Naphtha storage fraction and GHG emissions in the Korean petrochemical industry

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Abstract

This paper demonstrates for a Korean case study how to estimate the naphtha storage fraction and CO_2 emissions from naphtha use in the petrochemical industry. We applied the NEAT model to estimate CO_2 emissions by subtracting from the total carbon input the share which is stored in final products. We also estimate the country's naphtha storage fraction by calculating carbon storage in basic chemicals. Since the naphtha storage fraction and the related CO_2 emissions from non-energy use of naphtha depend on a country's production and trade structure, it is appropriate for Korea (with its large production and net exports of chemicals) to estimate a county-specific fraction.

The naphtha storage fraction estimated with the NEAT model was more than 90% for the 2011 to 2015 period in Korea, which is much higher than the IPCC default fraction of 75%. 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 (production and trade structure) of their country. The Korean government is recommended to account for this finding in their national emission accounting.

Keywords: non-energy use and carbon emissions, naphtha storage fraction, NEAT model, CO_2 emissions accounting, Korean petrochemical industry

1. Introduction

Estimation of carbon emissions related to non-energy use is essential for accurate accounting of national GHG emissions. Carbon emissions related to energy (fuel) use of

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fossil fuels like petroleum products and coal can easily be calculated with readily 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 in order to calculate carbon emissions from non-energy (feedstock) use.

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. While carbon in basic chemicals such as benzene, ethylene and propylene is partially stored (depending on the subsequent pathways), carbon in final chemical products such as polyethylene (PE), polypropylene (PP) and polyvinylchloride (PVC) is completely stored (embodied). Thus, the carbon emissions in a country's petrochemical industry will be the difference between carbon inputs and carbon storage. This carbon storage can be calculated by multiplying the carbon inputs with the carbon storage fractions of individual chemicals or fossil fuels.

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% (Vol. 3: Energy, p. 1.28, IPCC, 1997). This naphtha storage fraction was determined based on Marland and Rotty (1984; Marland and Marland, 2003), who had estimated 80% as naphtha storage fraction for the 1950 to 1982 period. This naphtha storage fraction estimated based on the production principle corresponds to a world average value.

However, such storage fractions will vary according to a country's production and trade structure. This explains why the following countries applied a different naphtha storage fraction than the IPCC default storage fraction in their National Inventory Report (NIR) submitted to the UNFCCC (2014): Belgium (100%), France (100%), Finland (100%), Spain (80%), the Netherlands (78%), the USA (70%) and Italy (64%).

The IPCC Guidelines do not define any method to estimate a country-specific naphtha storage fraction. The NEAT 2.0 model (Non-Energy use Emission Accounting Tables model version 2.0) is able to estimate the naphtha storage fraction both on the consumption and production basis by considering a country's production and trade structure of chemicals.

Korea has been a large consumer of naphtha[1] as feedstock for petrochemicals. The

[1] According to the IEA statistics (2016c), the world naphtha consumption for the petrochemical industry was 236.9 Mt in 2014. Naphtha is the most important petrochemical feedstock. Its share in the world petrochemical production was about 50% in 2014 (IEA, 2016b). Major naphtha consumers were China (42.3 Mt), Russia (24.7 Mt), Japan (23.1 Mt), Taiwan (16 Mt), Germany (12.4 Mt), the USA (9.9 Mt) and India (7.8 Mt). Most Asian countries use naphtha as their main petrochemical feedstock, whereas natural gas reach countries in the Middle East and the USA use also ethane and LPG as petrochemical feedstocks.

Korean petrochemical industry processed naphtha in the amount of 39 Mt (million tonnes) or 16.5% of the world consumption to produce various chemicals in 2014 (IEA, 2016c). Thus, the amount of carbon emissions associated with the use of naphtha has been significant. Moreover, Korea has been a large exporter of petrochemicals. Following the national boundary principle (consumption basis) for emissions the carbon emission equivalents related to exported chemicals have to be excluded from the Korean emission inventory.

Park (2005) estimated 88.2% to 89.4% as the naphtha storage fraction for the 1999 to 2000 period in Korea by using the NEAT model. This study caused the Korean government to finance studies in 2012 and in 2015 for estimating the naphtha storage fraction in Korea. The 2015 study by a consulting firm Ecosian (Kim, 2015) came to an estimation of 77% as the naphtha storage fraction for the 2007 to 2013 period in Korea. Given the production structure and Korea's large net exports this seems unlikely, hence calling for further analysis.

This paper demonstrates for a Korean case study how to estimate the naphtha storage fraction and CO_2 emissions from the naphtha use in the petrochemical industry. The Neat model was applied to estimate the Korean naphtha storage fraction for the 2011 to 2015 period as to revise this fraction to be used for the estimation of the annual GHG inventories. 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." (IPCC guidelines, Vol. 3, Energy, p. 1.27).

