## Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Contents</td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>Nomenclature</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>1</td>
<td>Description of the Refinery Model</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>Allocation in the GaBi refinery model</td>
<td>6</td>
</tr>
<tr>
<td>2.1</td>
<td>Crude Oil Demand Allocation</td>
<td>7</td>
</tr>
<tr>
<td>2.2</td>
<td>Thermal Energy Demand Allocation</td>
<td>8</td>
</tr>
<tr>
<td>2.3</td>
<td>Electricity Demand Allocation</td>
<td>8</td>
</tr>
<tr>
<td>2.4</td>
<td>Allocation Example and Allocation method choice explanations</td>
<td>9</td>
</tr>
<tr>
<td>2.4.1</td>
<td>Crude oil demand</td>
<td>9</td>
</tr>
<tr>
<td>2.4.2</td>
<td>Thermal energy/ steam demand</td>
<td>10</td>
</tr>
<tr>
<td>2.4.3</td>
<td>Electricity demand</td>
<td>11</td>
</tr>
<tr>
<td>2.5</td>
<td>The Backpack Principle</td>
<td>11</td>
</tr>
<tr>
<td>3</td>
<td>Literature</td>
<td>14</td>
</tr>
</tbody>
</table>
Nomenclature

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Explanation</th>
</tr>
</thead>
<tbody>
<tr>
<td>ETBE</td>
<td>Ethyl-Tertiary-Butyl-Ether</td>
</tr>
<tr>
<td>FCC</td>
<td>Fluid Catalytic Cracking</td>
</tr>
<tr>
<td>HC</td>
<td>Hydro Carbon</td>
</tr>
<tr>
<td>ISO</td>
<td>International Organization for Standardization</td>
</tr>
<tr>
<td>LCA</td>
<td>Life Cycle Assessment</td>
</tr>
<tr>
<td>LCI</td>
<td>Life Cycle Inventory</td>
</tr>
<tr>
<td>LPG</td>
<td>Liquefied Petroleum Gas</td>
</tr>
<tr>
<td>MTBE</td>
<td>Methyl-Tertiary-Butyl-Ether</td>
</tr>
<tr>
<td>NCV</td>
<td>Net Calorific Value</td>
</tr>
<tr>
<td>RON</td>
<td>Research Octane Number</td>
</tr>
</tbody>
</table>

1 Description of the Refinery Model

Crude oil refineries are complex plants. The combination and sequence of a large number of processes is usually very specific to the characteristics of the crude oil input and the products to be produced. Additional influencing factors are the market demand for the products, the available crude oil quality and certain requirements of the petroleum products set by authorities determining the configuration and complexity of a refinery.

Simple Hydro-skimming refineries can process only a few crude oil qualities and produce few high-quality products. Complex refineries with many conversion plants can process different crude oil types and produce different product slates.

Crude oil refinery activities begin with the input of crude oil. After desalting, the crude oil is fed to the distillation column for atmospheric distillation (fractionation of the crude oil by separation according to density/boiling/condensation areas). The light ends (gases) go up to the head of the column and are dispatched to the liquid gas system to recover methane and ethane for use as refinery fuel and LPG (propane and butane) as marketable products. This light product separation occurs in almost every refinery. These gases can also be used in a steam-reforming process to produce hydrogen, which is necessary for the desulfurization processes, the hydrocracking and, to a lesser extent, the isomerization unit.
The straight-run naphtha of the atmospheric distillation, which is taken in the upper trays of the column are divided and fed to three different processes. The light naphtha fraction is introduced to the chemical sweetening process in some refineries. Some sweetened naphtha is directly blended to the gasoline. The main fraction is sent to the isomerization unit where the aliphatic paraffins are converted into iso-paraffins with a high octane value. Often there is a de-isopentanizer (distillation) downstream to increase the acquisition of iso-components. These iso-paraffins are very valuable components for gasoline production with high RON content.

After desulfurization, the heavy naphtha fractions are sent to the reformer for catalytic transformation from aliphatic paraffins to iso-paraffins and from cyclo-paraffins to aromatic compounds, with a reduction of the net calorific value. The specific feature of this process is the production of hydrogen (the only hydrogen producer besides additional plants, like steam-reforming). The outputs of the isomerization (often including a de-isopentanizer) and catalytic reforming go to the gasoline blending system and premium or regular gasoline follows as a product.

Kerosene is directly obtained from the atmospheric distillation and is separately treated from the rest of the middle distillates fraction. The main portion of the middle distillates produced in the atmospheric distillation is deployed into the hydrofiner (for desulfurization). The desulfurized product is fed to the middle distillate blender. The residue from the atmospheric distillation is introduced to the vacuum distillation. Here, distillation occurs in light vacuum gas oil, vacuum gas oil (wax distillate) and vacuum residue.

