissions are regarded industrial process emissions (E3 in Figure 1). In the 'NEAT, allocated' approach only the input finally embodied in the product is regarded as non-energy use, whereas the other part of the input is considered as fuel use. As a result of this approach, the industrial process emissions are zero (the carbon is embodied in the carbon black product) and all emissions are regarded as emissions from fuel combustion (E2 in Figure 1).

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. There are two pathways for CO₂ emissions from these processes. These are the use of carbon electrodes, which are partially oxidised, and the oxidation of other solid carbon inputs. While there is no doubt that the first emission source represents a form of non-energy use and should hence be included in NEAT, this is less obvious for the second pathway. The decision about whether or not to include the solid carbon inputs in the non-energy use depends on how the non-energy use of fossil carbon for metallurgical purposes is treated in the energy balance of the country studied. In industrialised countries the emissions from the second pathway are generally small and can be neglected. Further analysis may be required for

countries with higher production volumes of these products. The emission factors for all processes currently implemented in NEAT are given in Table 5.

2.3 Steam cracking

There is one other industrial process that is modelled in the NEAT model. It has not been included under the section on industrial process emissions (Section 2.2) since it does not lead to industrial process emissions according to the IPCC terminology. Steam cracking is by far the most important petrochemical process. Ethylene, propylene, butadiene and aromatics are produced out of a variety of feedstocks. In Western Europe, naphtha accounts for three quarters of the total steam cracker input (IPTS, 2002), while plants operating on Liquefied Petroleum Gas (LPG) or Natural Gas Liquids (NGL) dominate in the USA (Weissermel et. al., 1998). Next to the high value basic petrochemicals, low value fuel grade products are produced. These products are partly used to fuel the steam cracking process and are partly recycled back to refineries or used as fuel elsewhere in the petrochemical sector. For a variety of feedstocks, the ultimate yields are modelled in NEAT, based on a best available technique reference document (IPTS, 2002), enquiries among industry experts and own calculations based on information from literature (Table 6). The NEAT model calculates absolute values for the process energy and the backflows to refineries in CO₂ equivalents with the ethylene production and feedstock mix as model inputs. The emission factors are given in Table 7.

For steam cracking, the allocation to energy and non-energy use is particularly problematic. When the hydrocarbon input as a whole is regarded final non-energy use, the backflows might be double-counted in the energy balance both as final non-energy use and as energy use in the refineries. It goes without saying that the inclusion of the fuel use in steam crackers in the figure for the national non-energy use has a considerable effect on the correct storage fractions to be applied in the IPCC-RA (equation 1). These aspects will be further discussed in the next section.

2.4 Uncertainty of emissions factors

The emissions factors given in Tables 2 - 6 are subject to various uncertainties. In general, emission factors represent the *lower* range of emissions have been implemented in NEAT. The model results for emissions can therefore be regarded as conservative estimates. In the NEAT model, an uncertainty range around the mean emission factors given in the tables is operational, giving the user the opportunity to conduct uncertainty analyses and to vary the emission factors used based on country specific information.

3 Stage 2 of the NEAT model, comparing the results with the official inventories

In stage 2 of the NEAT model, the results obtained in stage 1 are compared with values from official sources. Various comparisons are made.

3.1 Total non-energy use

In the first place, the results obtained in stage 1 can be used to create an independent NEAT-based estimate for the total non-energy use in the country studied. The non-energy use estimate consists of three components:

1. The consumption of feedstocks in the petrochemical industry, estimated by taking the production values of all *basic* chemicals produced from non-energy use feedstocks.
2. The consumption of non-energy use refinery products.⁵
3. The consumption of feedstocks that are released as industrial process emissions.