This paper is organized as follows. Section 2 reviews studies on the naphtha storage fraction in Korea. Section 3 discusses carbon storage and release in the non-energy use and presents the NEAT model for the estimation of carbon storage in the petrochemical industry. Section 4 estimates the naphtha storage fraction by using a NEAT model and a simplified estimation method which both allow the chemicals production and trade structure in the Korean petrochemical industry to take into account. This paper ends with conclusions and policy recommendations.

2. Review of studies

There are three studies which estimated the naphtha storage fraction in Korea. Park (2005) estimated it by applying the so-called NEAT model for the years 1999 and 2000. The two other studies were carried out by a consulting firm Ecosian and commissioned in 2012 and in 2015 by the Korean government.

2.1 Park's study of 2005

In the course of estimating the CO_2 emissions in Korea, Park (2005) estimated the naphtha storage fraction at 88.2% to 89.4% for the 1999 to 2000 period. About five percent points of this storage fraction was related to net exports of ODU (oxidized during use) chemicals which are equivalent to short-lived products according to the IPCC terminology. This result raised interest by the Korean government in view of (potential) need to revise the naphtha storage fraction. A study each in 2012 and 2015 were commissioned by the Korean government through the GHG Inventory & Research Center of Korea.

2.2 Ecosian's study of 2012

Ecosian studied the naphtha storage fraction jointly with the Korea Petrochemical Industry Association (KPIA) and the Korea Petroleum Association in a study commissioned by the Korean government (Ecosian, 2012). For this study, Ecosian made use of the reports submitted by six NCC (naphtha cracking centers or steam crackers) firms. Such reports with steam cracking material flows are submitted by petrochemical firms to get import duties on naphtha refunded; these import duties amount to won 16 (about US cent 1.3) per liter. Ecosian estimated the naphtha storage fraction with a formula as follows:

$$\text{Naphtha storage fraction} = 1 - \frac{\text{Process heat use} + \text{Fuel type byproduct sale}}{\text{Gross deliveries} + \text{Recycled input}} \qquad (1)$$

where the process heat use (also known as internal backflows) means the use of fuels for the heat needed for petrochemical processes (steam cracking) amounted to 4.284 Mt of naphtha in 2011 as shown in Table 1. The fuel type byproduct sale of 1.209 Mt is the amount of byproducts sold to consumers or returned to refineries, which is a part of backflows to refineries (external backflows). The gross naphtha deliveries in the petrochemical sector are those amounts of naphtha delivered from refineries to the petrochemical sector. These amounted to 21.138 Mt of naphtha in 2011. The recycled input refers to those byproducts in the cracking process which are recycled to the cracking process. The recycled input amounting to 8.862 Mt of naphtha comes mostly from the byproducts own use (9.568 Mt) according to Table 1.

The external backflows consisting of sales of categories of "Exports", "Fuel type" and "Others" of the fuel type byproducts amounted to 1.656 (= 0.168 + 1.209 + 0.279) Mt of naphtha in Table 1. The net naphtha deliveries, the difference between the naphtha gross deliveries and the external backflows, amounted to 19.482 (= 21.138 – 1.656) Mt. The non-energy, the difference between the net naphtha deliveries and the internal backflows or the process heat, amounted to 15.198 (= 19.482 - 4.284) Mt.

Table 1: Material balance table used by six producers for refunding import duties on naphtha, 2011 (in 1,000 tonnes)

			Material flow	Sales				Own use	Total
				Exports	Feedstock type	Fuel type	Others		
Input	Gross input		29,990						
	Recycled		8,862						
	Gross deliveries (Net input)		21,138						
Output	Main products	Ethylene	6,877						
		Propylene	3,340						
		etc.							
		Sub total	14,389	1,101	5,996		5	7,863	14,964
	Byproducts	Hydrogen	35						
		CH4	49						
		etc.							
		Sub total	11,053	168	1,143	1,209	279	9,568	12,388
Fuel (Process heat)		4,284							
LOSS		285							
Fuel & LOSS		4,568							

Source: Ecosian, 2012.

Note: 1) The term gross deliveries means deliveries from refineries to NCC crackers who name it as "net input".

2) The amounts of non-energy use (petrochemicals), exports, process heat use and own use are exempted from paying import duties of won 16 per liter. Thus, only the amounts of sales (1.493 Mt) of "Fuel type" (1.209 Mt) and "Others" (0.284) are not refunded. The refunding ratio is calculated as 0.929 [= 1 - (1.493/21.138) * 1.0053]. The factor 1.0053 is the amount of raw material required to convert into one unit of the product.

3) The amounts of main products and byproducts are different from those of their totals due to stock changes.

Ecosian estimated 79% to 81% as the naphtha storage fractions for the 2007 to 2011 period. In reality they did not estimate the naphtha storage fraction but estimated the share of non-energy in the naphtha use, which was 81.7% [= 1 – (4.284 + 1.209)/29.990] in 2011. The share of non-energy in the naphtha use should be 73.5% (= 15.532/21.138) rather than 81.7%. Thus, the denominator of the fraction in Eq. 1 should only contain the gross naphtha deliveries as to estimate the share of non-energy in the naphtha use. Ecosian's study counted twice the amount of the recycled input in the denominator of the fraction in Eq. 1. In conclusion, Ecosian's 2012 study did not lead to corrected values for the naphtha storage fraction.

