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Naphtha storage fraction and green house gas emissions in the Korean petrochemical industry

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Abstract

This paper shows for a Korean case study how the naphtha storage fraction and CO_2 emissions from naphtha use in the petrochemical industry can be estimated. We have used the Non-Energy use Emission Accounting Tables model to estimate CO_2 emissions by subtracting the carbon stored in products from the total carbon input. We also value the country's naphtha storage fraction by calculating carbon storage in basic chemicals. The naphtha storage fraction and associated CO_2 emissions from non-energy use depend on the production and trade structure of a country. Therefore, it is reasonable for Korea (with its large production and net exports of chemicals) to estimate a county-specific storage fraction. The naphtha storage fraction estimated using the Non-Energy use Emission Accounting Tables model was over 90% in Korea between 2011 and 2015. It is much higher than the Intergovernmental Panel on Climate Change default fraction of 75%. A revision of the naphtha storage fraction from 75 to 90% is proposed for Korea. The Intergovernmental Panel on Climate Change allows countries to apply their own values that more accurately represent their country's situation. The Korean government is advised to consider this finding in its national emission accounting.

Keywords

Non-energy use and CO_2 emissions, naphtha storage fraction, Non-Energy use Emission Accounting Tables model, Intergovernmental Panel on Climate Change Guidelines, Korean petrochemical industry

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Introduction

Estimation of carbon emissions related to non-energy use is essential for accurate accounting of national green house gas (GHG) emissions. Carbon emissions associated with energy (fuel) use of fossil fuels like petroleum products can be easily calculated using available carbon emission factors of individual fossil fuels. However, it is necessary to know the application of fossil fuels used for non-energy purposes, especially in the petrochemical industry. Carbon contained in non-energy materials is partly converted into CO_2 emissions during use and is partly stored in products like polymers unless these are incinerated. Carbon in basic chemicals like ethylene and propylene is partially stored (depending on the subsequent pathways). However, carbon in final chemical products like polyethylene (PE) and polyvinylchloride (PVC) is completely stored (embodied). Therefore, carbon emissions in a country's petrochemical industry will make the difference between carbon inputs and carbon storage. This carbon storage can be calculated by multiplying the carbon inputs by the carbon storage fractions of individual chemicals.

The Intergovernmental Panel on Climate Change (IPCC) provides in its 1996 Guidelines for National GHG Emissions default storage fractions for petroleum products, coal and natural gas used for non-energy purposes. In the case of naphtha, the IPCC default storage fraction is 75%.[1] This fraction was determined based on Marland and Rotty[2] and Marland and Marland,[3] who had estimated 80% as naphtha storage fraction from 1950 to 1982. This production-based fraction corresponds to a world average value.

However, such storage fractions will vary according to a country's production and trade structure of chemicals. This explains why the following countries in their National Inventory Report (NIR), submitted to the United Nations Framework Convention on Climate Change,[4] used a different naphtha storage fraction than the IPCC. They are Belgium (100%), France (100%), Finland (100%), Spain (80%), the Netherlands (78%), the USA (70%) and Italy (64%).

The IPCC Guidelines do not define a method for estimating a country-specific naphtha storage fraction. The NEAT model is able to estimate both consumption- and production-based naphtha storage fractions, taking into account a country's chemical production and trade structure. Countries that produce more chemicals with higher storage fractions will have a higher naphtha storage fraction than others. And countries that are net exporters of short-lived chemicals will have also a higher naphtha storage fraction than others.

Taking into account the net exports of short-lived chemicals as carbon storage can be compared with the treatment of exported gasoline and diesel fuels which do not cause CO_2 emissions in the exporting country. The only difference in the exports between petroleum products and chemicals is the available statistics. The energy statistics on which the emissions calculation is based include imports and exports of fossil fuels, but not of chemicals.

Korea is a major consumer of naphtha[a] as a feedstock for petrochemicals. According to the International Energy Agency,[5] the Korean petrochemical industry processed naphtha in 2015 at 47.2 Mt (million tonnes) or 16.9% of world consumption. The share of long-lived chemicals like polymers in Korean petrochemical production is relatively high. In addition, Korea is a large net exporter of petrochemicals. Its exports and imports of petrochemicals in 2015 were 33.7 and 11.2 Mt, respectively, according to the Korea Petrochemical Industry Association.[6] Therefore, the naphtha storage fraction should be higher in Korea than in other countries.

Park[7] estimated 88.2% as a naphtha storage fraction in Korea in 2000 according to the NEAT model. This study prompted the Korean government to fund studies in 2012 and 2015 to estimate the naphtha storage fraction in Korea. The 2015 study of the consulting firm Ecosian[8] estimated a naphtha storage fraction of 77% in Korea from 2007 to 2013. Given the structure of production and Korea's large net exports, this seems unlikely and requires further analysis.

This paper shows for a Korean case study how the naphtha storage fraction and CO_2 emissions from naphtha use can be estimated. The NEAT model was used to estimate the Korean naphtha storage fraction from 2011 to 2015 to revise this fraction.

The IPCC allows countries to revise their fractions: 'Whenever possible, countries should substitute assumptions that represent more accurately the practices within their countries and provide documentation for these assumptions.'[1]

This paper is organized as follows. The next section describes the Korean petrochemical industry. This is followed by a section in which we review studies on the naphtha storage fraction. Section 'Method to estimate the naphtha storage fraction' discusses the carbon storage and release in the non-energy use and presents the NEAT model for estimating carbon storage. Section 'Estimation of Korean naphtha storage fraction' estimates the naphtha storage fraction using a NEAT model and a simplified estimation method. These methods take into account the chemical production and trade structure in Korea. This article ends with conclusions and policy recommendations.