It is important to realise that the calculation of the first two components of non-energy use in NEAT requires an analysis of carbon flows at a different level than discussed so far. To make this clear, we refer to Figure 1 and 2. In Stage 1 of the model, the aim was to estimate the

⁵ Note the difference compared to component 1. In line with the principles of (international) energy balances, refinery products are accounted for with their consumption values, while chemical products are accounted for with respective feedstock use, which is estimated by using production values rather than consumption values (compare Figure 1).

emissions from solvent and other product use related to the final consumption downstream (E4 in Figures 1 and 2). We are now interested in the non-energy use as it is reported in the energy balances; this is a feedstock value, thus representing an upstream flow. In the example of Figure 2, an estimate for non-energy use can be obtained by looking at the feedstock required for ethylene production. To analyse this, it is not necessary to study all the downstream material flows indicated in Figure 2. It is, in this case, sufficient to know the amount of ethylene produced in the country of study. In general terms, the feedstock equivalents ending up in products can be estimated by adding up the carbon equivalents of all basic chemicals produced in the country (element 1). The calculation is complicated by the fact that the total non-energy use is composed not only of feedstocks, but also of the consumption of non-energy use refinery products (compare Figure 1). These non-energy use refinery products therefore enter the calculation with their consumption values (element 2). The third element of the non-energy use estimate is the feedstock released as industrial CO₂ emissions during the production of chemicals. These emissions have already been calculated in stage 1 of the model. For some of these production processes (ammonia, methanol and carbon black), different allocation methods are introduced in the NEAT model (see tables 2-4). Stage 2 of the model allows calculating non-energy use according to all allocation methods introduced in stage 1. In stage 1, the CO₂ emissions from fuel combustion in steam cracking and the backflows from steam crackers to refineries (in CO₂ equivalents) are also calculated. In some countries, the CO₂ equivalents of these two elements are included in the non-energy use according to the energy balances. This results in further possible emissions from non-energy use (Compare **Figure X** in **Patel et al., 2004**).

The non-energy use estimate (in CO₂ equivalents) determined with the NEAT model is fully based on production statistics and is therefore independent from the non-energy use reported in the energy balance and used in the IPCC-RA (e.g. in Table 1.a(d) of the common reporting format; SBSTA, 1999). The comparison between the NEAT estimate for non-energy use and the non-energy use according to the energy balances can serve a number of purposes:

- The comparison is a check for the consistency and completeness of the NEAT model. If, for example, the NEAT results for non-energy use are clearly lower than the values according to the energy balance, this might be an indication that the production statistics used in the model are incomplete.
- The comparison can give an indication, which parts are and which parts are not included in the non-energy use figure in energy balances. Due to the relatively large flows, this is particularly visible for the components associated with steam cracking. The comparison between NEAT and the energy balance can help to clarify whether fuel use and backflows are included in the energy balance value for non-energy use or not.
- The comparison can help to identify erroneous non-energy use data in energy balances. If, for example, the coal use in the iron and steel industry is included in the non-energy use figure in the energy balance, this becomes clear from the comparison between NEAT and the energy balance.

3.2 Carbon storage, total fossil CO₂ emissions and emissions from fuel combustion

Based on the estimated non-energy use, the NEAT model provides estimates for the total fossil CO₂ of the country studied and for the total CO₂ emissions from fuel combustion in all sectors. In the methodology, emissions from waste treatment without energy recovery (E5 Figure 1) are not included in the total fossil CO₂ emission estimate. Emissions from waste incineration with energy recovery are included if the waste used is correctly reported in the energy balance as a produced energy commodity. An overview of the calculation procedure is given in Figure 3. The total primary energy supply multiplied with CO₂ emission factors for the various fuels yields a value for the total fossil CO₂ emission *potential* of the country (Flow 1 in Figure 3). Part of this total CO₂ emission potential is used for 'non-energy use purposes' (Flow 2). The CO₂ equivalents of non-energy use are partly emitted as industrial process emissions (Flow 4 in Figure 3 and Flow E3 in Figure 1) and partly as emissions from solvent and other product use (Flow 5 in Figure 3 and Flow E4 in Figure 1 and 2). The remainder of the non-energy use is stored (i.e. not emitted) in the country of study. A simple method for the calculation of this carbon storage is to deduct the non-energy use emissions (Flow 4 and 5)

from the total non-energy use (Flow 2). As already explained by Gielen (1997), the carbon storage consists of two parts:

1. Materials that are not oxidised during use, which are produced domestically from part of the non-energy use, and which are consumed either domestically or abroad.
2. The net export of materials that are oxidised during use, which are produced domestically from part of the non-energy use.

