Proposal for streamlining Tier 2 methodology for ethylene production and estimated emission factors based on Russian data

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Tier2 total feedstock carbon balance method for CO_2 emission estimation from ethylene production

EQUATION 3.17
OVERALL TIER 2 MASS BALANCE EQUATION

$$ECO2_i = \left\{ \sum_k \left(FA_{i,k} \bullet FC_k \right) - \left[PP_i \bullet PC_i + \sum_j \left(SP_{i,j} \bullet SC_j \right) \right] \right\} \bullet 44/12$$

Where:

$ECO2_i$ = CO_2 emissions from production of petrochemical *i*, tonnes

$FA_{i,k}$ = annual consumption of feedstock *k* for production of petrochemical *i*, tonnes

FC_k = carbon content of feedstock *k*, tonnes C/tonne feedstock

PP_i = annual production of primary petrochemical product *i*, tonnes

PC_i = carbon content of primary petrochemical product *i*, tonnes C/tonne product

$SP_{i,j}$ = annual amount of secondary product *j* produced from production process for petrochemical *i*, tonnes

SC_j = carbon content of secondary product *j*, tonnes C/tonne product

Carbon mass balance approach is proposed as Tier2 methodology for CO_2 emission estimation for all source categories in petrochemical industry (IPCC 2006 Guidelines, volume 3, part 1 p. 3.67 equation 3.17).

This approach is applicable in cases where activity data are available for both feedstock consumption and primary and secondary product production and disposition.

Problems with implementation of the Tier 2 Methodology

- **There are no technological CO_2 emissions from the process itself because it is carried on without access of air. (http://www.eea.europa.eu//publications/emep-eea-guidebook-2016, 2.B Chemical industry 2016.pdf, ethylene (040501) and propylene (040502), p. 34).**
- **Many secondary products including propylene, butadiene and aromatics are produced in the steam cracking process. Only some of these secondary products may be combusted as a fuel for the process or for some other purposes. It is the main source of CO_2 emissions from the process.**
- **The types and compositions of feedstocks for steam cracking process vary considerably from one facility to another. Consequently, the number, amount and compositions of secondary products may be different. Using of default feedstock-product matrix does not improve the emission estimates.**
- **The feedstock carbon content and some secondary products' carbon content may differ substantially. It will result in significant uncertainties of CO_2 emission estimates if default or inaccurate carbon content values are used in the calculations.**
- **Another reason for significant uncertainties of the CO_2 emission estimates from steam cracking process. Some secondary products may be omitted or incorrectly accounted because the collection of so much activity data is very difficult to implement.**
- **Carbon balance methodology seems to be time and resource consuming. A lot of data from many facilities should be received to implement this methodology properly. The Tier2 methodology looks more like Tier3 methodology.**
- **Despite a lot of work done, the implementation of this methodology will not result in reliable and solid emission estimates.**

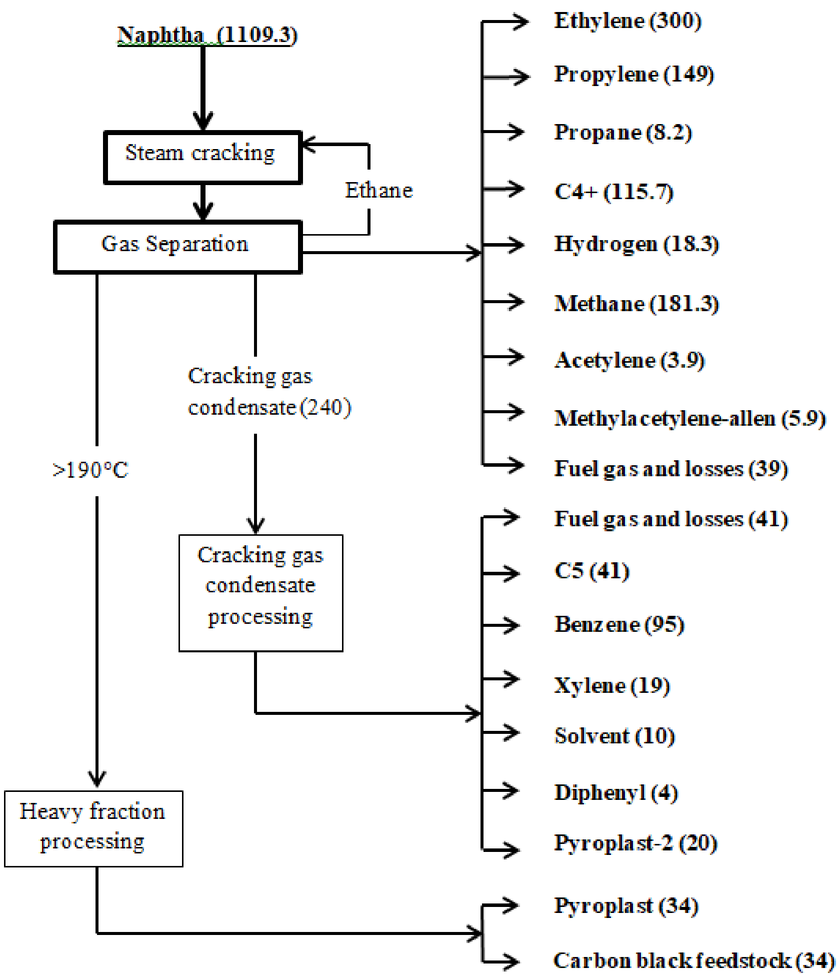
Default steam cracking feedstock-product matrix (IPCC 2006 Guidelines)