Korean petrochemical industry

Korea's petrochemical industry is located in three complexes Ulsan (Southeast of the country), Yeocheon (Southwest) and Daesan (West). It consists of six petrochemical companies (Naphtha Cracking Centres: NCC plants) and four oil refineries (Benzene Toluene Xylene (BTX) plants). The six companies, Korea Petrochemical, Lotte Chemical, Yeocheon NCC, Hanwha Total, LG Chemical and SK General Chemicals, operate NCC plants and produce BTX on the basis of pyrolysis gasoline (PG), which is produced in the NCC process. Four oil refineries, S-OIL, Hyundai Oilbank, GS Caltex and SK Energy, operate mostly BTX plants. Both NCC and BTX plants produce basic chemicals.

Korea's petrochemical industry is ranked fourth in terms of global ethylene production capacity of 8.6 Mt in 2015 after the United States (28.5 Mt), China (21.0 Mt) and Saudi Arabia (15.8 Mt). Domestic demand in 2015 was 7.842 Mt of ethylene, 6.227 Mt of propylene, 1.458 Mt of butadiene, 3.523 Mt of benzene, 1.921 Mt of toluene and 3.136 Mt of p-xylene.[6] The domestic demand for final chemical products has stagnated since the beginning of 2010.

Korea produced 29.404 Mt of naphtha and imported net 17.676 Mt (= imports of 23.304 – exports of 5.628) in 2015. Unlike other countries, Korean petrochemical and refinery companies use almost only naphtha as feedstock for petrochemical products.

Review of studies

There are three Korean studies that estimated the naphtha storage fraction. Park[7] estimated it by applying the so-called NEAT model for the year 2000. The two other studies were carried out by Ecosian and commissioned in 2012 and 2015 by the Korean government.

Park's study of 2005

In the course of estimating CO_2 emissions in Korea, Park[7] estimated the naphtha storage fraction at 88.2% in 2000.[b] About 5% points of this storage fraction was related to net exports of oxidized during use (ODU) chemicals, which according to the IPCC terminology correspond to short-lived products. This result has increased government interest in view of the (potential) need to revise this fraction. In 2012 and 2015, a study was commissioned by the government through the GHG Inventory & Research Center in Korea.

Ecosian's study of 2012

Ecosian studied the naphtha storage fraction jointly with the KPIA and the Korea Petroleum Association.[9] For this study, Ecosian used the reports of six NCC companies. Such reports with steam cracking material balances are being filed by petrochemical companies to get refunded import duties on naphtha. These duties amounted to won 16 (about US cent 1.45) per liter.

Ecosian estimated the naphtha storage fraction as the difference between one (1) and the emission factor. This emission factor is defined as the proportion of process heat use and fuel type by-product sales (as a numerator) to gross deliveries and recycled input (as a denominator).

The use of process heat (internal backflows), fuel use for the heat needed for cracking processes, was 4.284 Mt naphtha in 2011 as shown in Table 1. Gross naphtha deliveries (21.138 Mt) were the quantities of naphtha supplied by refineries to the petrochemical sector. The recycled input (8.862 Mt) refers to those by-products returned to the cracking process. It came mostly from the by-products own use (9.568 Mt) according to Table 1.

The external backflows (1.656 Mt), by-products sold to consumers or by-products returned to refineries consisted of 'Exports' (0.168 Mt), 'Fuel type' (0.129 Mt) and 'Others' (0.279 Mt) of the sales categories in Table 1. Naphtha's non-energy use was equal to the gross deliveries less internal backflows and external backflows (21.138–4.284–1.656 = 15.198 Mt).

Ecosian estimated the naphtha storage fractions from 2007 to 2011 at 79 to 81%. In actual fact, they did not estimate the naphtha storage fraction, but estimated the non-energy share in naphtha use to be 81.7% (= 1 – (4.284 + 1.209)/29.990) in 2011. The share of non-energy in the naphtha use should be 71.9% (= 15.198/21.138) and not 81.7%. This is because the denominator of the fraction for the emission factor should only include gross naphtha deliveries to estimate the non-energy share of naphtha use. Ecosian's study included twice the recycled input. In summary, this did not result in corrected values for the naphtha storage fraction.

Ecosian's study of 2015

Park's 2005 study, which estimates that Korea's naphtha storage fraction is well above 75%, prompted the Korean government to commission another study. Again, Ecosian was given the task for such an estimate. Ecosian estimated the naphtha storage fraction from 2007 to 2013 in three steps, NCC process, downstream process and carbon storage (described as products step in the study).

In the first step, Ecosian examined the process heat use of naphtha in six NCC plants which used 55% of the total naphtha consumption in 2013. They estimated the share of

Table 1. Material flow balances of six NCC crackers 2011 (in 1,000 tonnes).

			Material flow	Sales				Own use	Total
				Exports	Feedstock type	Fuel type	Others		
Input	Gross input		29,990						
	Recycled		8862						
	Gross deliveries (net input)		21,138						
Output	Main products	Ethylene	6877						
		Propylene	3340						
		etc.							
		Sub total	14,389	1101	5996		5	7863	14,964
	Byproducts	Hydrogen	35						
		CH_4	49						
		etc.							
		Sub total	11,053	168	1143	1209	279	9568	12,388
Fuel (process heat)		4284							
LOSS		285							
Fuel & LOSS		4568							

Source: Ecosian.[9]

NCC: Naphtha Cracking Centres.

Notes: 1. The term gross deliveries mean deliveries of refineries to NCC crackers (net input).