2.3 Ecosian's study of 2015

Park's 2005 study, according to which the naphtha storage fraction for Korea should be substantially higher than 75% as the IPCC's default naphtha fraction, caused the Korean government to commission another study. Again, Ecosian was given the task for such estimation. Ecosian estimated the naphtha storage fraction for the 2007 to 2013 period in three steps, NCC process, downstream process and carbon storage estimation (described as products step in the study).

In the first step, Ecosian surveyed the process heat use of naphtha in six NCC plants which used, in 2013, 55% of the country's total naphtha consumption and they estimated the share of naphtha used for process heat at 16%.

In the second step, Ecosian estimated 3% (= 1 – 84% * 97%, which should be 2.52%) as the share of the process heat in the remaining naphtha input of 84% in a sample survey of downstream petrochemical firms which convert basic chemicals to intermediates and final products.

In the third step, Ecosian distinguished chemicals produced in the first two steps between long-lived products and short-lived products by using the NODU (Not oxidized during use) and ODU (Oxidized during use) shares of Park's 2005 study. It estimated the share of the long-lived products at 94%. Ecosian multiplied all three ratios (84%, 97% and 94%) each other to estimate the naphtha storage fraction in Korea at 76.6% (rounded up to 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 country's total naphtha input in 2013 and as the production structure of BTX plants of the refineries, which use the remaining naphtha, is quite different from that of NCC plants.

Second, the consideration of NCC plants only in the first step resulted in an imbalance between input of basic chemicals produced in NCC plants and output of intermediates and final products which were manufactured with basic chemicals from both NCC plants and BTX plants (of refineries).

Third, although Ecosian tried to apply the NEAT model's concept on NODU and ODU products, it did not make use of the mass carbon balances to determine the use of basic chemicals and/ or intermediates and the input to produce intermediates and final products in each step of the flow path from a basic chemical through intermediates to final products. As a result, the amount of chemicals with storage was counted twice and trice. For instance, the amount of ethylene was counted once as ethylene itself and those portions of ethylene incorporated in ethylbenzene, styrene, polystyrene, SBR, ABS, SAN, etc.

Fourth, the first two steps to estimate the non-energy use of naphtha are not relevant to estimate the naphtha storage fraction.

3. Method to estimate the naphtha storage fraction

3.1 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 immediately emitted. When fossil fuels are used for non-energy purposes, carbon in the fossil fuels can be incorporated, i.e. stored in products and/or converted into CO_2 emissions. Petroleum products like bitumen and lubricants, and coal products like pitch, naphthalene and carbon black are used for non-energy purposes. A country's CO_2 emissions can be estimated by subtracting the total carbon stored in products from the total input of carbons (fossil fuels). The carbon storage ($E_{storage}$) and carbon release ($E_{release}$) can be calculated with the IPCC standard method (Reference Approach, RA) as follows.

$$\text{Carbon storage: } E_{storage} = \sum_i \{ Q_{NEU,i} * EF_i * P_i \} \qquad (2)$$

$$\text{Carbon release: } E_{release} = \sum_i \{ Q_{NEU,i} * EF_i * (1 - P_i)\} \qquad (3)$$

where Q_{NEUi} means non-energy use (in Joule); EF_i is carbon emission factor (in t CO_2/GJ); P_i is carbon storage fraction.

The carbon storage by non-energy use is obtained by multiplying the non-energy use ($Q_{NEU,\ i}$) identified in the energy statistics with the emission factors (EFi) and the carbon storage fractions (Pi) as shown in Eq. (2). The subscript i indicates the type of non-energy use like bitumen and lubricants. The carbon release (carbon emissions) by non-energy use can be obtained by replacing Pi (carbon storage fractions) on the right side of Eq. (2) with (1 – Pi) as shown in Eq. (3).