A portion of the atmospheric residue is fed into the visbreaker (mild thermal cracking). Small amounts are sometimes introduced directly into the heavy fuel oil blending system and the asphalt-blowing process. The light gas oil, as a product of the vacuum distillation, goes to the hydrofiner, is desulfurized, and employed to the middle distillate blender. Some of the vacuum distillate, which has been taken from the middle trays of the vacuum distillation, is introduced to the base oil production of lubricants and waxes (paraffins). Most of it is fed either to a catalytic cracker (often first desulfurized) or a hydrocracker, where the feeds are converted into shorter chains by molecule restructuring. The products are gases, gasoline, middle distillates and heavy cycle gas oils (components of the heavy fuel oil). The gases of the catalytic cracking are treated in an alkylation and polymerization unit to manufacture additional valuable gasoline components. These processes are used to combine small petroleum molecules into larger ones.

Butylene of the catalytic cracker is further used together with external supplied methanol to produce Methyl-Tertiary-Butyl-Ether (MTBE), a product used as octane booster. Externally purchased (bio-)ethanol is also often used in the esterification instead of Methanol. In this case
The product is called ETBE. The naphtha of the FCC has to be treated in a special desulfurization process to reduce the high sulfur content. The vacuum residues go into the coking process, which produces gases, gasoline, middle distillates and heavy fuel oil. A further product is petroleum coke, which is then purified. The vacuum residue, like some of the atmospheric residue, is also used as feed for the visbreaking, which also produces gases, naphtha, middle distillates and heavy fuel oil. The extracted hydrogen sulfides of all desulfurization processes are fed to a sulfur recovery unit to recover elemental sulfur.

The energy generation (heat, steam and electricity) requires a large amount of fuels. The fuel burned in refineries power plants and incinerators may be refinery gas, light fuel oil, heavy fuel oil (residual oil), petrol coke and sometimes LPG. In addition, purchased natural gas and electricity is also employed.

The main material and energy flows (input - output) are shown in the following graph “System Boundary of a Refinery”.

![System Boundary of a Refinery](image)

A simplified flow chart is shown below. The arrangement of these processes varies among refineries and few, if any, employ all of these processes.
Almost all refinery operations are multifunctional processes. Multifunctional processes create two or more simultaneous products (co-products). The challenge is to allocate the individual loads of the material and energetic input as well as the emissions released by the process to each product. ISO standards 14040 and 14044 define allocation as “partitioning the input or output flows of a process or a product system between the product system under study and one or more other product systems.”

The inputs of nearly each of the refinery unit processes are thermal energy, steam (both from now on called simply “energy”), electricity and crude oil (crude oil only fed in the atmospheric distillation, the other refinery processes only has a corresponding crude oil consumption). The environmental burdens associated with the provision of these energy and material inputs, e.g. emissions from the steam generation or the upstream emissions of the crude oil supply, must be allocated according to the relationship of the different products. This association is done using a distribution tool called allocation factors.
Furthermore, it is assumed that all emissions caused within the refinery (from thermal energy, steam, and electricity production as well as single processes and losses) arise in the refinery power plant and are allocated to the refinery products with the help of the amount of energy input of each unit process. This assumption is validated by the fact that nearly all emissions (>95%) are released by the energy supply and in particular by the on-site power plant.

Therefore, the environmental burdens of the following “processes” listed below must be allocated to the refinery products. These include:

- The emissions of the refinery power plant (incl. the power plant itself, converting plants, decentralized boilers, storage, losses)
- The impact of the crude oil supply (crude oil mix)
- The impacts of the electricity supply (purchased electricity which is used in addition to the one produced in the power plant; electricity mix)
- The impacts of the natural gas supply (if natural gas is used; natural gas mix)
- The impacts of the methanol/ethanol supply (if MTBE/ETBE is produced)
- The impacts of the hydrogen supply (if hydrogen from external sources is used)

An appropriate allocation factor must be chosen and its suitability must be justified.

The emissions caused by refining are allocated similarly to the impacts of the upstream chains external electricity and natural gas following a mass allocation. The impacts related to the crude oil supply are allocated by energy content to the products. Impacts from methanol/ethanol and hydrogen supply are assigned directly to the applicable products, e.g. the methanol and ethanol emissions to the produced gasoline.

In the next paragraph, the choice of the allocation method is described theoretically and in the following further explained by applying to an example.

In general, the allocation condition must be fulfilled, i.e. the inputs and outputs which have been allocated in a unit process must add up to the inputs and outputs before the allocation were performed.

