

**Fraunhofer** Institute  
Systems and  
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# **International Network Non-energy use and CO<sub>2</sub> emissions (NEU-CO<sub>2</sub>)**

**An Activity within the European Commission's  
ENRICH Programme,  
DG RTD, "Environment and Climate"**

**Final Report of the First Phase of the Network  
(January 1999-June 2000)**

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## Preface

The non-energy use of fossil fuels for the production of chemical, petrochemical and certain refinery products results in CO<sub>2</sub> emissions in the production, use and waste stages. This is still a "dark area" in emission inventories since the quantities and the relationships are not well understood. Hence, there are still large gaps and uncertainties in CO<sub>2</sub> emission accounting related to non-energy use. For this reason, non-energy use is addressed as a **priority area for future work** by the Revised 1996 IPCC Guidelines for National GHG Inventories (Vol. 3, page Overview.5) The need for consistent and comparable reporting of CO<sub>2</sub> emissions from non-energy use is also called for by the European Environment Agency, EEA (cited in Tenner, 1999, p.3-4).

The NEU-CO<sub>2</sub> network brings together experts in emission inventories and the chemical/petrochemical industry in order to gain deeper insight into the release of CO<sub>2</sub> emissions originating from non-energy use. The network is mainly devoted to international networking and not to research. Since its commencement, the network has continued to attract interest and it now comprises about two dozens of organisations, a smaller fraction of which receives funds from the European Commission. The other organisations participate at their own cost. These are mainly national environmental agencies and international organisations which have the important role of providing the link to statistics offices, administration and policy makers.

This report concludes the **first phase of the NEU-CO<sub>2</sub> network**, covering the period from January 1999 to June 2000. Within this period, two **workshops** were held, one in Paris in September 1999 and the other in Brussels in April 2000. The results of these workshops represent the basis of this report. The workshop papers have also been compiled in workshop proceedings which are publicly available.

Due to the success of the NEU-CO<sub>2</sub> network, the partners decided to apply for the continuation of this activity which was recently accepted by the European Commission. The **second phase of the of the NEU-CO<sub>2</sub> network** will start in Fall 2000 and will continue for 18 months. This will allow the NEU-CO<sub>2</sub> network to improve the methods applied, to close data gaps, to check the preliminary conclusions given in this report and to provide consolidated results and recommendations by mid 2002. The ultimate goal of the NEU-CO<sub>2</sub> network is to contribute to an improvement of the IPCC Guidelines in the area of non-energy use and and to provide inventorists with tools and methods to estimate more accurately non-energy CO<sub>2</sub> emissions.

## 1. Introduction

### 1.1 Background

In the context of greenhouse gas emissions, so far most attention has been paid to CO<sub>2</sub> emissions from the combustion of fossil fuels. But a significant fraction of fossil fuels is used for non-energy applications. **Non-energy use** is here defined as the consumption of fossil feedstocks for the manufacture of synthetic organic materials and chemical products, e.g. plastics, fibres, lacquers and varnishes, solvents, fertilisers, lubricants, greases, waxes, petroleum coke and bitumen (see Appendix 1). In Western Europe, non-energy use represents approx. 12% of the total amount of fossil fuels for final consumption. In other parts of the world, the manufacture of non-energy products is increasing at a tremendous pace, e.g. in Asia. Only a part of non-energy use is emitted as CO<sub>2</sub> within short periods of time, whereas carbon incorporated in long-lived products is first stored in the economy during the economic life-span of the product. When a product becomes waste, the waste management option determines the amount of carbon released to the atmosphere. For example, waste incineration results in the release of the full carbon content.

The IPCC issued **Guidelines** (IPCC/IEA/OECD/UNEP 1997) which include a method to account for CO<sub>2</sub> emissions from non-energy use, but there are still **large uncertainties** connected to the proposed procedures. The NEU-CO<sub>2</sub> network has been set up to discuss the related issues in order to come up with recommendations. The main final goal of the network is to **improve the methodology for estimations on CO<sub>2</sub> emissions from non-energy use**. Attention is thereby paid to aspects of feasibility (data availability, data gaps) and to methodological problems. The recommendations provided by the network will also include the identification of further research requirements, the outcome of which will contribute to an improvement of the Guidelines and to the harmonisation of ongoing activities.

### 1.2 Membership and organisation of the NEU-CO<sub>2</sub> network

The NEU-CO<sub>2</sub> network comprises experts in emission inventories and the chemical/petrochemical industry. To account for the global character of the issue, the network is composed of an **international team**<sup>1</sup> of experts from seven European countries, India, Japan, Korea, Russia and the U.S. The seven European countries covered are Austria, Denmark, France, Germany, Italy, United Kingdom and the Netherlands. Recently two further partners, from Belgium and Poland, joined the network. In addition, national environmental agencies and international

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<sup>1</sup> The full names of the organisations, the addresses and the names of the experts involved is given in Appendix 4.

organisations are actively involved in or affiliated to the NEU-CO<sub>2</sub> network. The national agencies participating in this activity are ANPA (Italy), RIVM (Netherlands), SFT (Norway) and UBA (Germany). The list of international organisations comprises EEA (Copenhagen), EUROSTAT (Luxembourg), IEA (Paris) and UNEP (Paris). These organisations have the important role of providing the link to statistics offices, to administration and policy makers.

The network activity of the seven European partners mentioned above, the Russian and the Indian partner was funded for the period 1.1.1999-30.6.2000 by the **European Commission**, DG RTD, under the ENRICH Programme (European Network for Research into Global Change). All the other organisations participated at own costs. The network was co-ordinated by the Fraunhofer Institute for Systems and Innovation Research (ISI, Karlsruhe, Germany) and the Netherlands Energy Research Foundation (ECN, Petten/Amsterdam, Netherlands).

The network is mainly devoted to international networking and not to research. Two two-day **workshops** were held, one in Paris in September 1999 and the other in Brussels in April 2000. The first workshop was preceded by a questionnaire which was prepared by ISI and ECN and which was answered by the country representatives of the network. The purpose of this survey was to obtain an overview of data availability and methodological work done to date. The papers presented at the workshops have been compiled in **workshop proceedings** (ECN/ISI 1999/2000). In an early phase of the network a **reader** was prepared (ISI, 1999) and a **homepage** was set up ([www.eu.fhg.de/NENERGY/](http://www.eu.fhg.de/NENERGY/)) as a general working basis for the network. The homepage presents the goals of the network and the most important background documents.

This report presents the results of the work of the NEU-CO<sub>2</sub> network in the period 1.1.1999-30.6.2000. With support from the European Commission, the network will continue its work for another 18 months, starting from Fall 2000. Consolidated calculation results and final recommendations on methodological issues are expected to become available by mid 2002.

### **1.3 Relationship between non-energy use and GHG emissions**

Data on non-energy use are published in national energy balances. Non-energy use can be split into a number of refinery products (such as bitumen and lubricants), products from the petrochemical industry (plastics, synthetic fibres, solvents etc.) and some coal products (such as tar by-products from coke production).

The carbon balance for non-energy use is complex for a number of reasons:

- Carbon is stored in synthetic organic products, but this carbon is released if these products are oxidised or incinerated. As a consequence, the storage and the release must be accounted for properly;
- It is not clear how petrochemicals produced in and/or handled by refineries are accounted for in energy statistics;

- The petrochemical industry is characterised by co-production of energy and materials and integration of energy and material flows with the refining sector, which complicates CO<sub>2</sub> emission accounting based on energy statistics;
- Petrochemical industries are usually highly integrated complexes. Energy statistics report flows to and from them expressed as "standard" petroleum products. It is difficult, if not impossible, to validate these data and to relate them to the materials used in the complexes;
- Some petrochemical products have (potentially) a long life span, others oxidise rapidly during use (e.g. detergents);
- Petrochemical products are traded internationally.

#### **1.4 Structure of the petrochemical industry and other relevant industrial sectors**

The petrochemical industry converts fossil fuels (oil and natural gas) and biomass carbon (e.g. vegetable oil) into synthetic organic products. These products can be split into energy carriers (e.g. pyrolysis gasoline) and other products. These other products include amongst others plastics, synthetic fibres, elastomers, solvents, resins, lubricants, and detergents. This list is not complete. Thousands of products can be discerned, based on a differing chemical structure. However, fine chemicals are excluded from this analysis, because the quantity is not significant in physical production volumes (GHG emissions are closely related to the physical production volume). This selection limits the number of products to several hundred. Less than fifty make up the bulk of the production.

The key process in the petrochemical industry is currently steam cracking of either refinery products or natural gas fractions. The refinery products used include naphtha, gas oil, liquefied petroleum gas (LPG). The natural gas fractions include NGL and ethane. Steam cracking results in a broad array of intermediary chemical products (ethylene, propylene, butadiene, BTX) and by-products used for energy purposes (hydrogen, methane, pyrolysis gasoline). They are either used for heating within the petrochemical industry or recycled to the refineries. The intermediates serve as input for the production of a broad array of petrochemicals.

The structure of the petrochemical industry is generally similar around the world, but some remarkable national differences should be noted. The US industry is to a much larger extent based on steam cracking of gas derived feedstocks than are the petrochemical industries in Europe and Asia, which largely rely on oil feedstocks (mainly naphtha). The production of ammonia and methanol is generally based on reforming of natural gas, but in some countries, substantial amounts are also produced from heavy fuel oil (e.g. Germany). Regarding conversion routes, some petrochemicals can be produced via a number of production routes, based on

differing intermediates. These differences must be accounted in the analysis. Fortunately the main process routes for plastics etc. are generally the same from a chemical process route point of view.

Refineries produce bitumen and lubricants. Both are accounted for as non-energy use. Bitumen is mainly used for production of asphalt. Lubricants are predominantly used in the transportation sector. Some overlap exists between refineries and the petrochemical industry. For example, propylene, an important petrochemical product from steam cracking, can also be produced from refinery gas. The same applies to many aromatic compounds such as benzene and xylenes. It has been stated before that important quantities of so-called pyrolysis gasoline are recycled into the refining sector. Other petrochemical products such as MTBE and ETBE are important petrochemical products which serve as input for gasoline production. Lubricants are still predominantly produced in refineries, but the production is gradually shifting into the petrochemical industry, which is able to produce superior quality lubricants.

A part of the CO<sub>2</sub> produced during ammonia production is re-used for chemical purposes, thus complicating CO<sub>2</sub> accounting. Most importantly, CO<sub>2</sub> is used to produce urea which is both an important nitrogen fertiliser and an intermediate for some resins (urea resins, melamine resins). CO<sub>2</sub> from this source is also used for other purposes, e.g. for welding and for carbonated beverages.

The distillation of tar, a by-product from coke ovens, also results in organic chemicals. A part of the products from tar distillation are used as feedstocks for petrochemical products, e.g. for carbon black and aromatics.

The use of fossil fuels as a reducing agent in iron and steel production – most importantly the use of coke in blast furnaces – is addressed by some authors as non-energy use. However, the entire area of metallurgical production is outside the area covered by the NEU-CO<sub>2</sub> network which concentrates on the chemical and petrochemical industry and selected refinery products (mainly lubricants and bitumen).

## 1.5 Principles of current carbon accounting

In its Guidelines, the IPCC introduces two different approaches for reporting on the national CO<sub>2</sub> emissions from fuel combustion, the so-called **"Reference Approach" (RA) and the "Sectoral Approach" (SA)** (IPCC/IEA/OECD/UNEP 1997). The RA is a simple method to estimate C-flows based on the supply data for fuels as published in energy balances. On the other hand, the SA is more general and provides methods for estimating all anthropogenic emissions of GHGs from each of the source categories within defined sectors of activity. The methods subsumed under the SA are arranged into "Tiers" differing in the detail and

complexity of their approach. For estimation of emissions from fuel combustion the methods range from the use of fuel delivery data found in energy statistics to estimation procedures based on the production volumes of certain goods, multiplied by specific emission factors. Hence, the SA provides information on the relative importance of the source categories and on the types of products. The RA can play an important role in checking the totals from the SA but cannot provide the sectoral detail. The RA is the reporting method applied by many of the non-Annex-1 countries, since it has the advantage of requiring less data than the SA.

## 1.6 The RA and non-energy use

The principle idea behind the RA is depicted in Figure 1. The total apparent consumption of fossil fuels in the country studied (second column from the left) is given by the following formula (IPCC/IEA/OECD/UNEP 1997):

$$\text{Apparent consumption} = \text{Primary fuel production} + \text{Imports} - \text{Exports} - \text{International bunkers} - \text{Stock change} \quad (1)$$

According to Figure 1 storage of fuel feedstock carbon in materials is deducted from total apparent consumption to determine the net carbon emissions. By multiplying the net carbon emissions by the fraction of carbon oxidised (ranging between 98% for coal and 99.5% for gas), a country's "Actual CO<sub>2</sub> emissions" are determined. "Actual CO<sub>2</sub> emissions" are generally regarded as CO<sub>2</sub> from fuel combustion. This implies that carbon storage, subtracted in the RA, must represent the total amount of fuel feedstock carbon stored in **all** chemical products,<sup>2</sup> including both short-lived and long-lived synthetic organic materials.