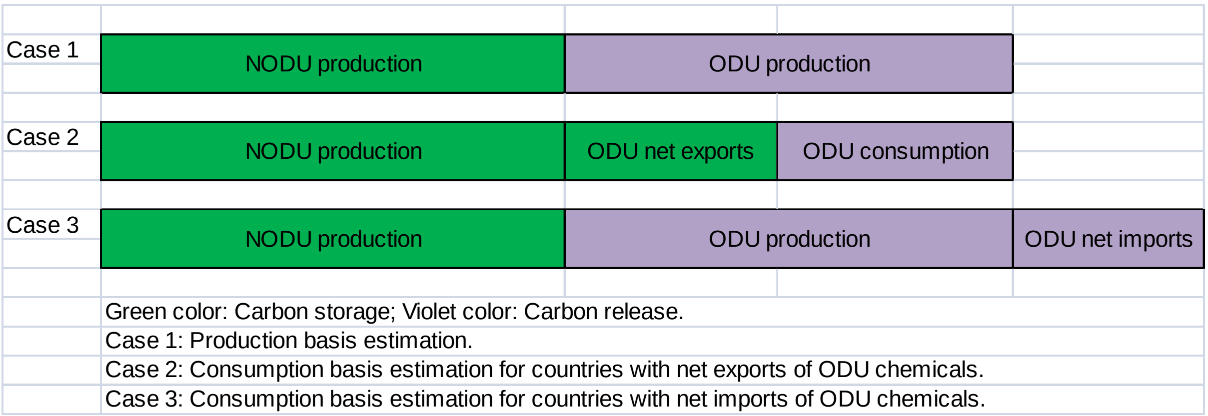
As this study is designed to estimate the carbon storage in the petrochemical industry, $Q_{NEU,i}$ at the right side of Eq. (2) should mean the production or use of petrochemicals like ethylene, propylene and benzene. Since default values for emission factors and carbon storage fractions of petrochemicals are not provided by the IPCC Guidelines, it is necessary to estimate them. The NEAT model, as described in the next Sub-section, provides a method to estimate carbon storage fractions by basic chemical and with it naphtha storage fraction and CO_2 emissions in the petrochemical industry.

3.2 NEAT model

NEU-CO2 group developed a bottom-up spread sheet model named NEAT 2.0 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 (Patel, 2001; Park, 2002, 2005; Neelis et al., 2003). It is consistent with the IPCC emissions estimates because it can calculate emissions in line with the national boundary principle (consumption basis), which takes into account the imports and exports of petrochemical products. Emissions from imported chemicals consumption are allocated to consuming countries.

Fig. 1 clarifies the distinction between the production basis and the consumption basis estimation of carbon storage and release. Net exports of ODU chemicals are considered as a part of carbon storage while net imports of ODU chemicals are considered as a part of carbon release.

Figure 1: Estimation scheme of carbon storage and release



The heart of the NEAT model is a mass carbon balance model which describes a country's production structure of the petrochemical industry, i.e. carbon flows from basic chemicals through intermediates to final products. This balance model was developed based on carbon intensities of chemicals published in C-Ströme (Patel et al. 1999), literature surveys and expert advises. Carbon usage by product (chemical) can be accurately calculated with the help of the mass carbon balance model which consists of two parts, upper balances (normalized transformation coefficients) and lower balances (absolute transformation flows).

The NEAT approach uses the mass carbon balances, so that the inputs and outputs of each process or flow are the same. However, it excludes the shift in stock due to inventory change and incomplete chemical conversion. The NEAT represents all main flows in terms of embodied CO_2 equivalents, so that implications of the GHG reduction policy can be directly derived from the results of the carbon flow analysis.

The upper balances are composed of a 67 by 67 matrix (input and output model) in the case of the Korean petrochemical industry. Their rows indicate the inputs (proportion) of basic chemicals and/ or intermediates for the production of one unit of an intermediate or a final chemical product. For instance, 0.8 Mt CO_2 of p-xylene and 0.2 Mt CO_2 of methanol are required to produce 1 Mt CO_2 of DMT which is one of the raw materials used 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 one unit of intermediates or final chemical products. For instance, production of 1 Mt (CO_2) of aniline requires 1 Mt (CO_2) of benzene and the respective benzene quantities for producing cumene, cyclohexane and ethylbenzene are 0.65 Mt, 1 Mt and 0.75 Mt.

The rows of the lower balances, which are also composed of 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) of DMT, the inputs needed are 0.14 (= 0.8 × 0.17) Mt of p-xylene and 0.04 (= 0.2 × 0.17) Mt of methanol, with 0.8 and 0.2 being the input ratios from the rows of the upper balances. The columns of the lower balances provide the absolute flows in the country (in terms of CO_2 equivalents) of how much of a product is needed for the production of another.

Figure 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 * B)	
Terephtalic acid (TPA) 1)	1.00	14.06	14.06	
Dimethyl terephtalate (DMT) 2)	0.80	0.17	0.14	
Sum of p-Xylene use				14.20
Other use of p-Xylene				0.30

Source : Neelis et al., 2003.

Notes: 1) Stoichometric factors. In the production of TPA(8 carbon atoms), all carbon atoms come from p-Xylene.

2) In the production of DMT (10 carbon atoms), 8 carbin atoms come from p-Xylene and 2 atoms from methanol. Hence, the specific consumption is 0.8 for p-xylene and 0.2 for methanol.

For instance, the input amounts of p-xylene for the production of DMT of 0.17 Mt CO_2 and TPA of 14.06 Mt of CO_2 are 0.14 (= 0.8 × 0.17) Mt CO_2 and 14.06 (= 1 × 14.06) Mt CO_2, with the factors 0.8 and 1 being 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 produce 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 Fig. 2.