### 2.1 Crude Oil Demand Allocation

Crude oil demand is how much crude oil is received by the refinery. This crude oil is processed to refinery products like diesel, gasoline, etc. Processing crude oil determines emissions in the crude oil supply (crude oil production and crude oil transport), which then must be attributed (called: allocated) to each product of the refinery.
The crude oil demand $CO_{i,\text{Process}}$ (expressed in mass), required for the production of product $i$, (product $i$ defined by its mass $m_i$ and its net calorific value of $NCV_i$) of a certain unit process is calculated proportionately to mass, $m_i$, and the average net calorific value, $NCV_{avg}$, of all products produced in the refinery process. The mass, $m_i$, is calculated with the weight percentage, $m_{pi}$, of the total mass of all products produced within this unit process and the crude oil input of the refinery process.

$$CO_{i,\text{Process}} = \frac{m_{pi}}{100\%} \cdot m_{\text{Crude oil}} \cdot \frac{NCV_i}{NCV_{avg}}$$  \hspace{1cm} (1)

with:

$$NCV_{avg} = \sum_{n=1}^{i} \frac{m_{pi}}{100\%} \cdot NCV_i$$  \hspace{1cm} (2)

The crude oil demand (or better: the burden of crude oil supply) is allocated to the refinery products according to the quantity produced in the unit process and its energy content. Hence, crude oil consumption of product $i$, is allocated according to its net calorific value.

### 2.2 Thermal Energy Demand Allocation

The thermal energy demand, $ThE_{i,\text{Process}}$, needed for the production of product $i$, with mass, $m_i$, of the unit process is calculated with the total energy demand, $ThE_{tot,\text{Process}}$.

$$ThE_{i,\text{Process}} = ThE_{tot,\text{Process}} \cdot \frac{m_i}{\sum_{n=1}^{i} m_i} = ThE_{tot,\text{Process}} \cdot \frac{m_{pi}}{100\%}$$  \hspace{1cm} (3)

The energy demand required for the production of a product corresponds to a value that is relative to its weight percentage of the total mass.

Hence, the thermal energy demand is also allocated by mass.

### 2.3 Electricity Demand Allocation

The electricity demand, $El_{i,\text{Process}}$, required for the production of product $i$, with mass, $m_i$, of the unit process is calculated in the same way as the thermal energy demand with the total demand of electricity, $El_{tot,\text{Process}}$.

$$El_{i,\text{Process}} = El_{tot,\text{Process}} \cdot \frac{m_i}{\sum_{n=1}^{i} m_i} = El_{tot,\text{Process}} \cdot \frac{m_{pi}}{100\%}$$  \hspace{1cm} (4)
Hence, the electricity demand is allocated by mass as well.

### 2.4 Allocation Example and Allocation method choice explanations

Figure 2-2 shows the allocation of the atmospheric distillation (example).

**2.4.1 Crude oil demand**

Figure 2-1 demonstrates that products with higher net calorific values than the average (gases, naphtha, middle distillates), result in a higher amount of crude oil demand (consumption) compared with products with a lower net calorific value (atmospheric residue). For example, from 1 kg of crude oil input, 0.036 kg gases are produced. To produce a specific amount of product (in this case 0.036 kg), a corresponding amount of 0.036 kg of crude oil is necessary. Through allocation, the gases are attributed 0.04169 kg of the crude oil demand.

The atmospheric residue works contrary to those with high net calorific value. The “real” material consumption (corresponding crude oil demand) is 0.443 kg but the allocation attributes only 0.4214 kg due to its low net calorific value. Therefore, products with higher net calorific value are attributed higher input amounts, and therefore higher environmental impacts (associated with the crude oil supply), than products with a lower net calorific value. This allocation approach does make sense, because lighter fractions are usually the preferred refinery products and a lot of effort is undertaken to produce them. This sort of extra effort is expressed in slightly higher
associated burdens. For instance, a lot of processing steps are involved in converting heavy fractions to lighter fractions, ultimately to a higher calorific value. Note, light products have often a higher market demand and market price. As previously mentioned, all products are considered to be main products (outputs) and are taken into account in allocation, but there are also main products with a higher complexity than others, resulting from the lighter fractions and require more effort in production to obtain the required amount of refinery products in the end. The allocation of the crude oil input by net calorific value could also be explained from a physical point of view, because the energy content is a representative value relating to the crude oil consumption of the refinery products. Background is the predominant energetic applications of the refinery products, on which representative oil consumption should be based.