The amount of carbon stored to be entered in the scheme shown in Figure 1 is estimated from the following formula and the data given in Table 1 (IPCC/IEA/OECD/UNEP 1997):

$$\text{Total carbon stored (Gg C)} = \text{Non-Energy Use (TJ)} * \text{Emission factor (t C/TJ)} * \text{Fraction of carbon stored /1000} \quad (2)$$

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<sup>2</sup> To be precise, the assumption that the total amount of carbon which is not combusted is identical with the total amount of carbon stored in all chemical products is again an approximation. In reality, there will be a difference between the two which is caused to a large extent by carbon oxidation during the production of ammonia, methanol and carbon black. This aspect will be dealt with later on.

Table 1: Default carbon storage factors according to the IPCC Guidelines (IPCC/IEA/OECD/UNEP 1997)

	Fraction of carbon stored
Lubricants	0.5
Bitumen	1.0
Coal oils and tars from coking coal	0.75
Naphtha as feedstock	0.8
Gas/Diesel oil as feedstock	0.5
Natural gas as feedstock	0.33
LPG as feedstock	0.8
Ethane as feedstock	0.8

Data on non-energy use of fossil fuels are published in national energy balances. These data were studied for various countries with regard to the definition of non-energy use chosen (Patel, 1999a). The analyses confirmed the earlier presumption (Patel et al. 1999) that the non-energy use data published in national and international energy balances are very often inconsistent since they refer to different definitions (system boundaries). It has been shown that the differences in definitions can influence the reported amount of non-energy use by 30% (Patel et al. 1999). As shown in equation (2), data on non-energy use are used in the RA to estimate the amount of carbon stored in products. **Therefore, it is rather unlikely that the direct use of these data for the RA will yield reliable results.** Equally, use of the data in the simpler, Tier 1 method for the SA (IPCC/IEA/OECD/UNEP 1997; Volume 3, Chapter 1.4) will create the same uncertainty in the estimates. For each definition of non-energy use, a different set of carbon storage factors would be required (the various definitions of non-energy use are described in Box 1, see Chapter 2).

The UNFCCC's new **Common Reporting Format (CRF)**; SBSTA 1999) has emphasised the role of the RA as a tool for validation of the estimates of CO<sub>2</sub> from fuel combustion obtained from the SA by Annex-1 countries. However, the reconciliation of the RA estimates with those obtained from the SA is not a simple matter. It will depend on, amongst other things, the "Tier" levels used by Annex 1 countries for the many different methods within the SA and the manner in which the RA estimate has been calculated. In particular, the RA may be applied differently depending on the data available to the country using it:

1. IPCC RA with no calculation of carbon stored where a country does not have a petrochemical industry or significant other non-energy use or does not have

credible figures for the flows of fuel to them (see IPCC/IEA/OECD/UNEP 1997; Vol 2, boxes on page 1.7 or 1.11)

2. IPCC RA with calculation of carbon stored by default values where a country does not have national estimates for carbon storage factors (see IPCC/IEA/OECD/UNEP 1997; Vol 2, Tables on page 1.37 or 1.54; see also Table 1 in this report).
3. IPCC RA with calculation of carbon stored using country specific factors.

Despite these differences in procedural precision, the studies conducted by the NEU-CO<sub>2</sub> network have confirmed the importance of accurate data for non-energy use and appropriate carbon storage factors for the SA and RA. In many cases, the carbon storage factors which have been determined from modelling performed by the NEU-CO<sub>2</sub> network, differ considerably from the default values contained in the IPCC Guidelines. In addition it has become clear that not all default values (for example, for heavy fuel oil) are available in the Guidelines.

## **1.7 The SA and non-energy use**

The SA provides estimation methods for greenhouse gas emissions which are related to energy use and to other activities. The SA is a collection of methods grouped into Tier 1, Tier 2 and Tier 3 Approaches according to their levels of detail and complexity. Calculated emissions from energy use are largely based on sectoral data from energy balances. With regard to the other activities, the most important source categories, in which non-energy use of fossil fuel carbon can occur, are "Industrial processes", "Solvent use" and "Waste". The emissions from these sources are usually not reported in the category "Energy" within the SA (waste incineration is an exception to some extent). The category "Energy" comprises fuel combustion and fugitive emissions (IPCC/IEA/OECD/UNEP 1997, Vol. 1, p.1.3-1.7).

The characteristics of activities falling under fuel combustion are not defined explicitly within the Guidelines but there are examples of activities which are not included. Emissions from flaring of natural gas are placed in the fugitive emissions source category (rather than fuel combustion) and emissions from the exothermic oxidation of feedstock carbon in chemical processes are placed in the industrial processes source category. In the first case, flaring is not considered fuel combustion because it is not a productive activity and, in the second case, the primary purpose of the exothermic oxidation of carbon is not for heat raising although the heat produced may be used for energy purposes.

On this basis, a clear allocation of CO<sub>2</sub> emissions to the source categories seems possible for the most important processes related to non-energy use. This allocation is shown in Table 2. However, it must also be mentioned that the IPCC Guidelines

provide a large degree of freedom concerning the allocation of emissions to the various source categories as long as it is made clear what has been done and provided that double counting is avoided.<sup>3</sup> To estimate the emissions from "Industrial processes", "Solvent use" and "Waste", the IPCC Guidelines usually provide **emission factors** for multiplication with the physical flow, e.g. the output of the process. Table 2 provides an overview for which of these activities default emission factors are provided by the IPCC Guidelines (IPCC/IEA/OECD/UNEP 1997).

For ammonia production, a default CO<sub>2</sub> emission factor is provided but no distinction is made by type of the feedstock used (a distinction should be made since the CO<sub>2</sub> emissions differ depending on whether gas, oil or coke are used as feedstocks). Moreover, according to the NEU-CO<sub>2</sub> network's knowledge, the SA/CRF wrongly assume that CO<sub>2</sub> process emissions from methanol and carbon black are negligible and they thus only refer to CH<sub>4</sub> emissions from these production processes. However, considerable amounts of the feedstock are oxidised during the process and lead to instant CO<sub>2</sub> emissions. Similarly, CO<sub>2</sub> emissions from the fuel use for ethylene production (steam cracking) must be reported as process emissions unless these fuels are already covered by the energy use of the refinery and chemical sector. For ethylene and for methanol production, the amount of emissions again depend on the type of feedstock used. Finally, the IPCC guidelines provide no support data to estimate CO<sub>2</sub> emissions from solvents and from the waste treatment related to non-energy use. This information is neither provided by the the CRF (SBSTA 1999) nor by EMEP/CORINAIR's Atmospheric Emission Guidebook (EMEP/CORINAIR 1999; see below, Chapter 3).

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<sup>3</sup> On the one hand this pragmatic approach has advantages for those preparing the inventories; on the other, it makes comparisons by source categories among various countries impossible and it makes data verification more difficult. Depending on the value of the distinction by source categories for abatement policy work this will be seen as a problem or not. This issue will have to be discussed with national users of inventories.

Figure 1: Calculation scheme of the IPCC Reference Approach (RA) (IPCC/IEA/OECD/UNEP 1997)

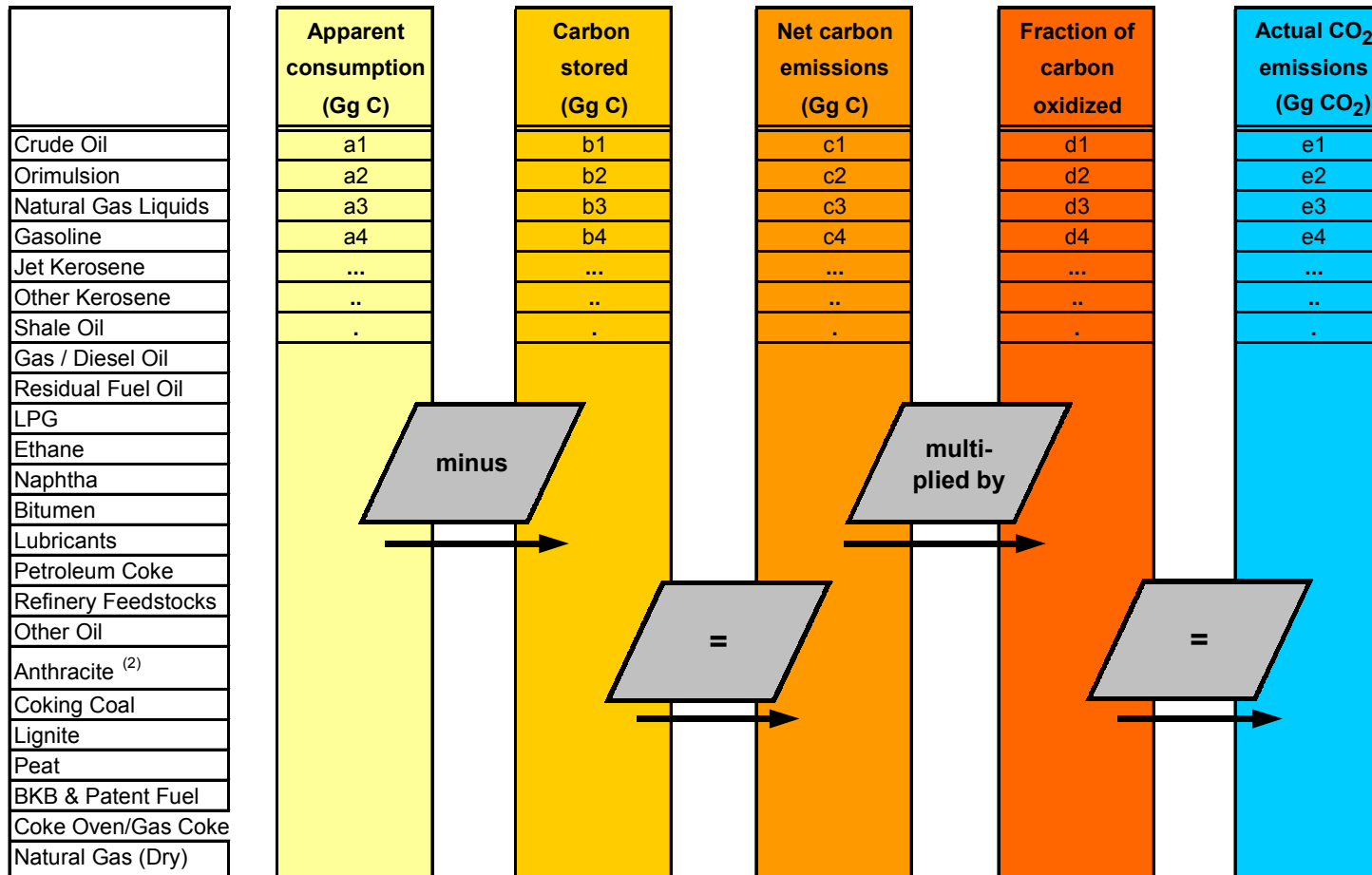


Table 2: Source categories of GHG emissions from non-energy use covered by the SA (Tier 2 and 3) and availability of default emission factors in the IPCC Guidelines (IPCC/IEA/OECD/UNEP 1997)

Activity	Methodology and/or default data provided (Y/N) <sup>1)</sup>	
	CO <sub>2</sub>	Other gases
Energy use (in the refinery and chemical sector)	Y	Y
Industrial processes		
Ammonia production	Y	Y
Carbide production <sup>2)</sup>	Y	Y
Carbon black production	N	Y
Ethylene production	N	Y
Methanol production	N	Y
Solvent use	N	N
Waste		
Wastewater	N	Y
Waste incineration	N	Y

<sup>1)</sup> For industrial processes and waste, both a methodology and default data are provided. For solvent use, none of the two is provided. For energy use, a methodology is provided but default data are not provided since they are not required (per definitionem).