3.3 Carbon storage fraction and emission factors of chemicals

The IPCC recommends the use of 75% as naphtha storage fraction unless member countries have established a more accurate value representing their production and trade structure.

The NEAT method distinguishes chemicals which are converted into CO_2 during use as ODU (oxidized during use) products as opposed to chemicals whose carbon is incorporated (stored) in the products as NODU (Not oxidized during use). The carbon embodied in these latter products is typically released no earlier than during waste management (if the product is incinerated while storage continues in the case of landfilling).

The shares of NODU and ODU depend on the usage of chemicals. Final products like polyethylene, 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 usage share distribution between ODU and NODU chemicals is based on data from literature like Weissermel and Arpe (1998), Chauvel and Lefebvre (1989) and Korea Petrochemical Statistics (KPIA, 2017). As there is some uncertainty, the NEAT approach introduces minimum release (maximum storage) and maximum release (minimum storage) apart from the mean release (Appendix 1).

4. Estimation of Korean naphtha storage fraction[2]

4.1 Korean petrochemical industry

The Korean petrochemical industry, which is located in three complexes Ulsan (Southeast of the country), Yecheon (Southwest) and Daesan (West), consists of six petrochemical companies (Naphtha Cracking Centers NCC plants) and four oil refineries (BTX plants). The six petrochemical companies, i.e. 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) produced in the NCC process. Four oil refineries, S-OIL, Hyundai Oilbank, GS Caltex and SK Energy, operate mostly BTX plants. Both NCC

[2] A preliminary result for the 2011 to 2013 period was published in the Korea Forum for Natural Gas Industry (Park, 2016 in Korean).

and BTX plants produce basic chemicals.

Korea's petrochemical industry is ranked fourth in terms of global ethylene production capacity of 8.6 Mt (million tonnes) 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 (KPIA, 2017). The domestic demand for final chemical products has stagnated since the beginning of 2010.

Korea produced 25.658 Mt of naphtha and net imported 20.042 Mt (= imports of 24.201 – exports of 4.159 Mt) in 2014. Unlike other countries, Korean petrochemical and refining companies use almost only naphtha as raw materials for petrochemical products.

4.2 Data

In order to estimate the naphtha carbon storage fraction, the naphtha flows in the petrochemical industry must be accurately determined. Naphtha is processed first to basic chemicals such as ethylene, propylene, butadiene, benzene, toluene and xylene in NCC and additionally in BTX plants of petrochemical companies and in BTX plants of refineries. In this process, fuel-type byproducts are formed apart from the basic chemicals. A part is used as process heat (also known as internal backflows). Another part of these byproducts is returned to refineries, which is called backflows (also known as external backflows). Thus, the non-energy use of naphtha is equal to the naphtha gross deliveries to the petrochemical industry minus process heat use and backflows, which corresponds to the notion of non-energy use of the IEA (https://www.iea.org/statistics/resources/balancedefinitions/).

Non-energy use and fuel (process heat) use of naphtha can be accurately determined with information given in the World Energy Statistics of the IEA (2016c). For instance, the gross naphtha use was 45.552 Mt in 2014, of which 6.590 Mt (14.47% of the total) were external backflows and 8.363 Mt (18.36%) whereas internal backflows. Thus, the naphtha non-energy use was 30.599 Mt or 67.17% of the total naphtha use.

In order to run the NEAT model, data on production and trade of 67 major petrochemicals, including 12 basic chemicals, 32 intermediates and 23 final chemicals, are required. About 30 of these 67 petrochemical production data have been published in the Korea Petrochemical Statistics of the Korea Petrochemical Industry Association (KPIA, 2017). However, the remaining production data are 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).

4.3 Estimation of naphtha storage fraction in Korea

This study estimates 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 as to distinguish between NODU (storage) and ODU (release) chemicals.

For instance, carbon storage and release of a basic chemical ethylene can be estimated as follows. The petrochemical industry produced in 2015 ethylene in the amount of 26.019 Mt CO_2 (8.279 Mt) in carbon terms, whereas 1.359 Mt CO_2 (0.433 Mt) of ethylene was net exported. The industry used the remaining ethylene of 24.659 (= 26.019 – 1.359 with a rounding difference of 0.001) Mt CO_2 for the production of intermediates and final products as shown in Fig. 3.

The amount of carbon storage and release from the use of ethylene can be established from four different sources. The first source is carbon storage and release calculated from the ethylene input for the production of various intermediates and final chemicals like ethylbenzene, styrene, polyethylene, epoxy resin, and polyvinylacetate as shown in Table 2. 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 2.