Due to the latter part, the NEAT result for carbon storage can become negative. This is for example the case in countries without a basic chemical industry. In these countries the total non-energy use is zero and a correction must be applied for imported products that are oxidised during use. In the NEAT methodology, this correction shows as a negative carbon 'storage' value. This negative value is deducted (see Figure 3), hence resulting in additional emission. In countries where this occurs, the total fossil CO₂ emissions might exceed the total primary energy supply of the country.

In the NEAT methodology, both the non-energy use emissions and the non-energy use 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 the product related emissions and storage, the allocation is more complex, because downstream emissions have to be allocated back to upstream fuels with the help of the carbon balance made in stage 1. All NEAT compounds made downstream from the steam cracking products are for example allocated back to the steam cracker inputs. The allocation to feedstock enables the model user to conduct analysis and comparisons on the level of individual fuels.

The carbon storage (Flow 3 in Figure 3) calculated with the NEAT methodology can be compared with the carbon storage used in the IPCC-RA calculation (equation 1). Differences between the two estimates can be caused by:

- A difference between the total non-energy use determined by NEAT (Flow 2 in Figure 3) and the total non-energy use used in the IPCC-RA calculation (the latter is usually taken from energy balances)
- A difference in the division 'Stored' (Flow 3 in Figure 3) versus 'Released' (Flow 4 and 5 in Figure 3) between NEAT (the division is calculated on basis on a material flow analysis) and the IPCC-RA (the division is usually based on the IPCC default storage fractions).
- A combination of the two.

The first reason can be a matter of non-energy use definition (e.g. different allocation methods for ammonia, methanol and carbon black production and/or inclusion of backflows from and fuel use in steam cracker. Regarding the second difference it should be emphasised that there is a contradiction between the purpose of the default carbon storage fractions determined by Marland and Rotty (1984) and the recent use of these fraction as validation tool for emissions from fuel combustion only (e.g. table 1.a(c) in the Common Reporting Format; STSBA, 1999). In contrast, the application of NEAT for validation of the IPCC-RA leads to a value that includes *all* fossil CO₂ emissions (except for emissions from waste without energy recovery) (**see also Patel et. al., 2004**).

3.3 Use of NEAT for the IPCC-SA

The NEAT model material flow analysis contains several elements that can be particularly useful also for experts preparing emission inventories according to the IPCC-SA. Examples are the emission factors for steam crackers and for ammonia, methanol and carbon black and metal/inorganics production by type of feedstock. The NEAT results for emissions related to solvent and other product use can be compared with those emissions in the IPCC-SA. The NEAT results for product-related emissions, i.e. for ODU products can be compared with the product related emissions as they are given in the 'Product and Other Solvent Use' emissions category in the IPCC-SA. The IPCC Guidelines provide a large degree of freedom concerning the allocation of emissions to the various source categories. Emissions from ammonia

production can therefore be allocated to the category 'Energy' or to 'Industrial process emissions'.

It should be noted that the IPCC-SA contains also non-fossil CO₂ emissions from for example the use of limestone in the 'industrial process emission' category. Comparing the IPCC-SA results on 'industrial process emissions' and 'emissions from fuel combustion' with the NEAT results in these categories is therefore 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.