TABLE 3.25
ETHYLENE STEAM CRACKING FEEDSTOCK-PRODUCT MATRIX

	kg product/tonne feedstock					
Product **Feedstock**	**Naphtha**	**Gas oil**	**Ethane**	**Propane**	**Butane**	**Others**
High Value Chemicals	**645**	**569**	**842**	**638**	**635**	**645**
Ethylene	324	250	803	465	441	324
Propylene	168	144	16	125	151	168
Butadiene	50	50	23	48	44	50
Aromatics	104	124	0	0	0	104
Fuel grade products and backflows	**355**	**431**	**157**	**362**	**365**	**355**
Hydrogen	11	8	60	15	14	11
Methane	139	114	61	267	204	139
Ethane and propane after recycle	0	0	0	0	0	0
Other C4	62	40	6	12	33	62
C5/C6	40	21	26	63	108	40
C7+ non-aromatics	12	21	0	0	0	12
<430C	52	26	0	0	0	52
>430C	34	196	0	0	0	34
Losses	5	5	5	5	5	5
Total	**1 000**	**1 000**	**1 000**	**1 000**	**1 000**	**1 000**

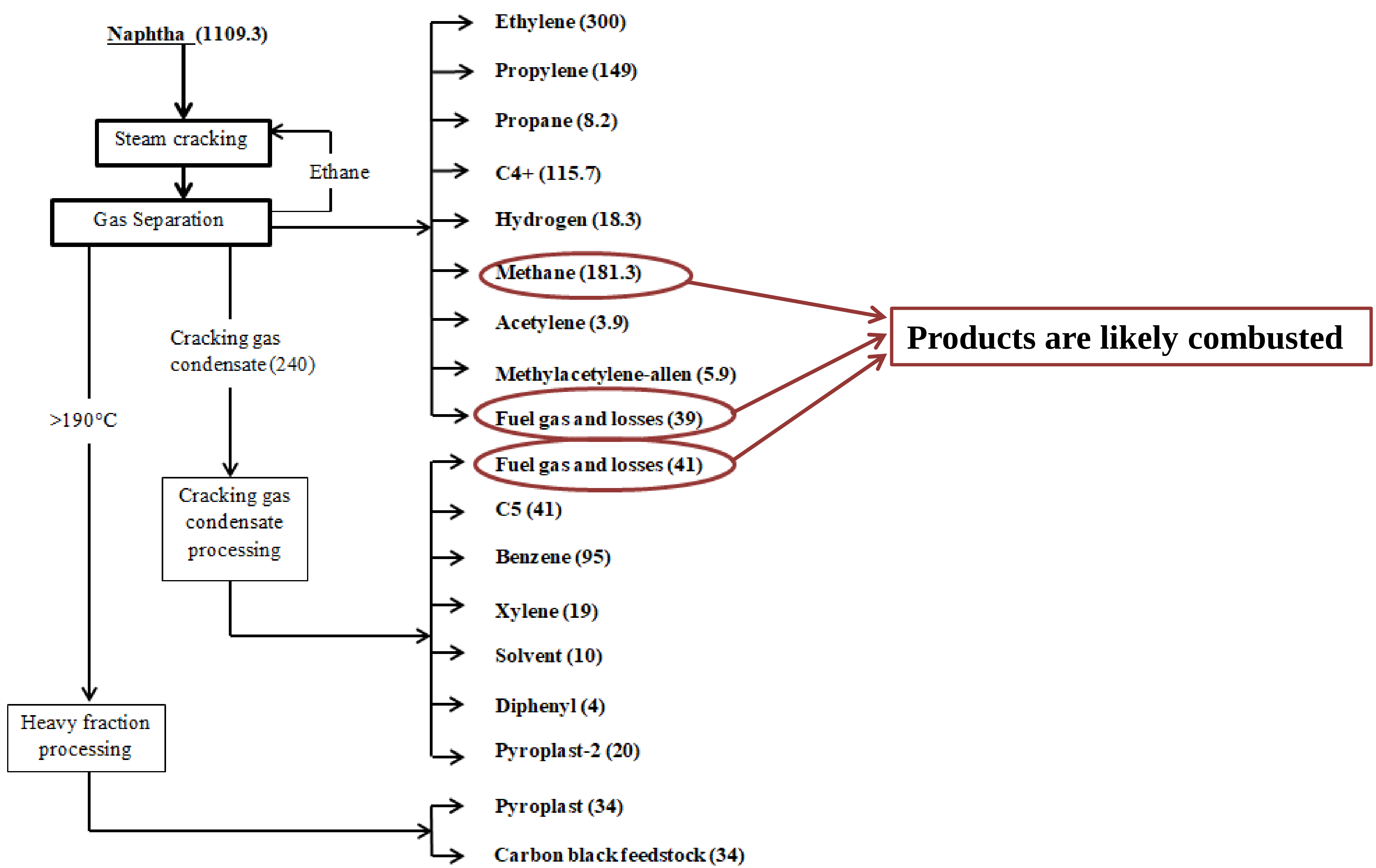
Source: Neelis, M; Patel, M; de Feber, M; Copernicus Institute, April 2003, Table 2.2, Page 24