2. The quantities of non-energy use (petrochemicals), exports, the use of process heat and own use are excluded from the payment of import duties of won 16 per litre. Thus, only the sales quantities of 'Fuel type' (1.209 Mt) and 'Others' (0.284 Mt) are not refunded. The refund rate is 0.929 (= 1–(1.493/21.138) × 1.0053). The factor 1.0053 is the quantity of raw material required to convert one unit of the product.

3. The quantities of main products and by-products are different from those of their total quantity due to inventory changes.

naphtha used for process heat to be 16%. In the second step, Ecosian estimated 3% ($= 1 - 84 \times 97\%$) of the process heat share in the remaining naphtha input of 84% in a sample survey of downstream petrochemical companies.

In the third step, Ecosian distinguished chemicals produced in the first two steps between long-lived products and short-lived products, using the not-oxidised during use (NODU) and ODU shares of the Park study. It estimated the NODU share of chemicals at 94%. Ecosian multiplied all three shares (84, 97 and 94%) to estimate the naphtha storage fraction at 77%.

Ecosian's study shows several shortcomings. First, the NCC plants do not represent the Korean petrochemical sector, as these plants use only 55% of the total naphtha input in 2013. And the production structure of the BTX plants, which use the remaining naphtha, differs significantly from those of the NCC plants.

Second, considering NCC plants only in the first step led to an imbalance between the input of basic chemicals produced in NCC plants and the output of intermediates and final products. This is because the production of basic chemicals was made by both NCC and BTX plants.

Third, Ecosian tried to apply the NEAT model to NODU and ODU chemicals. However, no mass carbon balances were used to determine the final use of basic chemicals and intermediates at each step of the flow path as to distinguish between NODU and ODU chemicals. As a result, the amount of storage chemicals was counted twice and three times.

For example, the amount of ethylene was counted as ethylene itself and as those parts of ethylene incorporated in ethylbenzene, styrene, polystyrene, Styrene Butadiene Rubber (SBR), Acrylonitrile Butadiene Styrene (ABS), Styrene Acrylonitrile (SAN) and so on.

Fourth, the first two steps to estimate the non-energy use of naphtha are not relevant to the estimation of the naphtha storage fraction. Therefore, this study also did not result in corrected values for this storage fraction.

Method to estimate the naphtha storage fraction

Carbon storage and release in the non-energy use

Fossil fuels are used both as energy and non-energy purposes. When fossil fuels are burned, heat is generated and CO_2 is emitted immediately. When fossil fuels are used for non-energy purposes, carbon can be incorporated/ stored in products and/or converted into CO_2 emissions. In the case of petrochemicals, the carbon storage is obtained by multiplying the production quantities with the associated emission factors and carbon storage fractions. The carbon release (CO_2 emissions) is in turn obtained by subtracting the total carbon stored in products from the total carbon input.

Since default values for emission factors and carbon storage fractions of petrochemicals are not included by the IPCC Guidelines, they must be estimated. The NEAT model provides a method for estimating carbon storage fractions by basic chemical and thus naphtha storage fraction and CO_2 emissions in the petrochemical industry.

NEAT model

The NEU-CO2 group developed a bottom–up spreadsheet model called NEAT model financed by the EU Commission. The NEAT model is an independent method of calculating CO_2 emissions by using petrochemical production, trade and consumption data.[7,10–12] It is in line with the IPCC emissions estimates because it can calculate emissions according to the national boundary principle (consumption-based estimation).

The NEAT model has a similar goal to the life cycle energy assessment (LCA). LCA is a method of estimating environmental impacts associated with all stages of product life, from raw material extraction through materials processing, manufacturing, use and disposal. However, the NEAT model does not analyse the entire life cycle of products. The NEAT model used in this study only estimates carbon storage and release by distinguishing the final use of basic chemicals and intermediates at each step of the flow path between NODU and ODU chemicals. In addition, this study does not analyse the carbon emissions associated with the disposal of chemicals, as these are dealt with separately in Volume 5: Waste of the IPCC Guidelines.

Figure 1 illustrates the distinction between production- and consumption-based estimates of carbon storage and release. Net exports of ODU chemicals are considered as part of carbon storage, while net imports of ODU chemicals are considered as part of carbon release.

At the heart of the NEAT model is a mass carbon balance model that describes the petrochemical production structure of a country, i.e. carbon flows from basic chemicals via intermediates to final products. This balance model was developed on the basis of carbon intensities of chemicals published in C-Ströme,[13] literature reviews and expert advices.

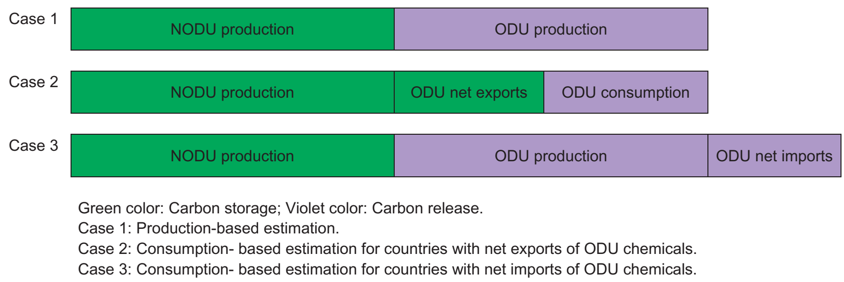

Figure 1. Carbon storage and release estimation scheme.
NODU: not-oxidised during use; ODU: oxidised during use.

Carbon usage by chemical can be accurately calculated using the mass carbon balance model, which consists of two parts, namely upper balances (normalized transformation coefficients) and lower balances (absolute transformation flows).