4 Stage 3 of the NEAT model, calculation of carbon storage fractions for use in the IPCC-RA

The NEAT model provides an overall country-specific storage fraction for non-energy use by dividing the carbon storage (Flow 3 in Figure 3) by the total non-energy use (Flow 2 in Figure 3). It must be emphasised again that waste treatment is not directly taken into account within the NEAT model and that emissions from waste⁶ are included in the calculated storage. If the emissions from this waste treatment were included, a lower storage fraction would be calculated. This approach is followed in work by Marland et. al. (1984) and Marland et. al. (2003). Except for emissions from waste management without energy recovery, all sources of fossil CO₂ emissions are taken into account in the calculated emissions. Because both the non-energy use storage and the non-energy use emissions are allocated to the various fuels used for non-energy purposes, storage fractions can also easily calculated by types of fuel. It should be noted that in countries where the overall storage is negative (compare Figure 4), the storage fractions are also negative. Although this is not very likely to happen for the overall storage fraction, this can easily happen for individual fuels. If for example, a country has no natural gas processing industries, but has considerable imports of natural gas derived chemicals that oxidise during their use, the non-energy use emissions that are allocated to natural gas might exceed the non-energy use of natural gas, leading to a negative storage fraction for the non-energy use for this fuel type.

Conclusions

The newest version of the NEAT model described here has so far been applied to Korea (**Park, 2004**), Germany (**Sjardin et. al., 2004**), Italy (**La Motta et. al., 2004**) and the Netherlands (**Neelis et. al., 2004**). These country analysis show that application of the NEAT model can yield the various valuable results claimed above. The most important drawback of the method is the extensive data requirement. By far the most time-consuming part of the NEAT model, requiring also most of the data inputs, is the bottom-up carbon balance, resulting in an estimate for emissions from solvent and other product use (ODU products). As a result of these major data requirements, the largest uncertainty is present in this part (e.g. Neelis et. al., 2004). To reduce this uncertainty, it is envisaged to study the possibility of replacing the carbon balance with more direct downstream estimates for products that are known to be released during their use. This approach is being successfully applied in the US (**Freed et. al., 2004**). This typically requires a comprehensive survey. Cross-country comparisons of such surveys may allow deriving generic values for implementation in NEAT.

Another area requiring further research is the position of CO₂ emissions from incineration of "non-specs", resulting from incomplete conversions in the chemical industry. In the NEAT methodology, these emissions are so far not explicitly modelled and are mainly included in the emissions from solvent and other product use. There are indications that the magnitude of these emissions might be substantial (Tonkovich et. al., 1995 and **Freed et. al., 2004**). The position of these residual fuel streams in energy balances and CO₂ emission inventories is rather unclear. Moreover, the final fate (oxidation during use or oxidation only during waste

⁶ To prevent double counting, the total consumption of products that are not oxidised during use is included in the storage. If waste is incinerated for energy recovery, the waste re-enters the energy balance as an energy commodity and the resulting emissions are calculated by multiplication with a certain emission factor.

treatment) of some complex products like lubricants should also be studied further; this will help to generate reliable estimates for emissions from solvent and other product use.

The NEAT model can be extended in order to include the elements just described (e.g. emissions from waste incineration). This requires substantial additional data analyses, which is strongly recommended for future research. By doing so, all CO₂ emissions from fossil fuel origin will be covered by the model. With such an extended mode it will be possible to estimate the fraction of non-energy use which is finally incinerated and to investigate the relative amount of waste emissions versus the non-energy use over the years.

Acknowledgements

This research was supported by the European Commission (Research Directorate General), 5th framework European Network for Research in Global Change (ENRICH) programme, through research contracts ENV-CT98-0776 and EVK2-CT-2000-80003 (International network Non-Energy Use and CO₂ emissions, NEU-CO₂). The network's homepage can be found on <http://www.chem.uu.nl/nws/www/nenergy/>.