This method is therefore providing a cause-oriented assignment of environmental impacts. The physical factor “net calorific value” as opposed to “market price” is preferred for allocation, because the assessment of plant-internal interim products with “market prices” is simply not possible as there are no market prices on intermediates. Moreover, economic allocation is already not the preferred allocation method following ISO 14044. Because there is a correlation (not linear and within limits) between market price and heating value, the conclusion of both allocation methods should anyway yield similar results.

2.4.2 Thermal energy/steam demand

The first step to find an adequate method for the allocation is to clarify the scope of the parameters (in this case thermal energy and steam) used in the processes. Then a fair assessment must be developed according to the input involved. The preheating phase to heat the different refinery process input materials to process temperature is the primary energy consumer in most of the refinery processes.

Equation (5) shows that heat, \( Q \), which is the affiliated energy of a medium, depends on the specific heat capacity, \( c \). The mass is \( m \), and the temperature difference \( \Delta T \).

\[
Q = m \cdot c \cdot \Delta T
\]  

(5)

Based on the aforementioned information the following conclusion can be made: An allocation based on crude oil demand, similar to that based on “net calorific value,” would increase the environmental impact associated with the provision of thermal energy, associated with producing heavier fractions. Since the heavier fractions have a higher specific heat capacity \( c \) compared to the lighter products, a higher amount of energy is needed to heat them to the same temperature, resulting in a higher \( \Delta T \). For example, for the separation via distillation (higher boiling point) an allocation by mass was chosen for the energy demand. As a result, a
“preferential treatment” toward the heavier products is avoided (compared to the allocation with net calorific value).

2.4.3 Electricity demand
The allocation by mass can also be used for the electricity demand. The mass of the product is used for the allocation, not because of higher specific heat capacity \( c \), but rather the higher density of heavier products. The electricity is primarily used to run the equipment, which includes pumps and mixers. The pump performance increases with the density of the medium, so allocation by mass is argued to be sufficiently efficient to demonstrate the higher burden of the heavy fractions.

Figure 2-1 shows a fulfilled allocation constraint: The sum of allocated inputs and outputs to a process are equal to the sum of inputs and outputs before allocation. This point can be observed at the bottom of Figure 2-1, where a comparison of the sums of the inputs and outputs are made.

2.5 The Backpack Principle
To quantify and assess the energy and material (crude oil) demand that is essential to produce refinery-finished products, the consideration of the atmospheric distillation process alone is not sufficient. Since most of the products pass through a great number of processes within the refinery, all refinery processes must be considered and allocated to the final products. More complex products (which undergo many more processes), such as fuel, require a higher electricity and energy demand (and therefore higher environmental loads) compared to products which undergo fewer refinery processes, such as vacuum residue which can be used directly as bitumen.

This requirement is achieved through the “Backpack Principle”. Each output of the refinery unit processes is assigned a “backpack” of allocated crude oil, energy and electricity demand. Thereby the backpack (crude oil, energy and electricity demand) of the feedstock plus the energy and electricity demand of the subsequent processes are allocated to the products and hence, the backpack continues to accumulate during subsequent “travel” through the refinery.

The formula for the distribution of the feedstock backpack’s content is the same as for the crude oil, energy and electricity demands of the atmospheric distillation process. In their respective backpacks, the products carry a proportionate amount of the feedstock, as well as a proportionate amount that has been redefined in each process stage.
To the three products of the vacuum distillation unit (gas oil, wax distillates and vacuum residue) a share of the crude oil (backpack of raw material), electricity (backpack of electricity and electricity demand of process) and energy demand (backpack of energy and energy demand of process) is allocated. The allocated crude oil demand of subsequent process inputs in the “downstream processes” is redistributed to the products (“subsequent processes are not allocated crude oil input”), during which the shares of energy and electricity in the backpack increase according to the energy required at the current process stage.

For processes with two or more hydrocarbon inputs, the respective input fractions of the backpacks are added together.

All subsequent processes of the atmospheric distillation consist of five corresponding inputs. Crude oil, energy and electricity of the input backpack, as well as energy and electricity at each specific step in the refinery process (in rare cases there are zero inputs, which means no consumption occurs, or even negative inputs, which means that energy or electricity is produced and hence credited) makes up the five inputs.

There are significant differences in the energy and electricity demands of each unit process. There are also differences in the number of processes a finished product undergoes over the course of its production route. But the backpack principle guarantees that each finished product is assigned the environmental impact of all processes over the course of its production pathway.
Gasoline derived from atmospheric distillation, which only undergoes gasoline desulfurization and passes through the catalytic reformer, has a smaller backpack than gasoline produced via atmospheric distillation followed by vacuum distillation, vacuum distillate desulfurization, and FCC because more processes are involved. Vacuum residue which can be sold directly as bitumen has a smaller backpack than the finished diesel fuel product.
3 Literature