Material balance (the feedstock-product matrix) of steam cracker EP-300 (10^3 t)



Source: Mukhina T.N., Baranov N.L., Babash C.E. et al. Steam cracking of hydrocarbon feedstock Moscow, Khimiya, 1987, 240 p. (in Russian)

Material balance (the feedstock-product matrix) of steam cracker EP-300 (10^3 t)



Proposal for Tier 2

- **Pick out secondary products which are likely to be combusted for energy in the steam cracking process or for other purposes.**
- **Based on feedstock-product matrix it is possible to calculate amounts of these products using proportion between ethylene and other products of the steam cracking process.**
- **It is not necessary to collect information on amounts of feedstock used and other secondary products output. Only data on ethylene production disaggregated by feedstock used should be collected.**

$$ECO_2 = \sum_j EF_j * MEP_j$$

$$EF_j = \frac{\sum_i (FP_{ij} * C_i) * 44/12}{EP_j}$$

ECO_2 = CO_2 emission from ethylene production, *tonnes*

EF_j = CO_2 emission factor for feedstock ***j***, *tonnes CO2/tonne ethylene produced*

FP_{ij} = output of secondary product ***i*** combusted for energy, for feedstock ***j***, *tonnes*

C_i = carbon content of combusted secondary product ***i***, *tonnes C/tonne product*

EP_j = ethylene output for feedstock ***j***, *tonnes*

MEP_j = total annual ethylene production from feedstock ***j***, *tonnes*

- **Outputs of ethylene and secondary products should be taken from feedstock-product matrix for every feedstock type.**

Steam cracking feedstock-product matrix

<table>
<tr><th>Products</th><th colspan="4">Feedstock</th></tr>
<tr><td></td><td>NGL [1)]</td><td>Ethane</td><td>Propane</td><td>n-Butane</td></tr>
<tr><td>Hydrogen</td><td>14.5</td><td>60</td><td>15</td><td>13</td></tr>
<tr><td>Methane</td><td>225</td><td>90</td><td>260</td><td>207</td></tr>
<tr><td>Butadiene</td><td>27</td><td>-</td><td>-</td><td>25</td></tr>
<tr><td>Propane - Butane</td><td>137</td><td>45</td><td>30</td><td>105</td></tr>
<tr><td>Propylene</td><td>174</td><td>35</td><td>150</td><td>190</td></tr>
<tr><td>Ethylene</td><td>334</td><td>750</td><td>420</td><td>330</td></tr>
<tr><td>Light steam cracking gas condensate</td><td rowspan="2">88.5</td><td>20</td><td>90</td><td>100</td></tr>
<tr><td>Heavy steam cracking gas condensate</td><td>-</td><td>35</td><td>30</td></tr>
</table>

[1)] *Natural gas liquids; Broad fraction of light hydrocarbons*

Source: Akhmediyanova R.A., Rakhmatullina A.P., Shaykhutdinova L.M. Technological processes of natural gas processing and use., St. Petersburg , Professiya, 2016, 368 p. (in Russian)

Assumptions and parameters used for calculations of feedstock specific emission factors

Feedstock	Combusted secondary products	Parameters	
Naphtha	Methane	Methane carbon content 0.749	Default losses value 0.5%
	Fuel gas (refinery gas)	default net calorific value 49.5 Tg/Gg, default carbon content 15.7 kg/GJ	
Ethane	Methane	Methane carbon content 0.749	
Ethane	Methane	Methane carbon content 0.749	
	Light steam cracking gas condensate (refinery gas)	default net calorific value 49.5 Tg/Gg, default carbon content 15.7 kg/GJ	
Propane **n-Butane** **NLG**	Methane	Methane carbon content 0.749	
Propane **n-Butane** **NLG**	Methane	Methane carbon content 0.749	
	32% Light steam cracking gas condensate (refinery gas) similarly to naphtha	default net calorific value 49.5 Tg/Gg, default carbon content 15.7 kg/GJ	

Feedstock specific CO_2 emission factors estimated on the base of Russian ethylene producing industry information

tonnes CO_2/tonne ethylene produced				
Naphtha	NGL	Ethane	Propane	n-Butane
2.37	**1.88 - 2.07**	**0.33 - 0.41**	**1.70 - 1.90**	**1.72 - 2.00**

- **Supplemental fuel combustion was not taken into account.**

Thank you for your attention!