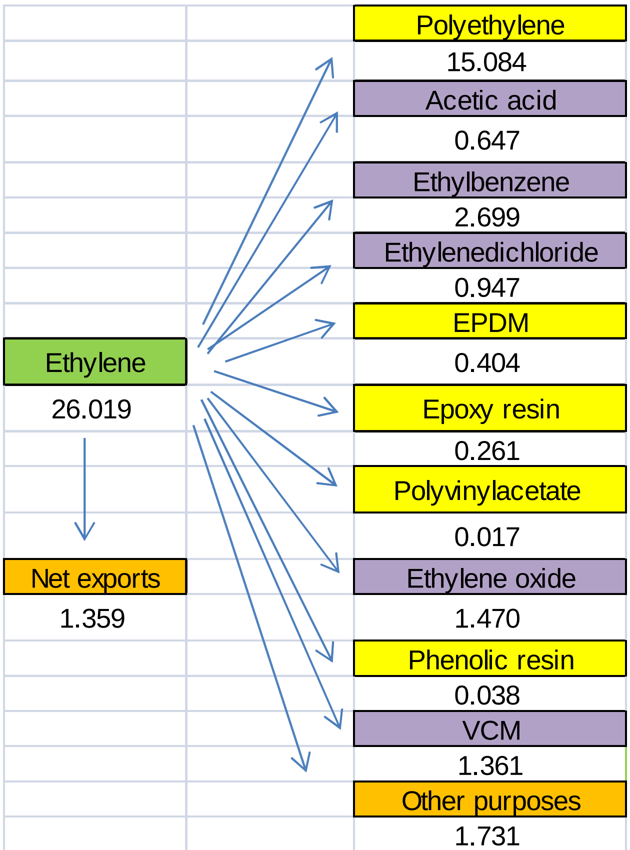
Gross carbon storage of intermediates and final products, which are produced with ethylene, is estimated as the sum of production of NODU chemicals and net exports of ODU chemicals. And gross carbon release of intermediates, which are produced with ethylene, is estimated as the product of use of intermediates for the production of other chemicals with the corresponding ODU shares. There is no gross carbon release for final products in Table 2 as the ODU shares of final products and intermediate like ethylbenzene and styrene are zero (0). Carbon storage and release of intermediates and final products are calculated as the product of gross carbon storage and release with the ethylene content of the corresponding chemical, respectively.

Table 2 shows a minus (-) sign of the carbon storage of ethanol. The reason is because, Korea did not produce any ethanol based on naphtha and there was a net export of -0.258 Mt CO_2 or a net import of 0.258 Mt CO_2.

The second source is carbon storage and release in the amount of 0.866 (= 0.5 * 1.731) Mt CO_2 each, which are calculated from the use of ethylene (1.731 Mt CO_2) for other purposes (other products than the chemicals listed in Fig. 2), as shown in Table 3. In the case of ethylene, an ODU factor of 0.5 is estimated for NODU versus ODU. The third source is carbon storage related to net exports of ethylene, which amounted to 1.359 Mt CO_2 in

2015.

Figure 3: Ethylene flow path in NEAT model in 2015



Notes: Chemicals in million tonnes (Mt) CO_2.

Green: basic chemicals; Violet: intermediates; Yellow: final products;

Orange: Other purposes and net exports.

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 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 first to third sources. This study allocates the difference of 0.892 Mt CO_2 to storage (97%) and release (3%) share shown in Table 2 and Table 3 (0.865 Mt CO_2 storage versus 0.027 Mt CO_2 release).

Table 2: Carbon storage & release from the use of ethylene to produce 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

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.

Table 3: Carbon storage & release from the use of ethylene, consumption basis, 2015 (Mt CO_2)

	Storage	Release	Sub-total
1. Production of intermediates & 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%

In summary, the carbon storage and release from the use of ethylene were 24.467 Mt CO_2 (94.04%) and 1.552 Mt CO_2 (5.96%) in 2015, respectively. Carbon storage and release for other basic chemicals can be estimated by analogy with the estimation of basic chemical ethylene. Table 4 represents the estimation of carbon storage and release of basic chemicals in 2015.

The most important basic chemicals with regard to carbon storage were found to be p-xylene, ethylene, propylene and benzene which recorded high shares of carbon storage (NODU shares). Toluene, other C4 and m-xylene are characterized high shares of carbon release (ODU shares).

Table 4: Carbon storage & release by basic chemical, consumption basis, 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			114.455	104.641	9.814
in %			100.0	91.4	8.6

The composition of carbon storage and release for the 2011 to 2015 period is summarized in Table 5. For instance, Korea produced in 2015 NODU and ODU chemicals amounting to 97.149 Mt CO_2 (84.9%) and 17.305 Mt CO_2 (15.1%), respectively. Thus, the naphtha storage fraction was 84.9% on the production basis.

However, Korea only used (consumed) the ODU products equivalent to 9.810 Mt CO_2 and net exported an equivalent of 7.495 Mt CO_2 (6.5%) in 2015. As the exported ODU products will release carbon in the importing countries, these ODU products can be considered as carbon storage for the exporting country. Making this correction, the carbon storage and the naphtha carbon storage fraction increased to 104.644 Mt CO_2 and 91.4% for the year 2015, respectively.