The NEAT model assumes that the inputs and outputs of each process or flow are the same. However, it excludes stock shift due to stock changes and incomplete chemical conversion. It represents all main flows in terms of embodied CO_2 equivalents.

The upper balances in the Korean case consist of a matrix of 67×67 (input and output model). Their rows show the inputs (proportion) of basic chemicals and/or intermediates for the production of a unit of intermediate or final chemical. For example, 0.8 Mt CO_2 of p-xylene and 0.2 Mt CO_2 of methanol are needed to produce 1 Mt CO_2 dimethyl terephtalate (DMT), which is one of the raw materials for the production of PET (0.8 and 0.2 are input ratios).

Their columns indicate the input ratios of a basic chemical or intermediate for the production of a unit of the intermediate or final chemical. For example, the production of 1 Mt CO_2 aniline requires 0.94 Mt CO_2 benzene and the corresponding benzene quantities for production of cumene, cyclohexane and ethylbenzene are 0.65, 1 and 0.75 Mt CO_2, respectively.

The rows of the lower balances, also a 67×67 matrix, indicate in absolute terms the required input of basic chemicals or intermediates for the production of a given amount of an intermediate or final product. For the production of 0.17 Mt (CO_2) DMT, the inputs required are 0.14 ($= 0.8 \times 0.17$) Mt p-xylene and 0.04 ($= 0.2 \times 0.17$) Mt methanol where 0.8 and 0.2 are the input ratios from the rows of the upper balances.

The columns of the lower balances indicate the absolute flows in the country (in terms of CO_2 equivalents) how much of a product is needed for the production of another. For example, the amounts of p-xylene used to produce DMT of 0.17 Mt CO_2 and TPA of 14.06 Mt CO_2 are 0.14 ($= 0.8 \times 0.17$) Mt CO_2 and 14.06 ($= 1 \times 14.06$) Mt CO_2. Factors 0.8 and 1 are the input ratios of p-xylene for the production of DMT and TPA. Accordingly, 14.20 Mt CO_2 of p-xylene was used to make DMT and TPA and the remaining 0.30 Mt CO_2 of 14.50 Mt CO_2 was consumed (used) for other products as shown in Table 2.

Carbon storage fraction and emission factors of chemicals

The IPCC recommends using 75% as a naphtha storage fraction unless the member states have established a more accurate value. The NEAT method distinguishes chemicals that are converted to CO_2 during use as ODU products, as opposed to chemicals whose carbon is

Table 2. Example of a mass balance calculation for chemical products in NEAT.

				($Mt\ CO_2/yr$)
p-Xylene				14.50
p-Xylene derivatives				
	Specific consumption ($Mt\ CO_2/Mt\ CO_2$) (A)	Annual production ($Mt\ CO_2/yr$) (B)	Absolute consumption ($Mt\ CO_2/Mt\ CO_2$) ($A \times B$)	
Terephtalic acid (TPA)[a]	1.00	14.06	14.06	
Dimethyl terephtalate (DMT)[b]	0.80	0.17	0.14	
Sum of p-xylene use				14.20
Other use of p-xylene				0.30

NEAT: Non-Energy use Emission Accounting Tables.
Source: Neelis et al.[12]
a) Stoichometric factors. In the production of TPA (8 carbon atoms), all carbon atoms are derived from p-xylene.
b)In the production of DMT (10 carbon atoms), 8 carbon atoms are derived from p-Xylene and 2 atoms from methanol. Therefore, the specific consumption is 0.8 for p-xylene and 0.2 for methanol.

stored in the products as NODU. The carbon embodied in these latter products is typically released no earlier than during waste disposal (if the product is burned while storage is continued in the case of landfilling).

The shares of NODU and ODU depend on the use of chemicals. Final chemicals like PE, PET, polystyrene and PVC have a NODU share of 100%, while intermediates like phenol, ethylenedicloride and ethanol have an ODU share of 100%. Intermediates like acetic acid and acetone have ODU shares of 65 and 40%, respectively.

The distribution of usage share between ODU and NODU chemicals is based on data from literature like Weissermel and Arpe,[14] Chauvel and Lefebvre[15] and Korea Petrochemical Statistics.[6] Since there are some uncertainties, the NEAT approach introduces a minimum release (maximum storage) and maximum release (minimum storage) in addition to the mean release (Appendix 1).

Estimation of Korean naphtha storage fraction[c]

Data

To estimate the naphtha carbon storage fraction, the naphtha flows in the petrochemical industry must be accurately determined. In NCC and BTX plants, naphtha is first processed into basic chemicals. In this process, fuel-type by-products are formed in addition to the basic chemicals. One part is used as process heat (internal backflows). Another part of them is returned to refineries, which is referred to as external backflows. Thus, the non-energy use of naphtha corresponds to the naphtha gross deliveries to the petrochemical industry less internal and external backflows.