<sup>2)</sup> Silicon carbide and calcium carbide

## 1.8 Starting points for the work of the NEU-CO<sub>2</sub> network

The two last chapters showed that estimations of CO<sub>2</sub> emissions from the non-energy use of fossil fuels are accompanied by considerable problems. The main conclusions, which at the same time represent the starting points for further work, are:

- Products manufactured from fossil fuel feedstock may be divided into two main groups, **short-lived materials and long-lived products**. The estimation of the CO<sub>2</sub> emissions from their manufacture **requires different approaches for each group** and, in some cases, for specific products or materials within the group.
- Within the IPCC Guidelines the simpler methods for estimating CO<sub>2</sub> emissions from the processing or combustion of fossil fuel carbon rely on statistics of fuels delivered to the manufacturing industries. In the case of the petrochemical sector the **statistics of feedstock deliveries (non-energy use) are subject to large uncertainties**. For most industries energy statistics cannot provide sufficient discrimination between the different uses of fossil fuel feedstock in enterprises to identify accurately the non-energy use. In particular, the

**definitions** of deliveries for non-energy use within the petrochemical sector **differ between countries** thereby making suspect the cross country comparisons of inventories based on the definitions.

- It is clear, therefore, that there is a strong need for countries to make explicit the bases used for reporting chemical feedstock consumption and to **harmonise the definitions used**. Equally, better energy data on the uses of fuels within enterprises would enable clearer distinctions between fuel combustion, non-energy and industrial processes uses of fuel carbon.
- There are also a number of **chemical processes**, most (but not all) of which are identified in the Guidelines and Atmospheric Emissions Guidebook, for which **CO<sub>2</sub> emission factors are either not suggested or could be improved**.
- In addition to the data issue described above, there are **problems of definition and conceptual consistency** within the various methodologies proposed or referred to in the IPCC Guidelines. These difficulties are particularly relevant for the allocation of emissions from non-energy use of fossil fuel carbon to the correct source categories. For example, the discussion of carbon storage factors, to be used in the RA and SA (Tier 1) methods for estimating emissions from fuel combustion, strongly suggests that emissions from the use of short-lived products, manufactured from fuel as feedstock, should be included in fuel combustion (IPCC/IEA/OECD/UNEP 1997, Vol 3, p.1.26). Short-lived products appear to be defined as those with a lifetime of less than twenty years (*ibid*, p.1.25). Elsewhere, however, the more detailed methodologies (SA, Tier 2 and Tier 3) allocate emissions from the use of these products to the sectors in which their carbon is released (e.g. for solvent use), i.e. the emissions are not included in the fuel combustion category.
- To contribute to a solution for these and other problems, **a model is required**. This should describe **the carbon flow through the various petrochemical processes** (with a distribution by types and characteristics), their **energy needs** and the way of satisfying these. Only with a model can the **emission mechanisms** be understood and estimated. Effects of the choice of definitions on emission estimates can also be examined.

The NEU-CO<sub>2</sub> network has been active in considering all of these important areas. In the following three chapters (Chapter 2 to 4) the approaches and results will be described.

## 2. Improvement of statistical data

As described in Chapter 1.6, non-energy use data published in national and international energy balances are very often inconsistent from country to country since they refer to different definitions (system boundaries). The NEU-CO<sub>2</sub> network came to the conclusion that the differences mainly originate from different ways of accounting for backflows and process energy (see below, Box 1). Non-energy use data published in energy balances play an essential part in the calculation of CO<sub>2</sub> emissions in the RA and the SA (Tier 1) and moreover, they provide checks on the estimates from the NEAT model. This raised the question about the possibilities of **improving the data quality by modifying the questionnaires** used for collecting the energy data. Together with IEA and EUROSTAT, which both participate in the NEU-CO<sub>2</sub> network, the joint IEA/EUROSTAT/UNECE annual gas, oil and coal questionnaires were revised with regard to non-energy use (Reece 2000). While it was felt that backflows are already adequately reflected by the current questionnaires, this was not considered to be the case for process energy. This refers exclusively to those processes which cover their energy requirements from a part of the feedstock. A further distinction can be made here between processes where

- a part of the feedstock is oxidised *inside* the chemical reactor, thereby acting as an internal energy source
- low-value process by-products are used to fuel the process, thereby providing the chemical reactor with heat via a heat exchanger.

The NEU-CO<sub>2</sub> network recommends that the first type of fuel/feedstock use should be reported under the heading "*non-energy use*" while the second type should rather be allocated to the (petro-)chemical industry's "*energy use*". The most important processes falling into the first category are ammonia and methanol production; the most important type of process pertaining to the second category is steam cracking (this process yields olefins and aromatics).

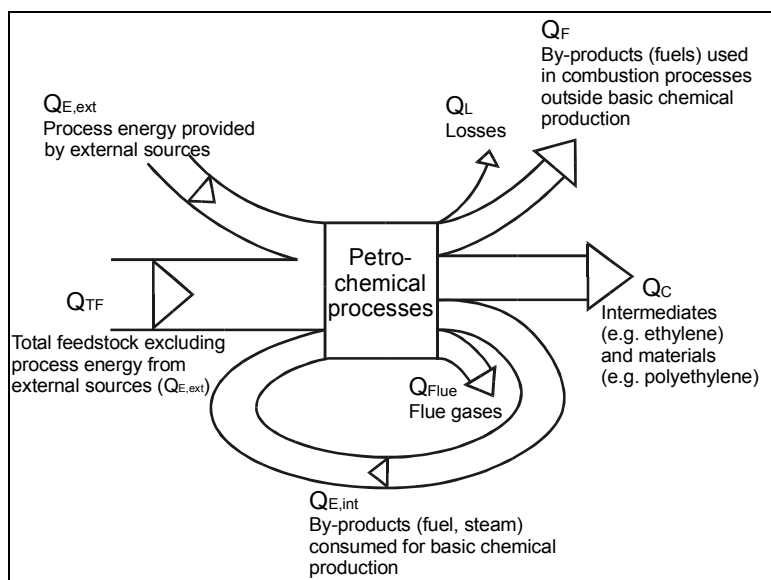
In detail, the latest changes to the IEA/EUROSTAT/UNECE energy questionnaire are given in Appendix 3. Future experience will show whether these changes are sufficient or further improvement will be required. For example, it is possible that different types of backflows need to be distinguished. In the current IEA/EUROSTAT/UNECE energy questionnaire only backflows to refineries are mentioned but it might be necessary to include also backflows to aromatic plants and moreover, those backflows to the motor fuel pool which do not pass through a refinery. There might be even further types of backflows which should also be taken into account.

## Box 1: Definitions used for non-energy use in energy balances

Netherlands (NL):  $Q_{NEU, NL, i} = Q_{TF, i} - Q_{F, i} - Q_{E, int, i}$  (1)

Italy (IT):  $Q_{NEU, IT, i} = Q_{TF, i} - Q_{E, int, i}$  (2)

Germany (FRG):  $Q_{NEU, FRG, i} = Q_{TF, i} - Q_{F, i}$  (3)



### 3. Emission factors for industrial processes

As shown in Table 2, the IPCC Guidelines provide default emission factors for only some of the industrial processes which generate CO<sub>2</sub> emissions. The NEU-CO<sub>2</sub> network has therefore generated preliminary data which are listed in Table 3. Table 3 also shows that the CRF (SBSTA 1999) and EMEP/CORINAIR's Atmospheric Emission Guidebook (EMEP/CORINAIR 1999) provide little information on these important processes. After detailed analysis and discussions with experts in the field, the NEU-CO<sub>2</sub> network will provide revised data for these processes and will recommend their inclusion in the IPCC Guidelines. Moreover, it will be checked whether emission factors for further processes related to the chemical/petrochemical industry should be included.

Table 3: Specific CO<sub>2</sub> emissions factors for industrial processes related to chemical/petrochemical industry

	EMEP/ CORINAIR	IPCC Guidelines	CRF	NEU-CO <sub>2</sub> *)
Ammonia	No methodology prepared	1.5 kg CO <sub>2</sub> /kg ammonia	Mentioned but no data	kg CO <sub>2</sub> / kg ammonia - from natural gas: 1.6 - from oil: 2.4
Olefins (ethylene, propylene)	Data on the contribution to a country's total CO <sub>2</sub> emissions	Not mentioned	Mentioned but no data	kg CO <sub>2</sub> / kg ethylene - from naphtha: 1.3 - from middle distill.: 1.8 - from LPG: 0.9
Methanol	Not mentioned	Not mentioned	Mentioned but CO <sub>2</sub> considered negligible	kg CO <sub>2</sub> / kg methanol - from natural gas: 0.4 - from oil: 1.3 - from soft coal: 2.1
Carbon black	No methodology prepared	Not mentioned	Mentioned but CO <sub>2</sub> considered negligible	kg CO <sub>2</sub> / kg carbon black - from oil: 1.6

\*) Preliminary values

As indicated earlier the CO<sub>2</sub> emissions released during the manufacture of the products listed in Table 3 are considered as process emissions and not as emissions from energy use because heat raising is not the primary purpose of the process. In general, energy statistics cannot provide sufficiently detailed figures of the different uses of oils or gases supplied to the enterprises undertaking the processes shown in Table 3. In the case of the petrochemicals industry, energy balances provide estimates of the feedstock supply but the quantities reported may meet both the non-energy needs and a part of the energy requirements in the industry. Equally, the figures may include or exclude the backflows to the fuel pool (gross vs. net values).

The need for consistent definitions when reporting the energy use of feedstock has already been mentioned above. Regarding emission inventories a common definition should enable to distinguish between emissions from fuel consumption and industrial processes (compare Appendix 3).

## 4. Model approaches

In view of the uncertainty of the statistical data on non-energy use and of the weakness of the methods proposed in the IPCC Guidelines, it was felt that a model was required which would also take into account the differences in the structure of the petrochemical industry in each country. To date, the NEU-CO<sub>2</sub> network developed two models, i.e.

- the **NEAT model** (Gielen et al. 1999) and
- the **Shortcut Method** (Patel 1999b).

Both of these are combined material flow and energy models. They have both been developed as spreadsheet models in Excel. Both models exclusively deal with the consumption of fossil feedstocks in the chemical/petrochemical and refining industries for the manufacture of synthetic organic materials and chemical products (e.g. plastics, fibres, lubricants, bitumen etc.) whereas other sources of non-energy CO<sub>2</sub> emissions, e.g. limestone use are excluded. In the following, further characteristics of the two models including their differences are described and results are presented for the NEAT model.

### 4.1 The NEAT model

#### 4.1.1 *Model philosophy*

With NEAT ("Non-Energy use Emission Accounting Tables", Gielen et al., 1999), a spreadsheet model of the carbon flow through the many petrochemical processes and non-energy refinery products has been developed. The underlying philosophy is:

- A material flow analysis for a specific year at a more detailed level (covering fossil energy carriers and synthetic organic materials) provides a better basis for estimation of GHG emissions in relation of petrochemical products, because the mass balance principle can be applied, which increases the accuracy.
- The basis of the spreadsheet is a systems analysis approach, where the industry is divided into processes (black boxes with a fixed relation between carbon process inputs and carbon process outputs).
- A carbon mass balance is applied. For each process and each flow, the total input must equal the total output. Storage within the industry is neglected. Carbon losses within the industry are neglected.
- A fixed relation exists between the chemical structure of a product, its carbon content and its CO<sub>2</sub> factor. The same applies to a large extent to the relation

between the flows of energy carriers, expressed in energy units, and CO<sub>2</sub> equivalents.

- The data from energy statistics (in PJ) must be linked to the mass flow statistics for the petrochemical industry (in Mt petrochemical product). For this purpose, all flows are translated into CO<sub>2</sub> equivalents. The translation in CO<sub>2</sub> equivalents allows a more easy interpretation of results for GHG policy purposes. It enables the generation of process carbon balances (contrary to mass flows) and it is a better measure of the relevance of flows for the GHG problem than carbon flows.
- The goal is to develop an easy-to-handle spreadsheet model which can be applied by national institutes which must calculate national GHG emissions according to IPCC Guidelines. The model should not require in-depth expert knowledge regarding the petrochemical industry. Running the model should not take more than half a day. The model results should be acceptable to petrochemical experts from industry and science.
- The spreadsheet input data consist of data regarding physical flows (production, consumption, and international trade). These flows are derived from publicly accessible sources.
- The model uses national averages. Data for specific industrial producers may differ. As a consequence, the method can only serve as a proxy regarding the emissions of specific producers within a country. However, the weighted total for all producers must represent the national average.

#### 4.1.2 *Scope of the model*

NEAT is a spreadsheet tool developed to enable a quick estimation of carbon emissions and carbon storage related to non-energy use.