Table 5 reveals that the share of NODU in the Korean petrochemical industry amounts to a share of 86.2% in the 2011 to 2015 period which is substantially higher than the IPCC default naphtha storage fraction of 75%. Furthermore, Korea net exported 45.7% (= 6.3%/13.8%) of the ODU products. This results in a naphtha storage fraction between 91.2% and 93.8%, with an average of 92.5% in the 2011 to 2015 period.

This study suggests a naphtha storage fraction of 90% to be used for the estimation of the annual GHG inventories by the Korean government. Applying this value instead of the officially used value (IPCC default storage fraction of 75%) would result in much lower CO_2 emissions in the national inventory report: Korea reported carbon emissions that are about 17.168 (= 114.455 * 15%; 15% is the difference between 90% and the officially used value of

75%) Mt CO_2 higher than its actual level of carbon emissions for the year 2015. The overestimated carbon emissions correspond to 2.7% of the country's total carbon emissions of about 630 Mt CO_2 in 2015.

Table 5: Composition of naphtha storage & release for the 2011 to 2015 period

	Production basis estimates			Consumption basis estimates						
	Production			Consumption			Net exports		Storage	Release
	NODU	ODU	Sum	NODU	ODU	Sum	NODU	ODU		
	(A)	(B)	(C = A + B)	(D)	(E)	(F = D + E)	(G)	(H)	(A + H)	(E)
	[Mt CO_2]	[Mt CO_2]	[Mt CO_2]	[Mt CO_2]	[Mt CO_2]	[Mt CO_2]	[Mt CO_2]	[Mt CO_2]	[Mt CO_2]	[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%

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.

4.4 Simplified estimation of naphtha storage fraction in Korea

It is not straightforward to estimate yearly the naphtha storage fraction by applying the (full) NEAT model due to difficulties to collect all the production data on chemicals. As explained earlier, only 30 of about 70 production data are published in the Korea Petrochemical Statistics of the KPIA. The other production data has to be collected directly from companies. Unless institutionalized, it may be adequate to conduct detailed analyses every three to five years and to apply a simplified method in-between. Based on this study it is suggested the use of the average values storage fractions of the three years from 2013 to 2015 as given in the last column of Table 6 in order to estimate the naphtha storage fractions for the years after 2015 without running the full NEAT model. These average values have to be multiplied by the equivalents of embodied CO_2 by basic chemical and production data in order to estimate the carbon storage in absolute terms.

For instance, the naphtha storage fraction on the consumption basis for the year 2016 is estimated as the ratio between the sum of carbon storage of all basic chemicals and the total carbon input in the petrochemical industry, which yields the weighted average value of carbon storage fractions of basic chemicals. The resulting estimated naphtha storage fraction is on the consumption basis.

Table 6: Storage fractions by basic chemical estimated with the NEAT method for the 2013 to 2015 period

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

This study uses the trade statistics of the Korea International Trade Association (KITA) for 67 chemicals and the NODU and ODU shares given in Appendix 1 to estimate the net export share of ODU products in the total carbon input of the petrochemical industry. The naphtha storage fraction on the production basis is the difference between the naphtha storage fraction on the consumption basis and the share of net exports of ODU products in the total carbon input. This approach allows for changes in the production and trade structure of chemicals.

4.5 Sensitivity Analysis

There are some uncertainties in the use of NODU and ODU shares in petrochemical products. This is because the exact use patterns of petrochemical products are unknown. In addition to the baseline mean release, 'maximum release' (maximum emissions) and 'minimum release' (minimum emissions) cases are considered. For the maximum release case the shares of ODU are increased by 10% points except for those ODU shares which are zero (0%). For the minimum release case these shares are decreased by 10% points except for those 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 represents 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 7. The naphtha storage fraction ranges from

90.9% to 92.6% for the year 2015.The results of this study indicate that the IPCC default storage fraction for naphtha is too low as the NODU share in the Korean petrochemical industry should be higher than the IPCC default factor of 75% and as Korea is a net exporter of ODU chemical products.

Table 7: Sensitivity analysis for the naphtha storage fraction for the year 2015

	Production basis estimates			Consumption basis estimates			
	Production			Net exports		Storage	Release
	NODU	ODU	Sum	NODU	ODU		
	(A)	(B)	(C = A + B)	(D)	(E)	(A + E)	(B - E)
	[Mt CO2]	[Mt CO2]	[Mt CO2]	[Mt CO2]	[Mt CO2]	[Mt CO2]	[Mt CO2]
Mean	97.149	17.305	114.455	56.153	7.495	104.644	9.810
Release	84.9%	15.1%	100.0%		6.5%	91.4%	8.6%
Maximum	97.149	21.481	118.631	52.994	10.654	107.803	10.828
Release	81.9%	18.1%	100.0%		9.0%	90.9%	9.1%
Minimum	97.149	13.755	110.905	58.057	5.591	102.740	8.165
Release	87.6%	12.4%	100.0%		5.0%	92.6%	7.4%

5. Conclusions and policy implications

Estimation of carbon emissions related to non-energy use is very important for accounting of national GHG emissions especially for countries with a large petrochemical industry like the Netherlands, Germany, Japan and Korea. However, the IPCC guidelines do not provide any method to estimate the carbon storage and release of the petrochemical industry. They only provide default storage fractions for petroleum products like LPG, bitumen, lubricant and naphtha, but not those of chemicals.