Non-energy use and fuel (process heat) use of naphtha can be determined exactly with the data in the World Energy Balances of the IEA.[16] For example, total naphtha supply in 2015 was 48.417 Mt, of which 8.547 Mt (17.65% of the total) was external backflows and 8.960

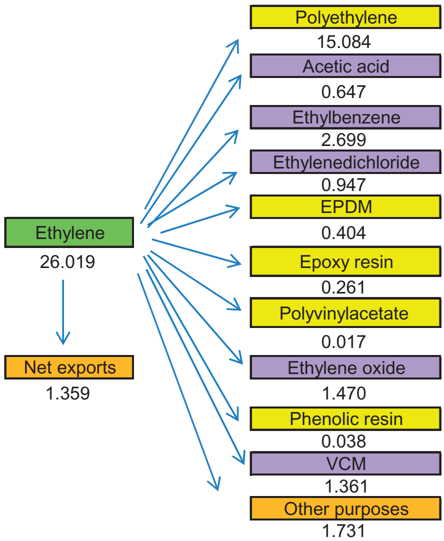

Figure 2. Ethylene flow path in NEAT model in 2015. Note: Chemicals in Mt CO_2. Green: basic chemicals; Violet: intermediates; Yellow: final products; Orange: other purposes and net exports.
NEAT: Non-Energy use Emission Accounting Tables.

Mt (18.51%) was internal backflows. Thus, the non-energy use of naphtha was 30.910 Mt or 63.84% of the total naphtha supply.

To operate the NEAT model, data are required on the production and trade of 67 major petrochemicals, including 12 basic chemicals, 32 intermediates and 23 final chemicals, are required. About 30 of these production data were published in the Korea Petrochemical Statistics of the KPIA.[6] The remaining production data are, however, to be collected directly from the manufacturers. Statistics on imports and exports of chemicals are obtained from the National Trade Information Portal of the Korea International Trade Association (KITA) (http://stat.kita.net/main.screen).[17]

Estimation of naphtha storage fraction in Korea

This study estimates the carbon storage and release by chemical in the flow path of the lower mass balances. It is important to determine the final use of basic chemicals and intermediates at each production step in the flow path to distinguish between NODU (storage) and ODU (release) chemicals.

For example, the carbon storage and release of basic chemical ethylene can be estimated as follows. Ethylene production in 2015 was 26.019 Mt CO_2 (8.279 Mt), while 1.359 Mt CO_2 (0.433 Mt) of ethylene was exported net. The remaining ethylene of 24.659 Mt of CO_2 was used to make intermediates and final products as shown in Figure 2.

The amount of carbon storage and release from ethylene use can be determined from four different sources. The first source is carbon storage and release calculated from the ethylene input to produce various intermediates and final chemicals like ethylbenzene, styrene and

PE. The amounts of carbon storage and release were 21.377 Mt CO_2 (97%) and 0.659 Mt CO_2 (3%), respectively, as shown in Table 3.

The gross carbon storage of intermediates and final products made with ethylene is estimated as the sum of the production of NODU chemicals and net exports of ODU chemicals. And the gross carbon release of intermediates made with ethylene is estimated to be the product of intermediates used to make other chemicals with the corresponding ODU shares. There is no gross carbon release for the final products in Table 3 because the ODU shares of final products and intermediates like ethylbenzene and styrene are zero (0). The carbon storage and release of intermediates and final products are calculated as the product of gross carbon storage and release (Columns A and B of Table 3) with the ethylene content (Column C) of the corresponding chemical, respectively.

Table 3 shows a minus sign (−) of carbon storage of ethanol. The reason for this is that Korea did not produce naphtha-based ethanol and had a net export (−0.258 Mt CO_2) or a net import (0.258 Mt CO_2).

The second source is the carbon storage and release of 0.866 ($= 0.5 \times 1.731$) Mt CO_2 calculated from the use of ethylene (1.731 Mt CO_2) for other purposes (products other than

Table 3. Carbon storage and release from ethylene for the production of intermediates and final products 2015 (Mt CO_2).

	Gross carbon storage (A)	Gross carbon release (B)	Ethylene content (C)	Carbon storage (= A × C)	Carbon release (= B × C)
Intermediates					
Ethanol	−0.258	0.258	1	−0.258	0.258
Ethylbenzene	1.241	0	0.25	0.307	0
Ethylenedichloride	0.003	0.036	1	0.003	0.036
Ethylene glycol	0.375	0.269	0.72	0.270	0.194
Styrene	1.947	0	0.25	0.481	0
Vinylchloride monomer (VCM)	0.250	0.419	0.40	0.100	0.168
Final products					
ABS	5.364	0	0.16	0.849	0
EPDM	0.673	0	0.60	0.404	0
Epoxy resin	1.177	0	0.22	0.261	0
Polyethylene (PE)	15.328	0	0.98	15.084	0
Polyethyleneterephthalate (PET)	3.629	0	0.33	1.198	0
Polystyrene (PS)	3.456	0	0.25	0.855	0
Polyvinylacetate	0.033	0	0.51	0.017	0
Polyvinylchloride (PVC)	2.124	0	0.75	1.599	0
SAN	0.649	0	0.13	0.083	0
SBR	1.609	0	0.08	0.123	0
Total				21.377	0.659
Share of storage and release				0.97	0.03

NODU: not-oxidised during use; ODU: oxidised during use.

Notes: (a) Gross carbon storage: production of NODU chemicals + net exports of ODU chemicals.

(b) Gross carbon release: use for the production of other chemicals × ODU share.

(c) Ethylene content: ethylene share in intermediates and final chemicals.

the chemicals listed in Figure 2). In the case of ethylene, both the ODU and NODU shares are estimated to be 0.5. The third source is carbon storage related to net exports of ethylene, which was 1.359 Mt CO_2 in 2015.

The fourth source is carbon storage and release calculated from the difference (0.892 Mt CO_2) between the ethylene production of 26.019 Mt CO_2 and the sum (25.127 Mt CO_2) of the carbon storage of 23.602 ($= 21.377 + 0.866 + 1.359$) Mt CO_2 and release of 1.525 ($= 0.659 + 0.866$) Mt CO_2 calculated from the previous sources. This study allocates this difference to the storage (97%) and release (3%) share shown in Tables 3 and 4 (0.865 Mt CO_2 storage versus 0.027 Mt CO_2 release).