In more detail, it provides estimates for carbon storage in long-lived materials (e.g. plastics and rubber) and short-lived materials (e.g. solvents) and it generates estimates of CO<sub>2</sub> emissions from industrial processes related to chemical/petrochemical industry<sup>4</sup> and from the fuel use of steam crackers. Carbon storage in long-lived and short-lived materials is determined taking an *upstream perspective* or, alternatively, a *downstream perspective* (see Figure 2). In the upstream perspective, the carbon flow is measured at level  $\alpha$  (this is also referred to as the "production

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<sup>4</sup> The NEU-CO<sub>2</sub> network deals with all CO<sub>2</sub> emissions from industrial processes which originate from fossil carbon feedstock and which imply manufacturing. The main processes belonging to this category are those to produce ammonia, methanol and carbon black (compare Table 3). Carbide production is a less important representative (Table 2). Processes leading to CO<sub>2</sub> of mineral origin, e.g. soda ash production and use, lime production and limestone use are not covered by the NEU-CO<sub>2</sub> network. Finally, products which release their embodied fossil carbon in the use phase, e.g. solvents and surfactants, are covered by NEU-CO<sub>2</sub> network by the category "short-lived materials/products".

approach"). In the downstream perspective, the carbon flow is measured at level  $\gamma_2$  (also referred to as the consumption approach").

Carbon storage according to the *downstream* perspective represents the amount of carbon inherent in the *materials* delivered to the domestic market (consumed) by a country (see Table 4); in contrast, carbon storage according to the *upstream* perspective represents the share of carbon *feedstocks* which is fixed in materials by subsequent chemical/petrochemical processes (Table 4). The NEAT model uses production and trade data of chemicals and products to infer the carbon flows both for the upstream and downstream perspective. Hence, the results generated by NEAT do not rely on feedstock data as published in energy balances, i.e. they represent **independent estimates**.

The difference between the *upstream perspective* and the *downstream perspective* for carbon storage originates mainly from the foreign trade of intermediates and materials ( $IM^C$ ,  $EX^C$ ,  $IM^D$ ,  $EX^D$ ); for example, for a country with large net imports of materials and intermediates, the downstream carbon storage (level  $\gamma_2$ ) is larger than upstream carbon storage (level  $\alpha$ ).

Table 4: Perspectives taken in the NEAT model to estimate carbon storage

	Carbon storage refers to carbon fixed in...	Level at which the carbon flow is measured
<b>Downstream</b> perspective	... <b>materials</b> , e.g. polymers and solvents for end users	$\gamma_2$ (compare Figure 2)
<b>Upstream</b> perspective	... <b>feedstocks</b> which will eventually be converted to materials (e.g. e.g. polymers and solvents for end users)	$\alpha_2$ (compare Figure 2)

The feedstock flow across  $\alpha$  into the upstream petrochemical processes is, for most countries, conceptually identical to that used within energy balances for the supply of feedstock to the petrochemical sector. The *upstream perspective* therefore provides a basis for the carbon storage factor applied to the feedstock supply within the RA and SA (Tier 1). It would be the fraction of feedstock carbon which is not oxidised in the processing of the incoming fossil fuel feedstock and activities supporting the processing.

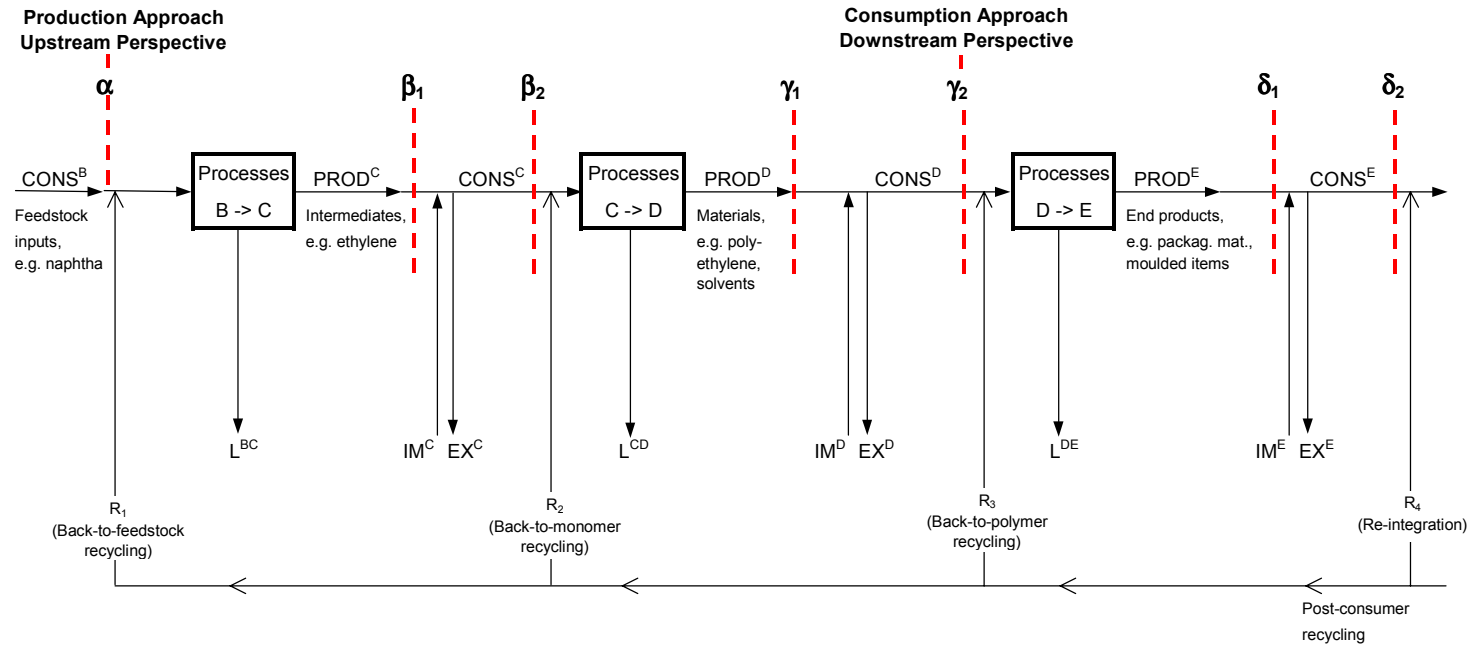
In contrast, carbon storage according to the *downstream* perspective is more in line with some of the detailed calculation methods applied within the SA (Tier 2, Tier 3) for CO<sub>2</sub> emissions outside the energy combustion sector, e.g. when determining the

CO<sub>2</sub> emissions related to the oxidation of short-lived materials (e.g. solvents, surfactants) within the boundaries of a country.

This indicates that, depending on the **purpose of use** of the NEAT results within the IPCC's reporting framework, either the upstream or the downstream perspective is the appropriate choice. This issue will be dealt with in more detail in Chapter 4.1.5.

As described in Chapter 2, the inconsistencies in non-energy use data published in national and international energy balances mainly originate from different ways of accounting for backflows and process energy. NEAT provides estimates for non-energy use according to different definitions (see below, Chapter 4.1.4). By comparison with the values published in statistics a conclusion can be drawn which of the definitions might have been used in energy balances. Moreover, the comparison of this quantity with other sources can act as a consistency check for the NEAT model (see below).

Figure 2: A country's carbon flows connected with the production of synthetic organic materials



Carbon flows (in kt of CO<sub>2</sub> equivalents):

- CONSB<sup>i</sup> = domestic consumption of commodity i
- PRODC<sup>i</sup> = total production of commodity i
- IM<sup>i</sup> = imports of commodity i
- EX<sup>i</sup> = exports of commodity i
- L<sup>j</sup> = losses & leakages from processes j

Indices:

- i = commodity, e.g. i = B = feedstock inputs, i = C = intermediates, i = D = materials and intermediates, i = E = final products
- j = group of processes, e.g. j = BC for the conversion of feedstock inputs B to basic chemicals C

#### 4.1.3 *Model structure, data requirements and principles of validation*

In its current version, the NEAT model consists of **11 sheets**: The first sheet contains all the input data, while the second to fourth sheet presents the results in tables and in graphs. In sheet No. 5, the user of the NEAT model is asked to provide country-specific information on system boundaries and definitions. Sheet No. 6 and No. 7 provide an overview of different definitions of non-energy use and of carbon storage which are currently in use. Finally, sheet No. 8 to 11 provide model-endogenic data and interim results, i.e. material balances for steam crackers, materials balances for all intermediates and a list of conversion factors.

In sheet No. 1, the **input data** are divided into 3 categories. In the first part, production, import and export data are collected for basic chemicals, intermediates and materials, totalling about 75 products. In the second part, the model is fed with non-energy use data according to the national energy balance. Finally, in the third part, the feedstock consumption for the most important petrochemical processes - i.e. steam cracking and the production of ammonia, methanol and carbon black - are entered. Important model-endogenic data are the chemical composition of petrochemical products and various CO<sub>2</sub> emission factors which are used to calculate the yearly CO<sub>2</sub> equivalents in absolute terms.

In order to generate a complete overview of the carbon balance of the petrochemical industry, two types of **materials balances** must be applied:

- a production/consumption balance for individual products in the petrochemical complex
- input/output balances of individual production processes.

Fortunately a limited number of conversion routes are the basis of the petrochemical industry. The conversion efficiencies of these processes are generally similar all over the world for cost-efficiency reasons and for environmental reasons.

The balance of individual products is important because many petrochemical products are used by the industry as intermediates for the production of other petrochemicals. The whole network of petrochemical processes must be considered for proper balancing. The best approach is to eliminate any residual use of petrochemicals in the balance, thereby minimizing the modelling uncertainties related to the fate of these products. Where such residual applications remain, an expert estimate is required.

A balance has been developed for the following intermediates:

- acetic acid
- acetone
- acrylic acid
- acrylonitrile
- adipic acid
- aniline

- benzene
- bisphenol A
- butadiene
- butenes/butane (C4 fraction)
- caprolactam
- creosote oil
- cumene
- cyclohexane
- cyclohexanone/cyclohexanol
- dimethylterephthalate
- ethyl benzene
- ethylene
- ethylene dichloride
- ethylene glycol
- ethylene oxide
- formaldehyde
- methanol
- phenol
- phthalic anhydride
- propylene
- propylene oxide
- styrene
- terephthalic acid
- toluene
- toluene diisocyanate (TDI)
- vinylchloride monomer
- mixed xylenes
- ortho xylene
- para xylene

Moreover, a mass balance has been developed for the petrochemical steamcrackers. These crackers constitute the most important primary step in the petrochemical production complex. Because the product mix depends on the feedstock type, different cracker types with differing feedstocks are separately analysed and subsequently aggregated.

The data regarding petrochemical production routes and the selection of important applications of intermediates have been based on (Weissermel, Arpe, 1998). This source suggests that a limited number of production routes are applied for a given product. This allows the generation of materials balances for processes (input-output relations from process data) and materials balances for products:

Production = Consumption + Exports - Imports

Storage and losses between production and consumption have been neglected in the analysis.

The *downstream perspective* (see Chapter 4.1.2) is more in line with the basic principle that emissions should be accounted for where they really occur. However, the *upstream perspective* is slightly easier to follow from an emission accounting point of view, because no trade data for materials ( $IM^D$ ,  $EX^D$ ) are required. Both perspectives have been elaborated in the model since they are both relevant and since it is worthwhile to study the difference between the two perspectives.

In order to check the **validity** of the model, a number of quality checks have been applied:

- check of the materials balance of the physical inputs and outputs of the industry
- application to individual countries and comparison and analysis of the resulting differences
- comparison to the estimates for carbon storage from other bottom-up studies
- check of the carbon storage with estimates for the increasing product stock and waste volumes disposed and net carbon exports in products
- interviews with industry experts and environmental scientists whether the correct relations are represented.

The first step for validation is the mass balance for carbon: the total input (of fossil fuels, in carbon equivalents) should equal the total output (of plastics etc., in carbon equivalents) plus the losses during production. The input and output values should correspond with the values from energy statistics and industrial production statistics.

#### 4.1.4 Results

The NEAT model was applied to several countries and showed that specific trade and production aspects can have a strong impact on the results (Park, 2000). This proves that a country-specific procedure should be taken and that it is unsound to use default factors for carbon storage without considering their appropriateness.

The results generated are still preliminary since there are still data gaps for various countries and there are also methodological uncertainties which will need to be addressed in the future (see Chapter 5). Nevertheless it seems justified to present and discuss the general results since these are not expected to change in the future course of model development. The preliminary main results for Germany, Italy, Japan, South Korea, United Kingdom and the U.S. are the following (based on La Motta, 2000; Gielen, 2000; Park, 2000; Patel, 2000):

- The NEAT results for the **total carbon storage in short-lived and long-lived materials are higher than the results according to the RA** in nearly all cases (see Figure 3).
- The NEAT results for carbon storage in long-lived materials are mostly smaller than the total carbon storage according to the RA.