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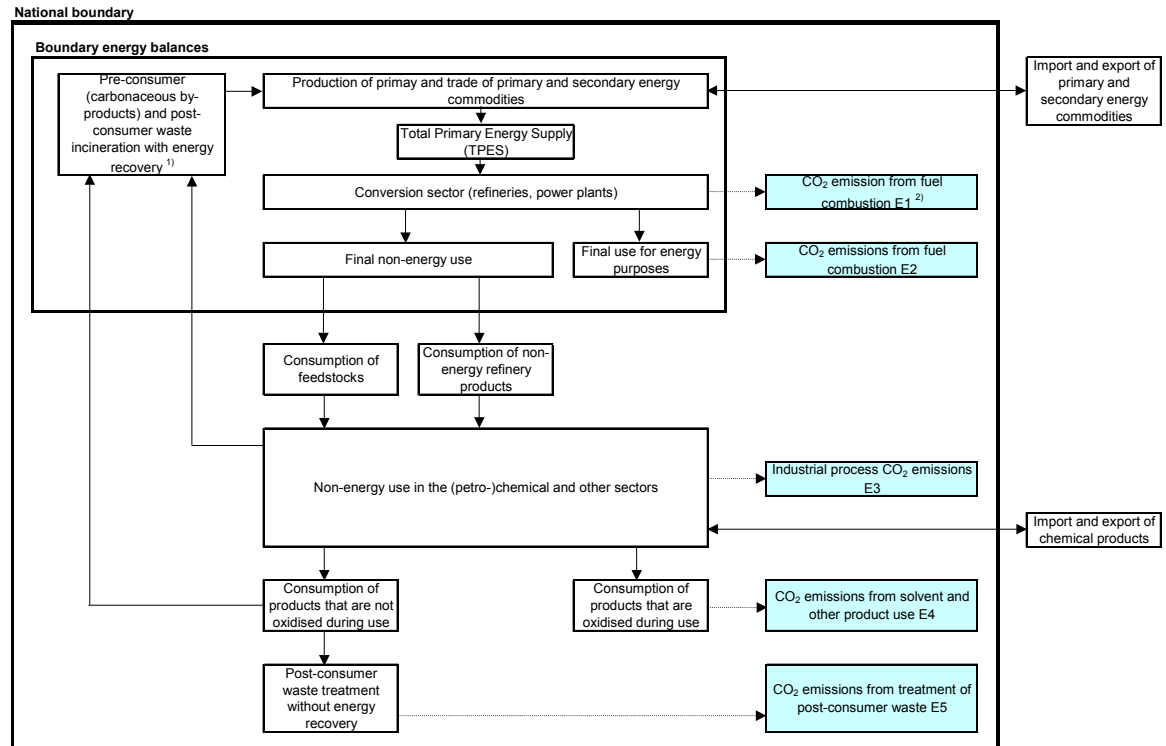
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Figure 1: Overview of CO₂ emissions from the energy and non-energy use of fossil fuels