Overall, carbon storage and release from the ethylene use in 2015 were 24.467 Mt CO_2 (94.04%) and 1.552 Mt CO_2 (5.96%), respectively. Carbon storage and release for other basic chemicals can be estimated by analogy with ethylene estimation. Table 5 shows the estimate of carbon storage and release of basic chemicals in 2015.

The composition of carbon storage and release from 2011 to 2015 is summarized in Table 6. For example, in 2015, Korea produced NODU and ODU chemicals of 97.149 Mt CO_2 (84.9%) and 17.305 Mt CO_2 (15.1%), respectively. Thus, the production-based

Table 4. Carbon storage and release from ethylene, consumption-based estimates 2015 (Mt CO_2).

	Storage	Release	Sub-total
1. Production of intermediates and final products	21.377	0.659	22.036
2. Production of other purposes (products)	0.866	0.866	1.732
3. Net exports	1.359	0	1.359
4. Allocation of difference between ethylene production and sum of above amounts	0.865	0.027	0.892
Total	24.467	1.552	26.019
Share	94.04%	5.96%	100%

Table 5. Carbon storage and release by basic chemical, consumption-based estimates 2015.

	Stored (%)	Released (%)	Production (Mt CO_2)	Stored (Mt CO_2)	Released (Mt CO_2)
Acetylene	100.0	0	0.496	0.496	0.000
Benzene	99.55	0.45	20.793	20.699	0.094
Butadiene	100	0	3.917	3.917	0.000
Other C4	21.10	78.90	2.721	0.574	2.147
CO-source	93.66	6.34	0.928	0.869	0.059
Ethylene	94.04	5.96	26.019	24.467	1.551
Propylene	97.96	2.04	22.137	21.685	0.451
Toluene	21.56	78.44	5.531	1.193	4.338
o-Xylene	90.97	9.03	1.192	1.084	0.108
m-Xylene	9.17	90.83	0.621	0.057	0.564
p-Xylene	98.33	1.67	30.101	29.599	0.502
Sum in %			114.455	104.641	9.814
			100.0	91.4	8.6

Table 6. Composition of naphtha storage and release from 2011 to 2015.

	Production-based estimates			Consumption-based estimates						
	Production			Consumption			Net exports		Storage	Release
	NODU (A) (Mt CO_2)	ODU (B) (Mt CO_2)	Sum (C = A + B) (Mt CO_2)	NODU (D) (Mt CO_2)	ODU (E) (Mt CO_2)	Sum (F = D + E) (Mt CO_2)	NODU (G) (Mt CO_2)	ODU (H) (Mt CO_2)	(A + H) (Mt CO_2)	(E) (Mt CO_2)
2011	78.422	10.615	89.037	35.417	5.550	40.966	43.004	5.065	83.487	5.550
	88.1%	11.9%	100.0%					5.7%	93.8%	6.2%
2012	87.802	13.779	101.582	35.676	6.909	42.584	52.127	6.871	94.673	6.909
	86.4%	13.6%	100.0%					6.8%	93.2%	6.8%
2013	88.055	13.460	101.515	40.005	7.000	47.005	48.050	6.460	94.515	7.000
	86.7%	13.3%	100.0%					6.4%	93.1%	6.9%
2014	93.022	16.300	109.322	40.099	9.606	49.705	52.923	6.694	99.716	9.606
	85.1%	14.9%	100.0%					6.1%	91.2%	8.8%
2015	97.149	17.305	114.455	40.996	9.810	50.806	56.153	7.495	104.644	9.810
	84.9%	15.1%	100.0%					6.5%	91.4%	8.6%
Average	86.2%	13.8%	100.0%					6.3%	92.5%	7.5%

IPCC: Intergovernmental Panel on Climate Change; NODU: not-oxidised during use; ODU: oxidised during use.
Notes: NODU means not oxidized during use or long-lived products according to the IPCC terminology. ODU means oxidized during use or short-lived products according to the IPCC terminology.

naphtha storage fraction was 84.9%, which was substantially higher than the IPCC default fraction of 75%.

This high naphtha storage fraction can be explained by the Korean petrochemical production structure as shown in Table 5. Most of the basic chemicals with large production volumes like p-xylene, ethylene, propylene and benzene had a storage share of more than 90%. For example, ethylene has been used mostly to produce final chemical products and intermediates like ethylbenzene and styrene, all of which have a NODU (storage) share of 100%, as shown in Table 3. But the production volume of basic chemicals with high share of carbon release, like toluene, other C4 and m-xylene, was relative small.

In addition, the net exports of ODU chemicals further increased the naphtha storage fraction. In 2015, Korea consumed only ODU products, which corresponded to 9.810 Mt of CO_2, and in 2015 exported net an equivalent of 7.495 Mt CO_2 (6.5%). Basic chemicals with large net exports of ODU products in 2015 were benzene (4.290), p-xylene (3.435), propylene (1.017) and ethylene (0.680), all in Mt CO_2. Since the exported ODU products release carbon in importing countries, these ODU products can be considered carbon storage for Korea. With this correction, the carbon storage and the naphtha carbon storage fraction increased to 104.644 Mt CO_2 and 91.4% for 2015, respectively.

According to Table 6, the NODU share in the petrochemical industry in Korea from 2011 to 2015 was 86.2%. This share was substantially higher than the IPCC default naphtha storage fraction of 75%. In addition, Korea exported a net 45.7% (= 6.3/13.8%) of ODU products. This results in a naphtha storage fraction between 91.2 and 93.8%, with an average of 92.5% over the same period.