- The NEAT results for **carbon release comprising**
  - the CO<sub>2</sub> equivalents of backflows of steam crackers to the fuel pool<sup>5</sup>,
  - the fuel use of steam crackers and
  - the industrial processes (production of ammonia, methanol and carbon black)**are mostly smaller than - or at the most equal to - the respective results according to the RA** (see Figure 4; exception: U.S.).
- The NEAT results for **carbon release comprising**
  - carbon storage in short-lived products
  - the CO<sub>2</sub> equivalents of backflows of steam crackers to the fuel pool<sup>6</sup>,
  - the fuel use of steam crackers and
  - the industrial processes (production of ammonia, methanol and carbon black)**is mostly larger than the respective results according to the RA.**

As mentioned in Chapter 4.1.2 carbon storage according to the *upstream* perspective is the relevant entity for the RA. In contrast, the data in Figure 3 giving the results for carbon storage according to the *downstream* perspective is not meant for use in the preparation of inventories. These *downstream* results are mainly of academic interest also because *carbon storage* is not explicitly determined in the detailed versions of the SA (Tier 2 and 3). To summarize, the *downstream perspective* is displayed to show the influence of foreign trade in intermediates (this determines the difference between the *upstream* and the *downstream perspective*).

The NEAT results for carbon storage are more reliable than those for carbon release. This is firstly due to the assumption in NEAT that steam crackers are operated in such a way that they are self-sufficient in energy terms; this is not always the case. Secondly it is assumed in NEAT that all backflows from steam crackers to the fuel pool are finally oxidised and therefore contribute to CO<sub>2</sub> emissions by combustion in other sectors. This assumption is irrelevant for those countries where these backflows have been netted off in energy balance data.

The results from the NEAT model are subject to **further uncertainties** firstly due to unclear and incomplete data and secondly, due to methodological uncertainties and limits (Patel, 2000). Data problems often originate from

- missing data or imprecise data , e.g. for solvents and other products
- unclear system boundaries of data, e.g. for MTBE, methanol and BTX

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<sup>5</sup> The CO<sub>2</sub> equivalents of these backflows should not be seen as emissions released by the petrochemical industry but by the sectors which use them as a fuel. Since it is unclear whether these emissions are really accounted for by the respective sectors, they have been included in the NEAT model.

<sup>6</sup> See previous footnote.

- feedstock and process alternatives, e.g. for PET which can be produced from both DMT and TPA.

For some countries, it is particularly difficult to provide the required data, e.g. for France, India and Russia (Sharma and Pachauri, 1999; Gritsevitch and Mikhailover, 2000).

The most important methodological difficulties originate from the simplification of the material flows and their interlinkages.

The possibilities for testing the accuracy of the NEAT model are very limited. Some insight can be gained by comparing the total non-energy use of fossil fuels as determined by NEAT with selected statistical data on non-energy use for which some details about the system boundaries are known. These comparisons are very encouraging since they indicate a **good coverage** of the NEAT model (Patel, 2000). For example, for Italy, the NEAT model results for non-energy use following the definition  $Q_{\text{NEU,NEAT}} = Q_{\text{TF}}$  is very close to the statistical data according to CEFIC (CEFIC, 1999) which follow the same definition (see Figure 5). Moreover, the statistical data according to the Bilancio Energetico are closest to the NEAT model result for the definition  $Q_{\text{NEU,NEAT}} = Q_{\text{TF}} - Q_{\text{E,int}}$  which confirms earlier analysis about the definition of non-energy use in Italian energy balances (Patel et al., 1999). Finally the NEAT calculations for Italy confirm that the EUROSTAT data have undergone some correction.

In spite of this good accordance further work will have to be done on the NEAT model to reduce the uncertainties listed earlier as far as possible and to test the model for further countries.

Figure 3 (Part 1): Carbon storage – Comparison of preliminary NEAT results with results generated by use of IPCC default factors

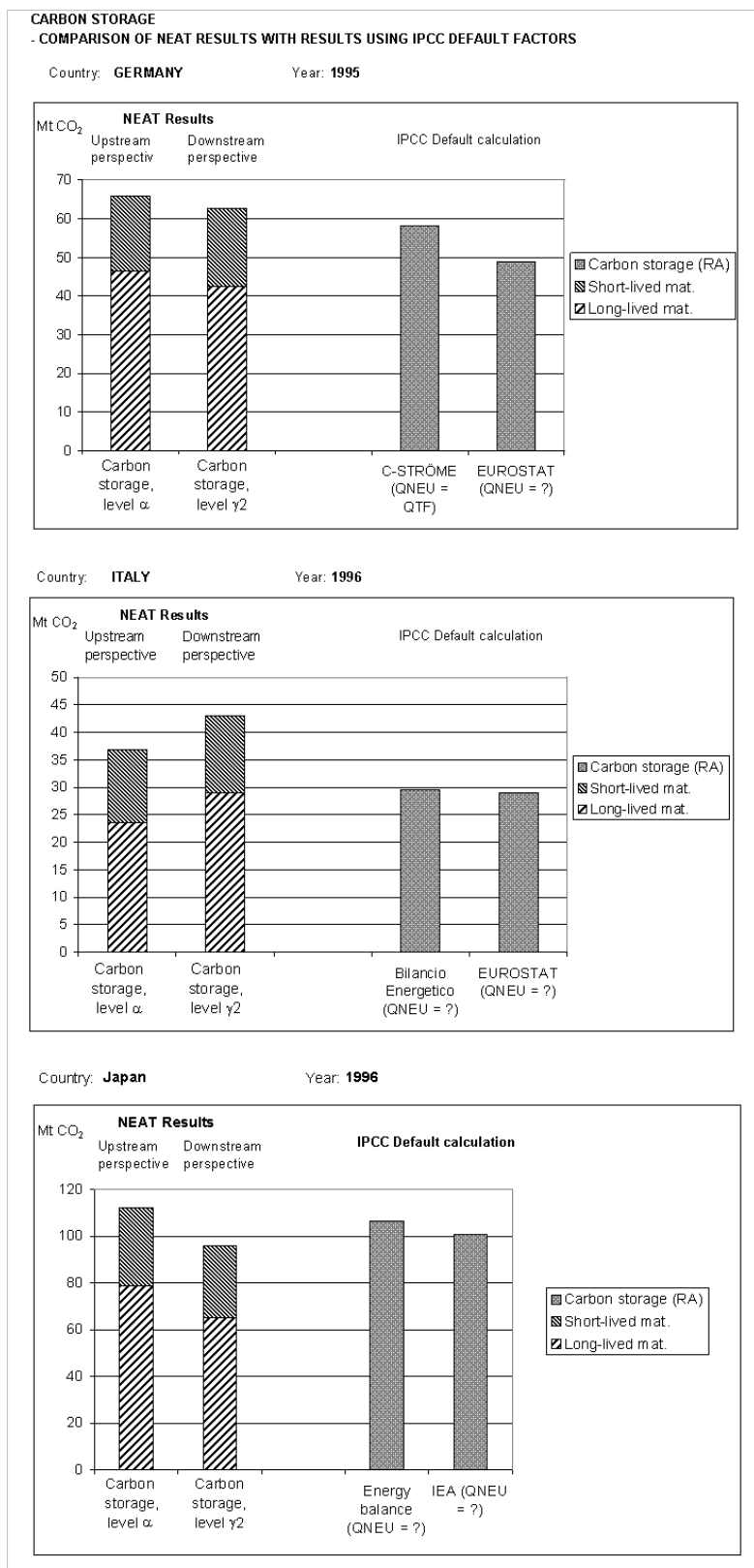


Figure 3 (Part 2): Carbon storage – Comparison of preliminary NEAT results with results generated by use of IPCC default factors

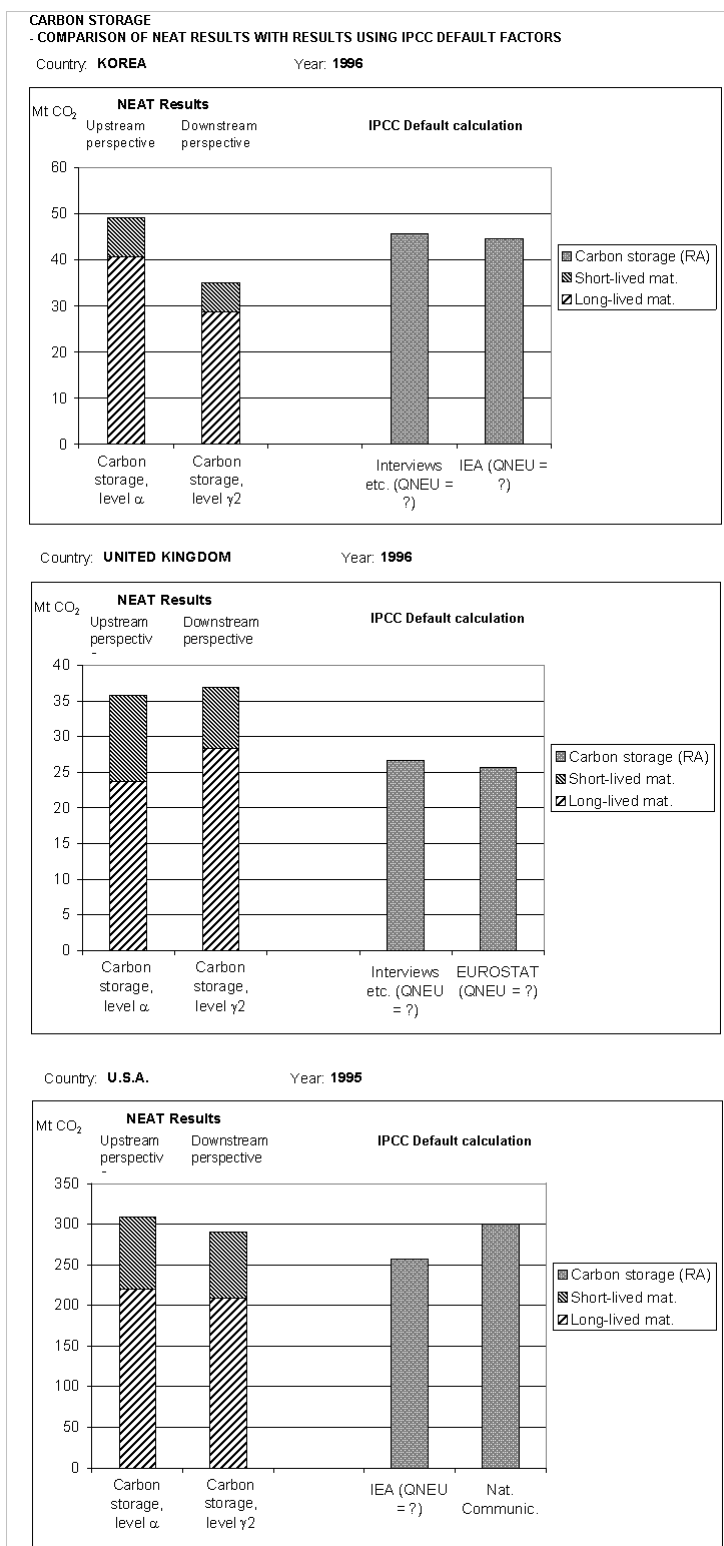


Figure 4 (Part 1): Carbon release – Comparison of preliminary NEAT results with results generated by use of IPCC default factors