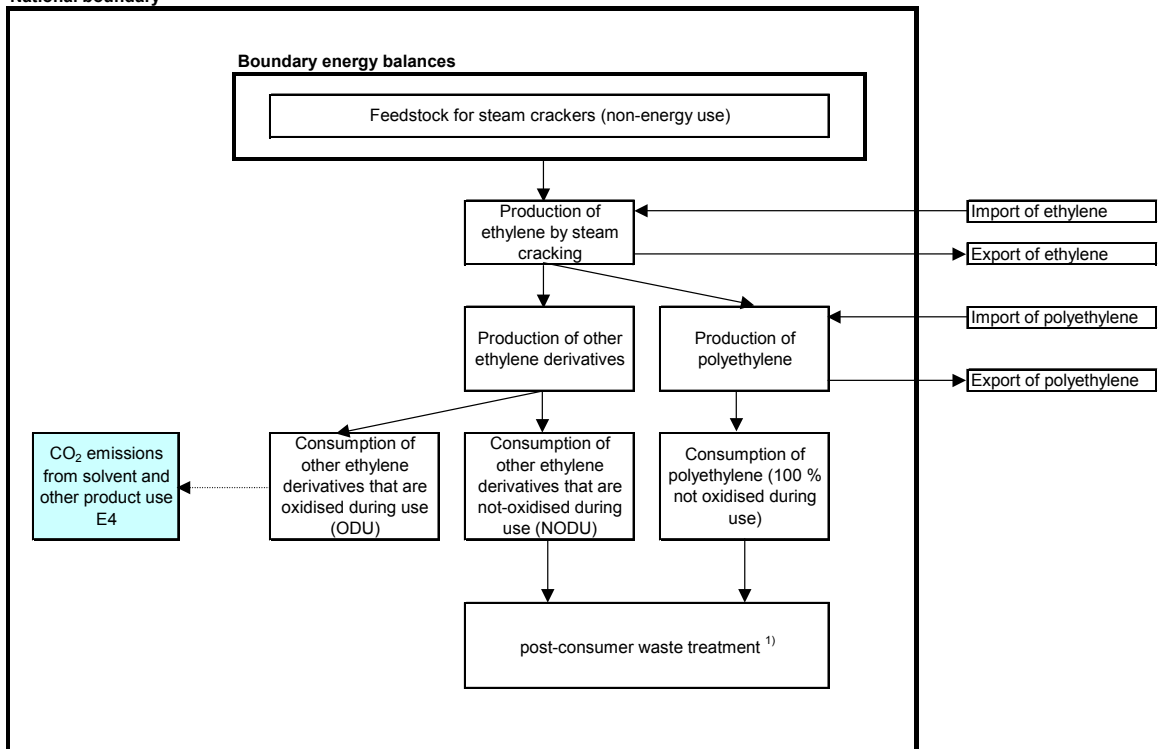


¹⁾ In line with the international energy balance (IEA, 2000), it is assumed that the waste used for energy recovery is in the energy balance reported as a produced energy commodity. The energy recovery (to e.g. electricity) is subsequently covered in the conversion sector and the CO₂ emissions are part of the emissions from fuel combustion (E1)

²⁾ Including emissions from waste incineration with energy recovery

Figure 2: Calculation of emissions from solvent and other product use in NEAT, simplified example for ethylene

National boundary



¹⁾ The post-consumer waste treatment leading to emissions in the category waste (E5 in Figure 1) or in the category fuel combustion (E1 in Figure 1) is not explicitly modelled in NEAT

Figure 3: Overview of CO₂ emissions and non-energy use storage according to the NEAT methodology