This study suggests a naphtha storage fraction of 90% to be used to estimate the annual GHG inventories in Korea. Using this value instead of the officially used value (75%) would result in significantly lower CO_2 emissions in the NIR: Korea reported carbon emissions of about 17.168 (= $114.455 \times 15\%$; 15% being the difference between 90 and 75%) Mt CO_2 higher than actual CO_2 emissions. The overestimated CO_2 emissions in 2015 represent 2.9% of the total CO_2 emissions of 586 Mt CO_2.[18,23]

Simplified estimation of naphtha storage fraction in Korea

It is not easy to estimate the naphtha storage fraction annually by applying the (full) NEAT model due to the difficulty of collecting all the chemical production data. As already mentioned, only 30 of about 70 production data are published by the KPIA. The other production data must be collected directly from the companies. Unless institutionalized, it may be appropriate to carry out detailed analyses every three to five years and to apply a simplified method in between.

Based on this study, it is proposed to use the average values of the storage fractions from 2013 to 2015, as indicated in the last column of Table 7. This allows estimating the naphtha storage fractions for the years after 2015 without using the full NEAT model. These averages have to be multiplied by the equivalents of the embodied CO_2 and production data by the basic chemical to estimate carbon storage in absolute terms.

For example, the consumption-based naphtha storage fraction for 2016 is estimated as the ratio between the sum of carbon storage of all basic chemicals and total carbon input in the petrochemical industry. The resulting estimated naphtha storage fraction is the weighted average of carbon storage fractions of basic chemicals.

Table 7. Storage fractions by basic chemical estimated by the NEAT method from 2013 to 2015.

Storage fraction by basic chemical	2013	2014	2015	Average
Acetylene	100.0	100.0	100.0	100.0
Benzene	98.57	98.93	99.55	99.02
Butadiene	100.0	100.0	100.0	100.0
Other C4	10.0	17.1	21.1	16.1
CO-source	95.87	92.07	93.66	93.87
Ethylene	93.74	94.64	94.04	94.14
Propylene	96.69	97.33	97.96	97.33
Toluene	61.76	39.94	21.56	41.09
o-Xylene	98.75	91.66	90.97	93.79
m-Xylene	3.65	15.52	9.17	9.45
p-Xylene	97.21	99.43	98.33	98.33
Naphtha storage fraction	93.17	91.21	91.43	91.94

NEAT: Non-Energy use Emission Accounting Tables.

Table 8. Sensitivity analysis for the naphtha storage fraction for 2015.

	Production-based estimates			Consumption-based estimates			
	Production			Net exports		Storage	Release
	NODU (A) ($Mt\ CO_2$)	ODU (B) ($Mt\ CO_2$)	Sum ($C = A + B$) ($Mt\ CO_2$)	NODU (D) ($Mt\ CO_2$)	ODU (E) ($Mt\ CO_2$)	($A + E$) ($Mt\ CO_2$)	(E) ($Mt\ CO_2$)
Mean release	97.149	17.305	114.455	56.153	7.495	104.644	9.810
	84.9%	15.1%	100.0%		6.5%	91.4%	8.6%
Maximum release	97.149	21.481	118.631	52.994	10.654	107.803	10.828
	81.9%	18.1%	100.0%		9.0%	90.9%	9.1%
Minimum release	97.149	13.755	110.905	58.057	5.591	102.740	8.165
	87.6%	12.4%	100.0%		5.0%	92.6%	7.4%

NODU: not-oxidised during use; ODU: oxidised during use.

This study uses KITA's chemical statistics for 67 chemicals and the NODU and ODU shares in Appendix 1 to estimate the net export share of ODU products in the total carbon input of the petrochemical industry. The production-based naphtha storage fraction is the difference between the consumption-based naphtha storage fraction and the share of net exports of ODU products in total carbon input. This approach allows for changes in the production and trade structure of chemicals.

Sensitivity analysis

There are some uncertainties when using NODU and ODU shares in petrochemicals. This is because the exact patterns of use of petrochemicals are unknown. In addition to the baseline mean release, the cases 'maximum release' (maximum emissions) and 'minimum release' (minimum emissions) are taken into account. For the maximum release case, the ODU shares will be increased by 10% points, with the exception of ODU shares, which will be zero (0%). In the minimum release case, these shares will be reduced by 10% points, except for the ODU shares, which are 1 (100%) as shown in Appendix 1.

The sensitivity analysis shows that the deviation of storage from the mean release case is 1.904 Mt CO_2 (1.8%) for the maximum release case and 3.159 Mt CO_2 (3.0%) for the minimum release case, as shown in Table 8. The naphtha storage fraction for the year 2015 ranges from 90.9 to 92.6%. These results show that the IPCC default naphtha storage fraction is too low for Korea. This is because Korea produces more chemicals with higher storage fractions than other countries and because Korea is a large net exporter of ODU chemicals.

Conclusions and policy implications

The estimation of carbon emissions related to the use of non-energy is very important for the accurate accounting of national GHG emissions. However, the IPCC Guidelines do not define a method for estimating country-specific storage fractions from non-energy use of fossil fuels. They only supply default storage fractions for petroleum products like LPG and naphtha, but not for chemicals. In addition, the IPCC Guidelines do not take into account the trade in chemicals.

The NEAT model is able to estimate both consumption- and production-based naphtha storage fraction, taking into account a country's chemical production and trade structure. Countries that produce more chemicals with higher storage fractions will have a higher naphtha storage fraction than others. And countries that are net exporters of short-lived chemicals will have also a higher naphtha storage fraction than others. In addition, this study provides a simplified method to estimate the naphtha storage fraction and hence carbon emissions in the petrochemical industry. This is necessary because it will be difficult to collect all the chemical production data annually.