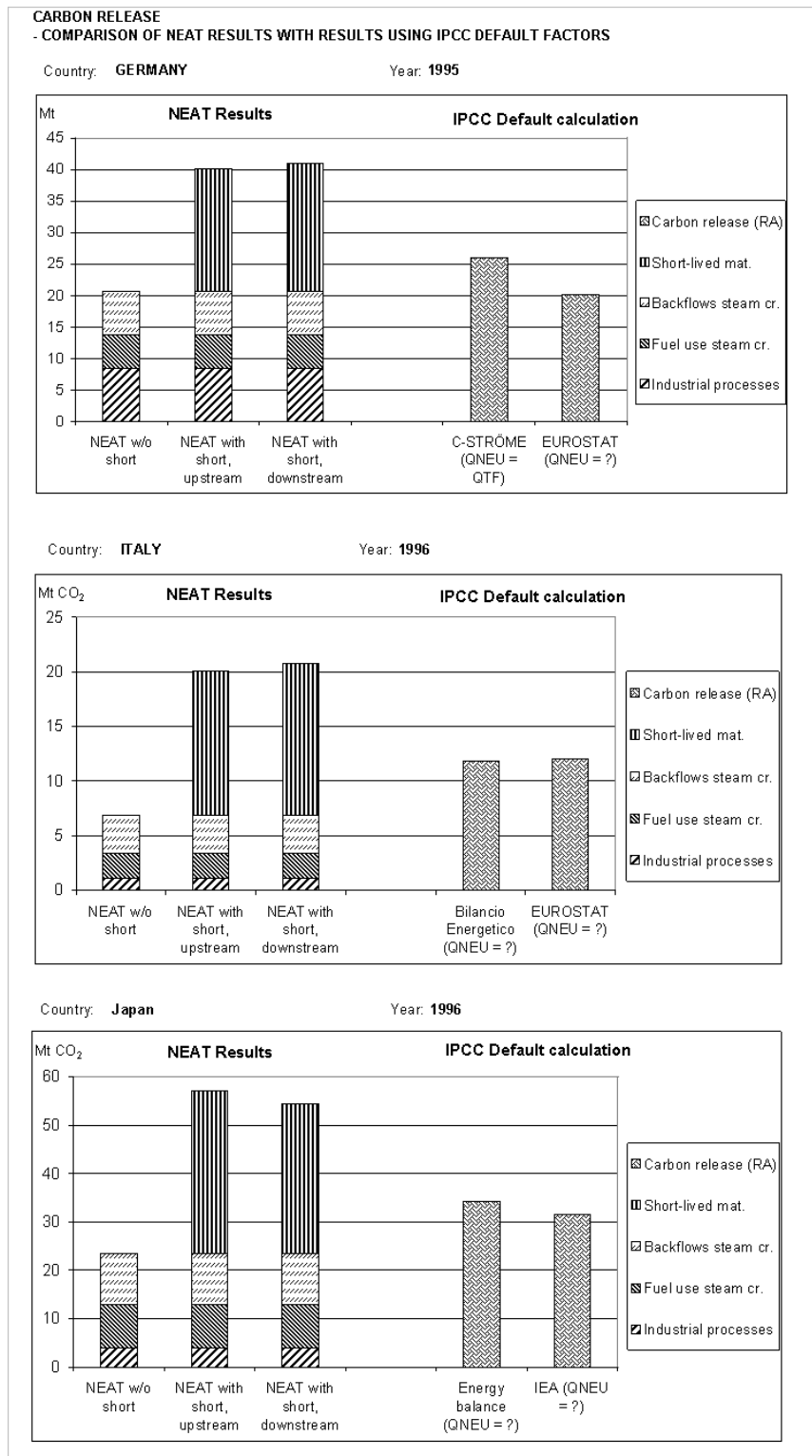


Figure 4 (Part 2): Carbon release – Comparison of preliminary NEAT results with results generated by use of IPCC default factors

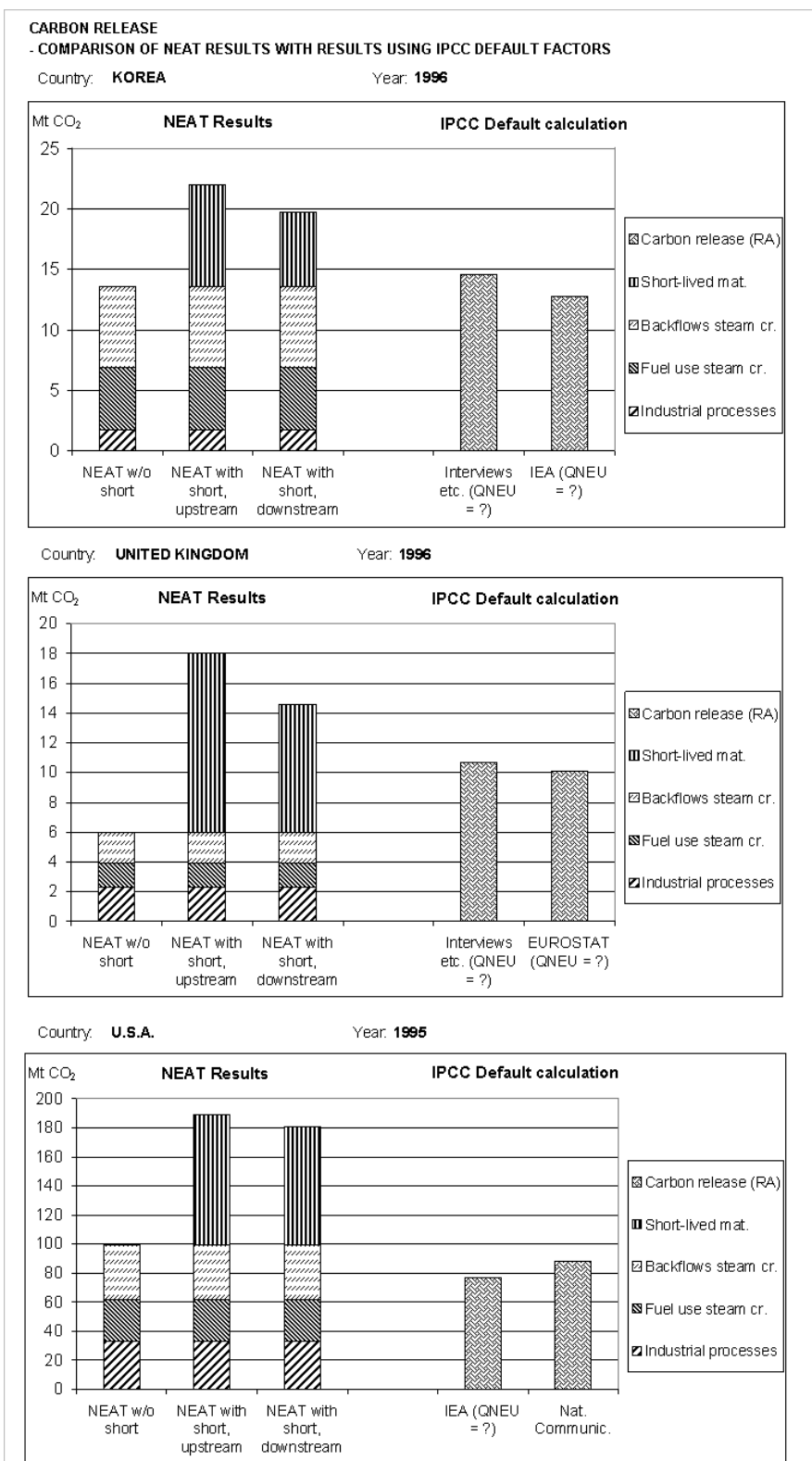
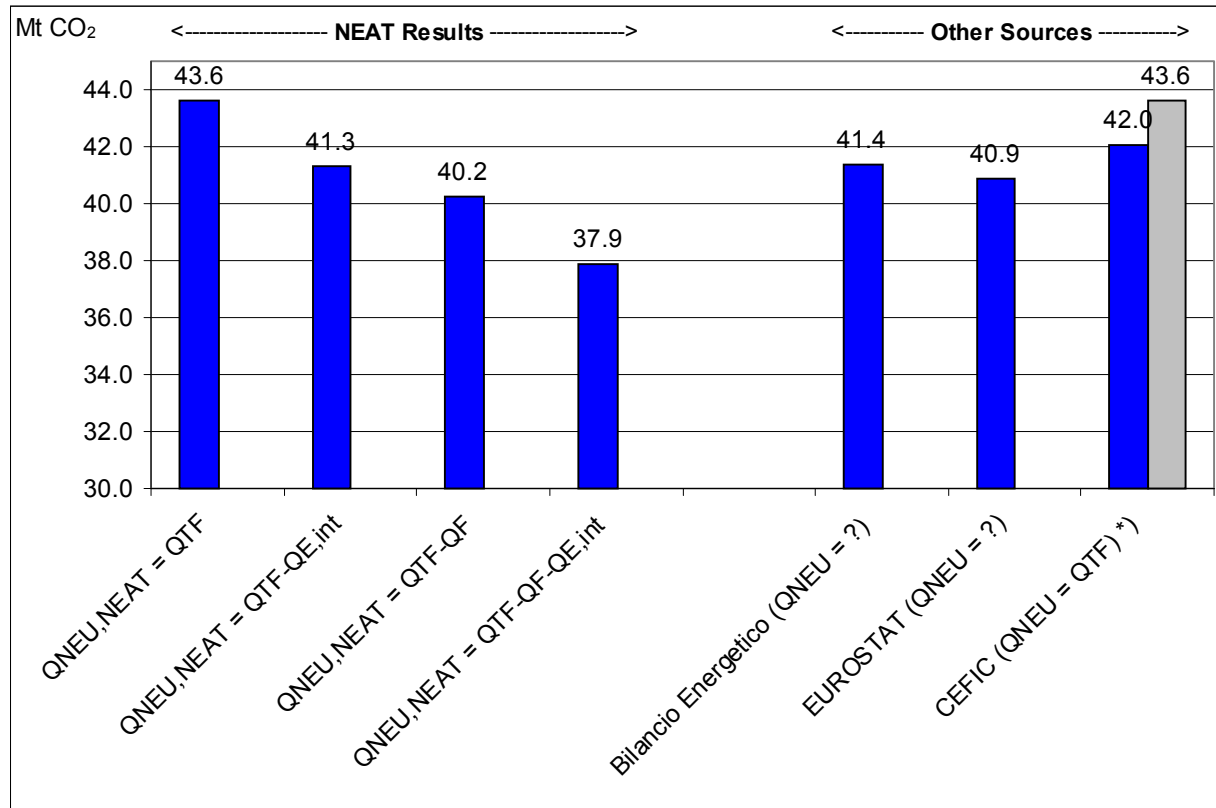


Figure 5: Italy, 1996 – Comparison of preliminary NEAT results for non-energy use with statistical sources



#### 4.1.5 Use of NEAT results within the reporting framework

Both the NEAT results taking an upstream perspective and those following the downstream perspective are meaningful entities. As Table 5 shows their relevance depends on the context of use. Further investigations on the feasibility of conducting calculations with NEAT, the concomitant uncertainties and alternative estimation methods will finally enable pragmatic choices among the options given in Table 5. The decision process is complicated due to the fact that a variety of methods is being applied both within the RA and the SA (see above, Sections 1.6 and 1.7). Once the decisions are made the methods will have to be developed in detail (e.g. derivation of storage factors by type of fuel for case 1b in Table 5).

Table 5: Possibilities to use the NEAT model results

	NEAT result	Purpose of use	Procedure
1.	Total carbon storage in short-lived and long-lived materials, taking an <b>upstream</b> perspective*)	a) Determine the country's total CO <sub>2</sub> emissions from fuel combustion according to the RA b) Generate corrected country specific carbon storage factors for further use in the RA	Subtract the NEAT result from the country's total apparent consumption of fossil fuels  Divide NEAT result for carbon storage by total feedstock input to the chemical/petrochem. industry according to energy balances
2.	Carbon release comprising: - Carbon storage in short-lived products, taking a <b>downstream</b> perspective - CO <sub>2</sub> equivalents of backflows of steam crackers - Fuel use of steam crackers - Industrial processes	a) Check or replace respective results of the SA b) Generate country-specific factors for further use	Comparison of NEAT results with SA  Divide NEAT result of choice by appropriate reference quantity

\*) The use of the respective NEAT result taking a downstream perspective is prohibited for this purpose.

## 4.2 The Shortcut Method

### 4.2.1 Scope of the model

The purpose of the Shortcut Method is to divide the total amount of carbon input into a two parts - one which ends up in short-lived materials and another which is fixed in long-lived products. The Shortcut Method can be adopted to provide carbon storage factors for the RA.

Compared to the NEAT model, the Shortcut Method is a rather simple model requiring a relatively small amount of data (unfortunately, this does not mean that all the data required are readily available). Another characteristic of the Shortcut Method is that it exclusively takes an upstream perspective (compare Figure 2). This is a loss of information compared to the NEAT model which also takes a downstream perspective. However, the difference between the two approaches is small for countries with a small net foreign trade. In contrast to NEAT, the Shortcut Method relies on statistical data for non-energy use; hence, a good understanding of the underlying system boundaries is required to use these data in an appropriate manner. This is a clear shortcoming compared to NEAT which provides independent estimates. Moreover, as a consequence of the new CRF (SBSTA, 1999), the distinction between short-lived and long-lived has become irrelevant for the RA.

Due to these shortcomings of the Shortcut Method, the NEU-CO<sub>2</sub> network is putting most efforts into the development of the NEAT model. For this reason, only a short explanation of the structure of the tool and the data requirements is given in the next section. For further details and for the results, the reader is referred to Patel (1999b).

#### 4.2.2 *Structure of the tool and data requirements*

The Shortcut Method starts from the most important (petro-)chemical processes. These are:

- steam cracking of naphtha, gas oil and LPG,
- methanol production from natural gas and fuel oil,
- ammonia production from natural gas and fuel oil,
- the production of carbon black,
- processing of tar,
- processing of coal-derived benzene and
- other products, which comprise
  - petroleum coke,
  - lubricants,
  - bitumen,
  - paraffins/waxes,
  - other products from natural gas and
  - other products from other feedstocks.