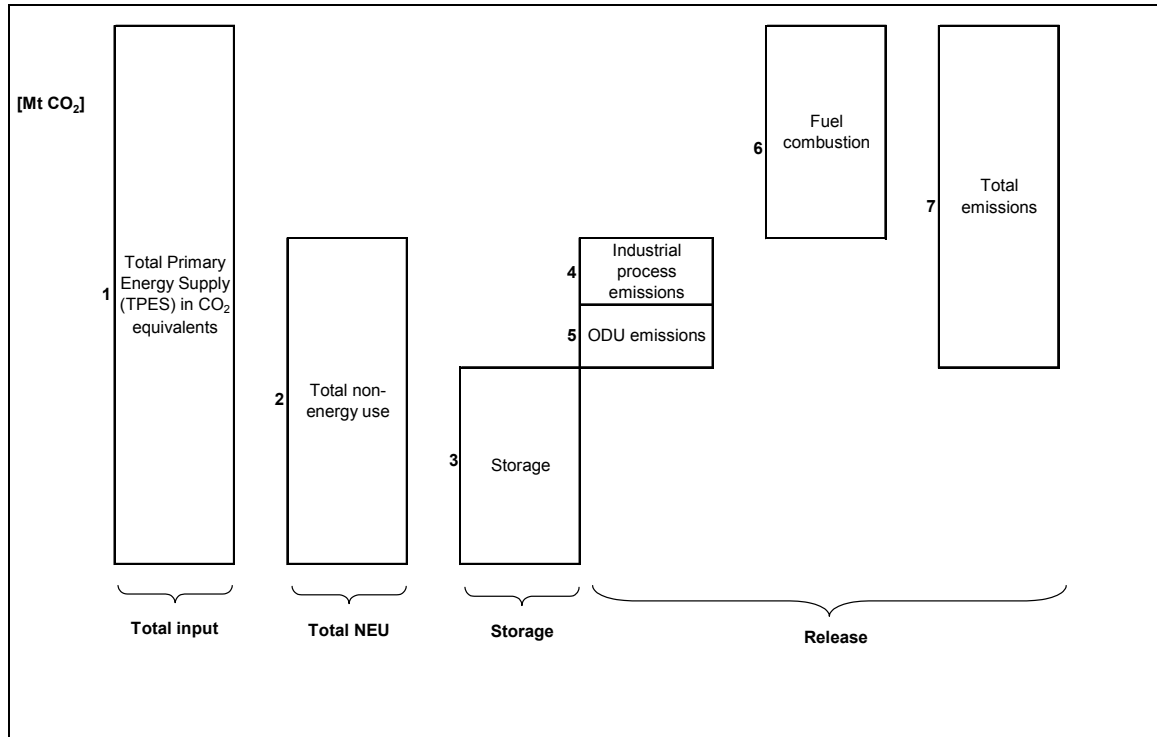


Table 1: Assumed fractions of ODU vs. NODU products for the 77 NEAT core products (the datasets 'MIN Release' and 'MAX Release' are used for a sensitivity analysis)

Compound ¹⁾	Total consumption or 'other use'	MEAN		MIN RELEASE	MAX RELEASE
		NODU ²⁾ [%]	ODU ²⁾ [%]	ODU ²⁾ [%]	ODU ²⁾ [%]
BASIC CHEMICALS					
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 (o-,m-,p-mixed xylene)	total	0	100	30	100
ortho-Xylene	other	0	100	30	100
meta-Xylene	total	0	100	30	100
para-Xylene	other	0	100	30	100
INTERMEDIATES					
Acetic acid	other	35	65	35	75
Acetone	other	60	40	45	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-Tert-Butyl-Ether (MTBE) 3)	total	0	0	0	0
Higher alcohols	other	50	50	10	90
Orthophthalates	other	100	0	0	50
Phenol	other	0	100	70	100
Phthalic anhydride (PSA)	other	0	100	30	100
Polyether-Polyols	other	100	0	0	50
i-Propanol	other	7	93	80	100
Propylene oxide	other	0	100	100	100
Styrene	other	100	0	0	0
Terephthalic acid (TPA)	other	100	0	0	0
Isocyanates	other	100	0	0	0
Urea	other	0	100	0	100
Vinylchloride monomer (VCM)	other	20	80	30	100
PRODUCTS					
Acrylonitrile-Butadiene-Styrene (ABS)	total	100	0	0	0
Butadiene Rubber (BR)	total	100	0	0	0
Ethylene-Propylene-Diene-Monomer (EPDM)	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 (PE)	total	100	0	0	0
Polyethyleneterephthalate (PET)	total	100	0	0	0
Polypropylene (PP)	total	100	0	0	0
Polystyrene (PS)	total	100	0	0	0
Polyurethane (PUR)	total	100	0	0	0
Polyvinylacetate	total	100	0	0	0
Polyvinylchloride PVC	total	100	0	0	0
Styrene-Acrylonitrile (SAN)	total	100	0	0	0
Saturated polyester	total	100	0	0	0
Styrene-Butadiene Rubber (SBR)	total	100	0	0	0
Unsaturated polyester/alkyd resin	total	100	0	0	0
Urea formaldehyde resin (UF)	total	100	0	0	0

¹⁾ Ammonia does not contain any embodied carbon and it is therefore not listed in this table. However, the production of ammonia results in CO₂ emissions which are dealt with in NEAT as industrial process emissions

²⁾ ODU = Oxidised During Use, NODU = Not-Oxidised During Use

³⁾ MTBE ends up as a antiknocking agent in the fuel pool and the emissions are thus taken into account in the CO₂ emissions from fossil fuel combustion

Table 2: Overview of NEAT CO₂ emission factors for ammonia production

Feedstock	Allocation method ¹⁾	Industrial process emissions	CO ₂ from fuel combustion
		kg CO ₂ /kg NH ₃	kg CO ₂ /kg NH ₃
Steam reforming of natural gas ²⁾	NEAT, standard	1.6	0
	NEAT, allocated	1.1	0.5
Partial oxidation of coal ³⁾	NEAT, standard	3.9	0
	NEAT, allocated	2.7	1.2
Partial oxidation of oil ⁴⁾	NEAT, standard	2.5	0
	NEAT, allocated	1.8	0.7

¹⁾ 30% of the total hydrocarbon input to ammonia production is allocated to energy use (fuel combustion), while 70% is allocated to industrial process emissions (see text).