The naphtha storage fraction estimated using the NEAT model was more than 90% in Korea between 2011 and 2015, much higher than the IPCC default fraction of 75%. This is because Korea produces more chemicals with higher storage fractions than other countries and because Korea is a large net exporter of ODU chemicals. Korea's carbon emissions, estimated using the naphtha fraction of 75%, are likely to overestimate 17.1 Mt of CO_2 (15% of emissions related to the use of naphtha) or 2.9% of total carbon emissions of the country (586 Mt CO_2) in 2015.

Finally, a revision of the naphtha storage fraction from 75 to 90% is proposed for Korea. The IPCC allows countries to apply their own values that represent more accurately the situation of their country. The Korean government is advised to consider this finding in its national emission accounting.

In addition, this study can help to improve the estimation of CO_2 emissions from non-energy (feedstock) use in the petrochemical industry worldwide. The NEAT method will be of particular interest to those countries that produce more chemicals with higher storage fractions and/or are net exporters of short-lived chemicals. It is also recommended to improve the IPCC Guidelines.

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Notes

a. According to the IEA,[16] global naphtha consumption was 279.4 Mt in 2015. Naphtha is the most important petrochemical raw material. Its share of global petrochemical production in 2015 was about 50%.[19] Other major naphtha consumers were China (45 Mt), Japan (35 Mt), Russia (26 Mt) and Taiwan (20 Mt). In most Asian countries, naphtha is used as the main raw material for petrochemical purposes, while natural gas suppliers also use ethane and LPG as petrochemical raw materials.
b. After applying the NEAT model, Neelis et al.[20] estimated the storage fraction of other oil products (naphtha) in the Netherlands between 1993 and 1999 at 87 to 93%. The U.S. Environmental Protection Agency[21] estimated the U.S. storage fraction of both naphtha and other oil at 65% for 2015 (in Tables 3–21 of the U. S. EPA report).
c. A preliminary result from 2011 to 2013 was published in the Korea Forum for Natural Gas Industry.[22]

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Appendix 1. NODU and ODU shares applied in the Korean NEAT model.

Compound	Total consumption or 'other use'	Mean NODU (%)	Mean ODU (%)	Min release ODU (%)	Max release ODU (%)
Basic chemicals					
Acetylene	Other[a]	50	50	40	60
Benzene	Total	50	50	40	60
Bitumen	Other	100	0	0	0
Butadiene	Other	100	0	0	0
Other C4	-	37	63	53	73
Carbon black	Other	100	0	0	0
CO-Source	Total	50	50	0	0
Ethylene	Total	50	50	40	60
Lubricants	Total[b]	67	33	67	33
Methanol	Other	50	50	40	60
Petroleum coke	Total	0	100	100	100
Pitch	Other	0	100	100	100
Creosote oil	Other	100	0	0	0
Naphthalene	Total	50	50	50	50
Other tar products	-	100	0	0	0
Propylene	Other	60	40	30	50
Toluene	Total	30	70	60	80
Waxes, paraffins	Other	0	100	100	100
Xylenes (o-,m-,p-,mixed xylene)	Total[b]	70	30	20	40
ortho-Xylene	Other	0	100	100	100
meta-Xylene	Other	80	20	10	30
para-Xylene	Other	80	20	10	30
Intermediates					
Acetic acid	Other	35	65	55	75
Acetone	Other	60	40	30	50
Acrylic acid	Other	100	0	0	0
Acrylonitrile	Total	100	0	0	0
Adipic acid	Other	100	0	0	0
Aniline	Other	80	20	10	30
Bisphenol A	Other	100	0	0	0
Butanol	Other	19	81	71	91
Caprolactam	Other	100	0	0	0
Cumene	Total	100	0	0	0
Cyclohexane	Other	20	80	70	90
Cyclohexanone	Other	5	95	85	100
Dimethylterephthalate	Other	100	0	0	0
Ethanol	Other	0	100	100	100
Ethylbenzene	Other	100	0	0	0
Ethylenedichloride	Total	0	100	100	100
Ethylene glycol	Other	0	100	100	100
Ethylene oxide	Other	29	71	61	81
Formaldehyde	Other	0	100	100	100
Methyl-tert-butyl-ether (MTBE)[b]	Other	0	0	0	0
Higher alcohols	Other	50	50	40	60

(continued)

Continued

Compound	Total consumption or 'other use'	Mean NODU (%)	Mean ODU (%)	Min release ODU (%)	Max release ODU (%)
Orthophtalates	Total	100	0	0	50
Phenol	Other	0	100	100	100
Phthalic anhydride (PSA)	Other	0	100	100	100
Polyether-Polyols	Other	100	0	0	0
i-Propanol	Other	7	93	83	100
Propylene oxide	Other	0	100	100	100
Styrene	Other	100	0	0	0
Terephthalic acid (TPA)	Other	100	0	0	0
Toluene diisocyanate	Other	100	0	0	0
Urea	Other	0	100	0	100
Vinylchloride monomer (VCM)	Other	20	80	70	90

NODU: not-oxidised during use; ODU: oxidised during use.

[a)]The category 'others' covers all types of applications that have not been worked out.

[b)]In NEAT, the total value assigned to the category 'others' is assigned to the ODU versus the NODU products based on information from the literature (see Neelis et al.[20]).

[c)]The NODU shares for the final products are not listed as they are all 100%.