Some of the processes listed only have one type of output (e.g. methanol production from natural gas) whereas others result in a whole array of outputs; for example, steam cracking yields ethylene, propylene and other olefins, various aromatics, hydrogen, methane and fuel oil. The main idea of the Shortcut Method is to weight these outputs of intermediates with the share which is stored in materials for longer

periods. The carbon storage factors required for this purpose differ depending on the use pattern of intermediates. Based on the information which is available for various countries and regions, ranges can be established for the share of intermediates which can be assigned to long-lived materials. By combining these data with the outputs of the processes listed above, the total amount of carbon fixed in long-lived and short-lived materials is determined.

## 5. Conclusions of the network and outlook

One of the main conclusions of the NEU-CO<sub>2</sub> network is that **use of the default carbon storage factors in the RA or the Tier 1 SA method for CO<sub>2</sub> emissions is not advised without careful consideration** of their relevance for the country. The NEAT model has shown that carbon storage varies considerably between countries. It has been concluded from this that the **statistical data on non-energy use must be clearly improved**. Secondly, **default factors for process emissions** from the production of ammonia, olefins, methanol and carbon black **should be generated** and should be recommended to the IPCC as a valuable extension of the SA.

In both points, good progress has already been made. It remains to be seen how the quality of non-energy use data collected with the **revised IEA/EUROSTAT/UNECE questionnaire** develops. Further work also be necessary to generate **consolidated default emission factors** for the processes mentioned above; the preliminary values given in Table 3 represent a good starting point.

With NEAT, a combined material flow and energy model has been developed which offers an improved insight into the complex matter of producing and using synthetic organic materials. The results generated to date are promising, indicating a good quality of the estimates. Nevertheless, further work is required to **reduce uncertainties** related to the data and the calculation method. With regard to **data**, the next steps are to

- close the data gaps and improve the data quality by interacting with experts in the field, especially with industry experts<sup>7</sup>
- to apply the model to further countries in order to further improve its accuracy and
- to ensure the applicability for countries where less data are available due to less developed survey systems or severe confidentiality rules.

Urgent **methodological** issues are

- to ensure the compliance of the NEAT model with CO<sub>2</sub> accounting from waste management (Kilde, 2000)
- to refine the method used in NEAT for distinguishing between short-lived and long-lived materials (especially for the upstream perspective)

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<sup>7</sup> Issues of high priority are for example the supply of improved data on

- the fraction of short-lived versus long-lived materials produced from the various chemicals and on
- material balances of the various basic chemicals used to produce intermediates and subsequent products.

- to decide upon how to use the NEAT model results within the reporting framework, followed by further development in the selected areas (see Chapter 4.1.5).

Moreover, an appropriate **documentation** of the NEAT model will be required, thereby using a clear and generally accepted terminology (Simmons, 2000).

Further issues which deserve attention in the future and are also related to NEAT are

- the estimation of carbon **losses due to incomplete conversion** in the chemical/petrochemical industry (Windsperger 1999),
- an in-depth analysis of CO<sub>2</sub> **emissions from solvents and other short-lived materials** which might best be done in close co-operation with associations and consultants and
- the extension of the NEAT model by **non-energy processes outside the chemical/petrochemical sector**, e.g. limestone production and electrode use in steel/aluminium production.

With regard to the reporting framework, the NEU-CO<sub>2</sub> network recommends to

- rephrase the **IPCC Guidelines** (IPCC/IEA/OECD/UNEP 1997) in some parts which refer to non-energy use and product-related carbon storage (and carbon release) in order to avoid inconsistencies (see Box 2).
- **improve the terminology chosen in the CRF**, thereby making it easier to comprehend (see Box 2).

The NEU-CO<sub>2</sub> network could contribute to the realisation of the suggested improvements.

Finally, the data collected and the enhanced understanding gained by the NEU-CO<sub>2</sub> network prepares the grounds for **wider modelling activities** related to synthetic organic materials, e.g. dealing with

- the **potential of CO<sub>2</sub> mitigation** by increased recycling of synthetic organic materials and the increased use of biomass as a feedstock (both simulation and optimisation tools could be applied for this purpose)
- detailed material flow models analysing the **dynamics of material accumulation and release** in the economy (Windsperger 1999; Windsperger 2000).

Box 2: Examples for inconsistencies and lack of clarity concerning non-energy use in the current reporting framework

- The IPCC Guidelines (IPCC/IEA/OECD/UNEP 1997) make very clear that they refer to "carbon storage" as carbon fixation in materials/products for longer periods of time (Vol.2, p.1.3; Vol. 3, p. 1.9, p. 1.26). By "long" the authors mean a time span in the range of decades or more (Vol. 2, p.1.9: "sometimes as long as centuries"; Vol. 2, p.1.25: "e.g., greater than 20 years"). However, on the other hand, by using these carbon storage figures in the RA (and SA, Tier 1) – i.e. by deducting carbon storage from a country's apparent fuel consumption - we determine the emissions from fuel combustion plus emissions that may occur in industrial processes, in the use phase of products or in waste disposal (compare Vol.3, p.1.27). Since the RA is referred to as a "simple method for fuel combustion" (Vol.3, p.1.7) this means that "fuel combustion" in this context comprises not only the incineration of fuels for heat raising but also the source categories just mentioned. This may easily lead to confusion or misunderstandings, also because the latter source categories are *not* included in the category "fuel combustion activities (1A)" in the Common Reporting Format (Vol.1, p.1.3).
- As mentioned above the IPCC Guidelines (IPCC/IEA/OECD/UNEP 1997) refer to carbon storage as carbon fixation for a time span in the range of decades. In contrast, the new IPCC Good Practice Report (IPCC, 2000) considers "long life waste" to originate from "products manufactured before the inventory year" which means that here, the threshold between "short" and "long" is in the range of just one year.
- It remains unclear in the IPCC Guidelines whether carbon storage refers to the quality of materials/chemicals or to the type of *end* product. In the first case, for example, *all* plastics would be allocated to "carbon storage". In the second case, only plastics used for long-lived products (e.g. pipes in buildings) would be allocated to "carbon storage" whereas, e.g., plastics used for packaging would be excluded if this packaging is incinerated after use. In most cases, the examples given in the IPCC Guidelines seem to indicate that a choice has been made for the first option (Vol. 2, p.1.3; Vol. 3, p.1.9; Vol. 3, p.1.32); but, at least in one case (Vol. 3, p.1.27, last section), it seems that the second option is supported (i.e. the allocation depends here on the type of end product and the waste management option).
- In Box 2 of Volume 3 of the IPCC Guidelines (p.1.26) the concept of potential and actual emissions of CO<sub>2</sub> is introduced. Potential emissions are defined here as carbon that is stored in products for a longer period of time while actual emissions is carbon that is oxidised immediately or within a short period of time. In contrast, the term "Actual CO<sub>2</sub> emissions" is used in Worksheet 1-1 and 1-2 (Vol.2, p.1.33-1.53) and also in Table 1.A(b) of the new Common Reporting Format (CRF; SBSTA 1999) to address CO<sub>2</sub> emissions from fuel combustion. It might be helpful to rename the categories in order to avoid misunderstandings.
- The issue of trade of non-energy products is addressed in paragraph (d) of the Overview Chapter of Vol.3 (page "Overview.5) but it seems necessary to expand the explanations here or in other parts of the IPCC Guidelines in order to avoid misunderstandings.

Note: This list is not complete. Not all the relevant quotations might be given.

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## **Appendix 1: Definition of fuels used for non-energy purposes**

This list originates from the IEA/EUROSTAT questionnaire.

### **1. Hard Coal**

Hard coal is made up of coking coal and other bituminous coal.

Coking coal refers to coal with a quality that allows the production of a coke suitable to support a blast furnace charge. Its gross calorific value is greater than 23 865 kJ/kg (5 700 kcal/kg) on an ash-free but moist basis.

Other bituminous coal is used for steam raising and space heating purposes and includes all anthracite coals and bituminous coals not included under coking coal. Its gross calorific value is greater than 23 865 kJ/kg (5 700 kcal/kg), but usually lower than that of coking coal.

### **2. Brown Coal**

Brown coal is made up of sub-bituminous coal and lignite.

Sub-bituminous coals are non-agglomerating coals with a gross calorific value between 17 435 kJ/kg (4 165 kcal/kg) and 23 865 kJ/kg (5 700 kcal/kg) containing more than 31 per cent volatile matter on a dry mineral matter free basis.

Lignite is a non-agglomerating coal with a gross calorific value of less than 17 435 kJ/kg (4 165 kcal/kg), and greater than 31 per cent volatile matter on a dry mineral matter free basis.

### **3. Peat**

Combustible soft, porous or compressed, fossil sedimentary deposit of plant origin with high water content (up to 90 per cent in the raw state), easily cut, of light to dark brown colour.

### **4. Coke Oven Coke**

Coke oven coke is the solid product obtained from the carbonisation of coal, principally coking coal, at high temperature. It is low in moisture content and volatile matter. Also included are semi-coke, a solid product obtained from the carbonisation of coal at a low temperature, lignite coke and semi-coke made from lignite.

### **5. Gas Coke**

Gas coke is a by-product of hard coal used for the production of town gas in gas works. Gas coke is used for heating purposes. The composition is very like Coke Oven Coke.

## **6. Patent Fuel**

Patent fuel is a composition fuel manufactured from coal fines with the addition of a binding agent (pitch). The amount of patent fuel produced is, therefore, slightly higher than the actual amount of coal consumed in the transformation process.

## **7. Brown Coal/Peat Briquettes (BKB)**

BKB are composition fuels manufactured from brown coal, produced by briquetting under high pressure. These figures include peat briquettes, dried lignite fines and dust, and brown coal breeze.

## **8. Crude Oil**

Crude oil is a mineral oil consisting of a mixture of hydrocarbons of natural origin, being yellow to black in colour, of variable density and viscosity. It also includes lease condensate (separator liquids) which are recovered from gaseous hydrocarbons in lease separation facilities.

## **9. Natural Gas Liquids (NGL)**

NGLs are the liquid or liquefied hydrocarbons produced in the manufacture, purification and stabilisation of natural gas. These are those portions of natural gas which are recovered as liquids in separators, field facilities, or gas processing plants. NGLs include but are not limited to ethane, propane, butane, pentane, natural gasoline and condensate. They may also include small quantities of non-hydrocarbons.

## **10. Refinery Gas**

Refinery gas is defined as non-condensable gas obtained during distillation of crude oil or treatment of oil products (e.g. cracking) in refineries. It consists mainly of hydrogen, methane, ethane and olefins. It also includes gases which are returned from the petrochemical industry. Refinery gas production refers to gross production.

## **11. Liquefied Petroleum Gases (LPG)**

These are the light hydrocarbons fraction of the paraffin series, derived from refinery processes, crude oil stabilisation plants and natural gas processing plants comprising propane ( $C_3H_8$ ) and butane ( $C_4H_{10}$ ) or a combination of the two. They are normally liquefied under pressure for transportation and storage.

## **12. Ethane**

Ethane is a naturally gaseous straight-chain hydrocarbon ( $C_2H_6$ ). It is a colourless paraffinic gas which is extracted from natural gas and refinery gas streams.

**13. Motor Gasoline**

This is light hydrocarbon oil for use in internal combustion engines such as motor vehicles, excluding aircraft. Motor gasoline is distilled between 35°C and 215°C and is used as a fuel for land based spark ignition engines. Motor gasoline may include additives (such as ethanol), oxygenates and octane enhancers, including lead compounds such as TEL (Tetraethyl lead) and TML (tetramethyl lead).

**14. Jet Kerosene**

This is medium distillate used for aviation turbine power units. It has the same distillation characteristics and flash point as kerosene (between 150°C and 300°C but not generally above 250°C). In addition, it has particular specifications (such as freezing point) which are established by the International Air Transport Association (IATA).

**15. Other Kerosene**

Kerosene comprises refined petroleum distillate intermediate in volatility between gasoline and gas/diesel oil. It is a medium oil distilling between 150°C and 300°C. In most refineries Jet Kerosene is the major product and heating kerosene is produced to the same specifications.

**16. Gas/Diesel Oil (Distillate Fuel Oil)**

Gas/diesel oil includes heavy gas oils. Gas oils are obtained from the lowest fraction from atmospheric distillation of crude oil, while heavy gas oils are obtained by vacuum redistillation of the residual from atmospheric distillation. Gas/diesel oil distils between 180°C and 380°C. Several grades are available depending on uses: diesel oil for diesel compression ignition (cars, trucks, marine, etc.), light heating oil for industrial and commercial uses, and other gas oil including heavy gas oils which distil between 380°C and 540°C and which are used as petrochemical feedstocks.