²⁾ Based on a natural gas consumption of 28.5 GJ/t NH₃ and an emission factor of 56 kg CO₂/GJ natural gas.

³⁾ Based on a total coal consumption of 42 GJ/t NH₃ and an emission factor of 93 kg CO₂/GJ coal.

⁴⁾ Based on a total oil consumption of 34.5 GJ/t NH₃ and an emission factor of 73 kg CO₂/GJ oil.

Table 3: Overview of NEAT CO₂ emission factors for methanol production

Feedstock	Allocation method ¹⁾	Industrial process emissions	CO ₂ from fuel combustion
		kg CO ₂ /kg methanol	kg CO ₂ /kg methanol
Steam reforming of natural gas ²⁾	NEAT, standard	0.4 ²⁾	0
	NEAT, allocated	0	0.4
Partial oxidation of coal ³⁾	NEAT, standard	2.9 ³⁾	0
	NEAT, allocated	0	2.9
Partial oxidation of oil ⁴⁾	NEAT, standard	1.4 ⁴⁾	0
	NEAT, allocated	0	1.4

¹⁾ In the "NEAT, standard approach", the feedstock is allocated to non-energy use and the resulting emissions are regarded industrial process emissions. In the "NEAT, allocated approach", part of the feedstock is allocated to energy use. To this end, the carbon content of methanol (1.38 kg CO₂/kg methanol) is deducted from the carbon content of the feedstock.

²⁾ Based on a natural gas consumption of 31.6 GJ/t methanol and an emission factor of 56 kg CO₂/GJ natural gas.

³⁾ Based on a total (brown)coal consumption of 38.6 GJ/t methanol and an emission factor of 111 kg CO₂/GJ soft coal (lignite).

⁴⁾ Based on a total oil consumption of 38.4 GJ oil/t methanol and an emission factor of 74 kg CO₂/GJ oil.

Table 4: Overview of NEAT CO₂ emission factors for carbon black production

Feedstock	Allocation method ¹⁾	Industrial process emissions kg CO ₂ /kg carbon black	CO ₂ from feedstock used as fuel kg CO ₂ /kg carbon black
Natural gas	NEAT, standard	0.15 ²⁾	0
Oil	NEAT, standard	1.77 ²⁾	0
Natural gas	NEAT, allocated	0	0.15 ²⁾
Oil	NEAT, allocated	0	1.77 ²⁾

¹⁾ In the "NEAT, standard approach", the feedstock is fully allocated to non-energy use and the resulting emissions are regarded industrial process emissions. In the "NEAT, allocated approach", the feedstock is completely allocated to energy use of the feedstock and emissions are regarded emissions from fuel combustion.

²⁾ 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 CO₂/GJ for natural gas and 74 kg CO₂/GJ for oil. The total oil input is therefore equivalent to 5.15 kg CO₂/kg carbon black and the total natural gas input to 0.43 kg CO₂/kg carbon black. The carbon content of carbon black is assumed to be 3.67 kg CO₂/kg carbon black. The total CO₂ emission therefore equal 5.15 + 0.43 - 3.67 = 1.91 kg CO₂/kg. 7.7% (0.43/(0.43+5.15)) of the emissions is allocated to natural gas and 92.3 % (5.15/(5.15+0.43)) is allocated to oil.

Table 5: Overview of CO₂ emission factors from the production of metals and inorganics

	Input raw materials (%)			Specific CO ₂ emissions (t CO ₂ /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

Table 6: Ultimate yields of steam crackers with various feedstocks

	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 7: Overview of CO₂ emissions from fuel use in steam crackers and carbon equivalents of backflows to refineries.

	Naphtha	Gas oil	Ethane	Propane	Butane
Specific CO ₂ emissions from fuel use steam crackers (Mt CO ₂ / Mt ethylene)	1.7	2.3	1.0	1.0	1.1
Specific CO ₂ equivalents of backflows steam crackers (Mt CO ₂ / Mt ethylene)	0.9	2.1	0.0	0.8	0.9