Furthermore, the IPCC guidelines do not consider the trade with chemicals. Importing rather than exporting countries should be responsible for the emissions of short-lived chemicals consumed. This is in line with the approach for exports of petroleum products such as gasoline and diesel in the emission accounting. The only difference in the exports between petroleum products and chemicals is the availability of the statistics. The energy statistics, which are the basis of emission accounting of fossil fuels, list imports and exports of fossil fuels but not those of chemicals.

The NEAT model for emission accounting provides a method to estimate carbon storage and release of non-energy use in the petrochemical industry and the storage fraction of naphtha which is the main feedstock for the petrochemical industry especially in Asian countries. It represents a country’s petrochemical processes in terms of mass carbon balances. A country’s carbon flows from naphtha through basic chemicals and intermediates to final chemical products can be exactly followed with help of these mass carbon balances. The NEAT model is also applied to calculate imports and exports of both ODU and NODU chemicals, which allows to estimate both the naphtha storage fraction and the carbon emissions in the petrochemical industry based on the domestic consumption (rather than the production) of chemical products .

Moreover, this study applied a simplified method to estimate the carbon emissions in the petrochemical industry and the naphtha storage fraction in Korea. This is necessary as it is difficult to collect all the data on chemical products on the yearly basis. The average storage fractions of basic chemicals can be used to estimate the carbon emissions in the petrochemical industry and the naphtha storage fraction for future years.

The naphtha storage fraction estimated with the NEAT model was more than 90% for the 2011 to 2015 period in Korea, which is much higher than the IPCC default fraction of 75%. Korea's carbon emissions estimated with the IPCC default naphtha fraction of 75% is likely to have resulted in an overestimation of 17.1 Mt CO_2 (15% of the emissions related to the use of naphtha in 2015) or 2.7% of the country's total carbon emissions (about 630 Mt CO_2).

To conclude, a revision of the naphtha storage fraction from 75% to 90% is proposed for the Korean petrochemical industry. The IPCC allows countries to apply their own values that represent more accurately the situation of their country. The Korean government is recommended to account for this finding in their national emission accounting.

Furthermore, this study can contribute to improve the estimation of CO_2 emissions from the non-energy (feedstock) use in the petrochemical industry worldwide. The NEAT method will be of particular interest for those countries which produce more chemicals with higher storage fractions and/or which are net exporters of short-lived chemicals. When using the IPCC default naphtha storage fraction, their reported CO_2 emissions will typically be overestimated.

Acknowledgements

The authors wish to express their gratitude to the Korean petrochemical community for the assistance to collect required data on petrochemicals production and trade, especially to Mr. Pyung Joong Kim, Director for Industrial Research, Korea Petrochemical Industry Association.

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

Compound	Total consumption or 'other use'	MEAN NODU [1] [%]	MEAN ODU [1] [%]	MIN RELEASE ODU [1] [%]	MAX RELEASE ODU [1] [%]
BASIC CHEMICALS					
Acetylene	other [2]	50	50	40	60
Benzene	other	50	50	40	60
Butadiene	other	100	0	0	0
Other C4	other	37	63	53	73
CO-Source	other	50	50	0	0
Ethylene	other	50	50	40	60
Methanol	other	50	50	40	60
Propylene	other	60	40	30	50
Toluene	other	30	70	60	80
Xylenes (o-,m-,p-,mixed xylene)	total [3]	70	30	20	40
ortho-Xylene	other	0	100	100	100
meta-Xylene	total	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	other	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	total	19	81	71	91
Caprolactam	other	100	0	0	0
Cumene	other	100	0	0	0
Cyclohexane	other	20	80	70	90
Cyclohexanone	other	5	95	85	100
Dimethylterephthalate	other	100	0	0	0
Ethanol	total	0	100	100	100
Ethylbenzene	other	100	0	0	0
Ethylenedichloride	other	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) [3]	total	0	0	0	0
Higher alcohols	other	50	50	40	60
Orthophtalates	other	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	total	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
Isocyanates	other	100	0	0	0
Urea	other	0	100	0	100
Vinylchloride monomer (VCM)	other	20	80	70	90

[1] ODU = Oxidised During Use, NODU = Not-Oxidised During Use

[2] The category "others" includes all types of applications, which have not been elaborated.

[3] In NEAT, the total assigned to the category "others" is allocated to ODU versus NODU products by means of information from literature (see Neelis et al., 2005).

[4] The NODU shares for final products are not listed as these are all 100%.

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