**17. Heavy Fuel Oil (Residual)**

This heading defines oils that make up the distillation residue. It comprises all residual fuel oils, including those obtained by blending. Its kinematic viscosity is above 10 cSt at 80°C. The flash point is always above 50°C and the density is always more than 0.90 kg/l.

**18. Naphtha**

Naphtha is a feedstock destined either for the petrochemical industry (e.g. ethylene manufacture or aromatics production) or for gasoline production by reforming or isomerisation within the refinery. Naphtha comprises material in the 30°C and 210°C distillation range or part of this range.

### 19. Petroleum Coke

Petroleum coke is defined as a black solid residue, obtained mainly by cracking and carbonising of residue feedstocks, tar and pitches in processes such as delayed coking or fluid coking. It consists mainly of carbon (90 to 95 per cent) and has a low ash content. It is used as a feedstock in coke ovens for the steel industry, for heating purposes, for electrode manufacture and for production of chemicals. The two most important qualities are "green coke" and "calcinated coke". This category also includes "catalyst coke" deposited on the catalyst during refining processes: this coke is not recoverable and is usually burned as refinery fuel.

### 20. White Spirit and SBP

White spirit and SBP are refined distillate intermediates with a distillation in the naphtha/kerosene range.

- They are sub-divided as:
- *i) Industrial Spirit (SBP)*: Light oils distilling between 30°C and 200°C, with a temperature difference between 5 per cent volume and 90 per cent volume distillation points, including losses, of not more than 60°C. In other words, SBP is a light oil of narrower cut than motor spirit. There are 7 or 8 grades of industrial spirit, depending on the position of the cut in the distillation range defined above.
- *ii) White Spirit*: Industrial spirit with a flash point above 30°C. The distillation range of white spirit is 135°C to 200°C.

### 21. Lubricants

Lubricants are hydrocarbons produced from distillate or residue; they are mainly used to reduce friction between bearing surfaces. This category includes all finished grades of lubricating oil, from spindle oil to cylinder oil, and those used in greases, including motor oils and all grades of lubricating oil base stocks.

### 22. Bitumen

Solid, semi-solid or viscous hydrocarbon with a colloidal structure, being brown to black in colour, obtained as a residue in the distillation of crude oil, vacuum distillation of oil residues from atmospheric distillation. Bitumen is often referred to as asphalt and is primarily used for surfacing of roads and for roofing material. This category includes fluidized and cut back bitumen.

### 23. Paraffin Waxes

Saturated aliphatic hydrocarbons (with the general formula  $C_nH_{2n+2}$ ). These waxes are residues extracted when dewaxing lubricant oils, and they have a crystalline structure with carbon number greater than 12. Their main characteristics are that: they are colourless, odourless and translucent, with a melting point above 45°C.

**24. Other Petroleum Products**

Includes the petroleum products not classified above, for example: tar, sulphur, and grease. This category also includes aromatics (e.g. BTX or benzene, toluene and xylene) and olefins (e.g. propylene) produced within refineries.

**25. Natural Gas**

Natural gas comprises gases, occurring in underground deposits, whether liquefied or gaseous, consisting mainly of methane. It includes both "non-associated" gas originating from fields producing only hydrocarbons in gaseous form, and "associated" gas produced in association with crude oil as well as methane recovered from coal mines (colliery gas). Production is measured after purification and extraction of NGL and sulphur, and excludes re-injected gas, quantities vented or flared. It includes gas consumed by gas processing plants and gas transported by pipeline.

**26. Gas Works Gas**

Gas works gas covers all types of gas produced in public utility or private plants, whose main purpose is the manufacture, transport and distribution of gas. It includes gas produced by carbonisation (including gas produced by coke ovens and transferred to gas works), by total gasification (with or without enrichment with oil products), by cracking of natural gas, and by reforming and simple mixing of gases and/or air. This heading also includes substitute natural gas, which is a high calorific value gas manufactured by chemical conversion of a hydrocarbon fossil fuel.

**27. Coke Oven Gas**

Coke oven gas is obtained as a by-product of the manufacture of coke oven coke for the production of iron and steel.

**28. Blast Furnace Gas**

Blast furnace gas is produced during the combustion of coke in blast furnaces in the iron and steel industry. It is recovered and used as a fuel partly within the plant and partly in other steel industry processes or in power stations equipped to burn it. Also included here is oxygen steel furnace gas which is obtained as a by-product of the production of steel in an oxygen furnace and is recovered on leaving the furnace. The gas is also known as converter gas or LD gas.

## Appendix 2: Glossary

**Actual emissions:** is a synonym for "immediate emissions"; in the new CRF "actual emissions" is used as a synonym for emissions from fuel combustion.

**Apparent consumption:** Production - export + import;

In the IPCC methodology: Production – export + import – bunkers +/- stocks

**Back-to-Feedstock Recycling:** A process using chemical techniques to recycle materials (here: carbon-based) to raw materials, e.g. crude oil substitute, naphtha substitute etc. (hence a recycling from waste materials to energy carriers)

**Back-to-Monomer Recycling:** Recycling of plastics waste to the monomer stage

**Back-to-Polymer Recycling:** Mechanical recycling (see below)

**Carbon losses:** Losses of carbon in conversion processes, due to imperfect yields (<100%)

**Carbon storage:** The amount of fossil carbon that is stored in short-lived materials, long-lived materials or both (to be specified in the respective context). In the new CRF, carbon storage is referred to as the total fossil carbon that is stored in short-lived materials plus long-lived materials.

**CRF, Common Reporting Format:** Decision on Guidelines for the Preparation of National Communications by Parties, decided by the Conference of Parties on its Fifth Session in Bonn, 25 October – 5 November 1999

**End users:** (1) Final users. (2) Consumers of energy carriers, materials and products which are not further processed

**Energy efficiency:** The amount of energy that is used per unit of product (in physical units e.g. GJ/t; in monetary units e.g. GJ/ECU); is a synonym for "specific energy consumption" (SEC)".

**Energy recovery:** A process to recover the energy content of waste

**Energy system:** Total of energy production and energy use in a country or region, characterised by energy production, conversion, and energy use process activities and energy flows

**Global Warming Potential:** Relative contribution of gaseous emissions to the greenhouse effect compared to CO<sub>2</sub> (on a per tonne basis)

**Gross Calorific Value (GCV):** Heating value that does not account for the evaporation of water that is generated in the combustion process (also: Higher Heating Value, HHV)

**Intermediate:** substance which is chemically further transformed before consumption

**Life cycle:** Consecutive and inter-linked stages of a product or service system, from the extraction of natural resources to the final disposal

**Life Cycle Assessment (LCA)** (depending on the context): (1) LCA is a concept to evaluate the environmental consequences of any given activity holistically from the initial gathering of raw material from the earth until the point at which all residuals are returned to the earth (2) A systematic set of procedures for compiling and examining the inputs and outputs of materials and energy and the associated environmental impacts directly attributable to the functioning of a product or service system throughout its life cycle

**Long-lived materials (made from carbon):** Materials which have a long life; in contrast to short-lived materials they are not oxidised to CO<sub>2</sub> very easily.

**Long-lived products:** Products which have a long residence time in the economy; they are stocked in the economy for a relatively long time before they end up as (post-consumer) waste.

**Material:** Commodity, excluding energy carriers, food and fodder, produced by industry.

**Materials efficiency:** The amount of material that is used per unit of product

**Material Flow Analysis (MFA):** MFA refers to accounts in physical units (usually in the terms of tonnes) comprising the extraction, production, transformation, consumption, recycling and disposal of materials (e.g. substances, raw materials, base materials, products, manufactures, wastes, emissions to air, water or soil). According to different subjects and various methods, MFA covers approaches such as Substance Flow Analysis (SFA), product flow accounts, material balancing and overall material flow accounts.

**Material recovery:** A process to convert waste into a material which is recovered for further application.

**Mechanical recycling:** A recycling process where the chemical structure of the material remains unchanged, only the shape is changed (examples: plastics, bitumen). Mechanical recycling is a synonym for "Back-to-Polymer recycling".

**National boundary system:** The systems boundaries are identical with the frontiers of the country analysed.

**Net Calorific Value (NCV):** Heating value that accounts for the evaporation of water that is generated in the combustion process (also: Lower Heating Value, LHV).

**Non-energy use:** Use of carbon sources (here: fossil feedstocks) to produce materials, e.g. plastics, fibres, rubber, lacquers & varnishes, solvents, fertilisers, lubricants, greases, waxes and bitumen/asphalt.

**Plastics converter:** is a synonym for "Plastics processors", see below

**Plastics processors:** the industry that produces plastic products from polymer resins, e.g. by injection moulding, extrusion, thermoforming or blow moulding; "plastics processors" is a synonym for "plastics converters".

**Post-consumer waste:** Waste from consumers

**Process:** Subsystem, treated as black box, defined by the relation between its physical inputs and outputs and/or by its technological characteristics

**Process waste:** Waste from processing industry

**Product:** Materials in their final physical shape that is delivered to the consumer

**Recovery:** Operations listed in Annex IIB in Commission Decision of 24 May 1996 (96/350/EC). Recovery includes Energy Recovery (R1).

**Recycling:** All Recovery Operations except Energy Recovery (R1).

**Reference Approach (RA):** A simple method to estimate CO<sub>2</sub> emissions, based on the supply data for fuels as published in energy balances. The RA is laid down in the Revised 1996 IPCC Guidelines for National Greenhouse Gas Inventories.

**Renewables:** Natural resources that are capable of regeneration on a time scale of 0-100 years

**Reuse:** Reclaiming products or product parts in order to use them for the same purpose again

**Sector:** Set of processes, defined as an economic subsystem

**Short-lived materials (made from carbon):** Materials which have a short life; they are usually oxidised to CO<sub>2</sub> during use (e.g. solvents in open applications) or shortly afterwards (e.g. surfactants in sewage treatment plants).

**Short-lived products:** Products which have a short mean residence time in the economy; they end up as (post-consumer) waste rather quickly.

**Specific energy consumption (SEC):** The amount of energy that is used per unit of product (in physical units e.g. GJ/t; in monetary units e.g. GJ/ECU); is a synonym for "energy efficiency".

**Standard Approach (SA, now named Sectoral Approach):** A variety of detailed methods to determine Greenhouse Gas emissions released from the processes in the various sectors. The SA is laid down in the Revised 1996 IPCC Guidelines for National Greenhouse Gas Inventories.

**Stock:** Products or materials which are accumulated in the economy during their in-use phase (without waste)

**Substance:** Matter characterised by its chemical composition

**System:** A dynamic, interconnected set of processes that collectively perform a function

**System boundary:** Interface between the product or service system being studied and its environment or other systems

**Users:** Either "end users" (see above) or users of energy commodities as feedstocks.

**Waste:** Output of process in life cycle stage beyond the final use

## Appendix 3: Changes to the joint IEA/EUROSTAT/UNECE annual energy questionnaire

The following changes to the joint IEA/EUROSTAT/UNECE energy questionnaire were proposed by the NEU-CO<sub>2</sub> network on its second workshop, which was held in Brussels on 13-14 April, 2000 (changes are printed in italics).

### 1. Solid Fuels questionnaire:

Definition of Non-Energy Use: *report coal and coal derived fuels used for non-energy purposes in the chemical/petrochemical industry, e.g. solid fuels used as feedstocks in the production of ammonia and methanol.*

### 2. Natural Gas questionnaire:

- a) **Non-energy use:** report by sector and sub-sector non-energy use of natural gas. This category includes
- Natural gas feedstocks in processes such as cracking and reforming for the purpose of producing ethylene, propylene, butylene, aromatics, butadiene and other non-energy hydrocarbon based raw materials. Not included are the amounts of energy consumed as fuel for petrochemical processes such as steam cracking.
  - *Natural gas inputs (total) to ammonia and methanol production plants.*
- b) **Energy use:** report by sector and sub-sector all energy use of natural gas. Report amounts of energy consumed as fuel for petrochemical processes such as steam cracking. *Excluded are the inputs for ammonia and methanol production.*

### 3. Oil questionnaire:

- a) **Energy use:** report quantities of oil used as fuel for petrochemical processes such as steam cracking. *Do not include any inputs to ammonia and methanol production.*
- b) **Non-Energy use:** report quantities of petroleum products used in the petrochemical sector for the purpose of producing ethylene, propylene, butylene, synthesis gas, aromatics, butadiene, *carbon black* and other hydrocarbon-based raw materials in processes such as steam cracking, aromatics plants and steam reforming. Exclude amounts of oil used for fuel purposes. *Please note that total inputs of petroleum products for ammonia and methanol production are included in this category.*

## Appendix 4: Overview of the consortium

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