Sphera® GaBi
The GaBi LCA Refinery Model 2022

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Background – How a refinery works?

Crude oil refineries are complex plants. The combination and sequence of many processes is usually very specific to the characteristics of the crude oil and the refinery products to be delivered. Available crude oil quality, the market demand for specific refinery products, as well as product requirements 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, 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 further treated at the gas treatment 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 mainly necessary for desulfurization processes, hydro cracking 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 often divided and fed to three different processes. 1) In some refineries, smaller quantities of light naphtha fraction are fed to the chemical sweetening process. Depending on the spec, some sweetened naphtha is directly blended to the gasoline. 2) The middle 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-iso-pentanizer (distillation) downstream to increase the yield of iso-components. These iso-paraffins are very valuable components for gasoline production with high a Research Octane Number (RON). 3) 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. The catalytic reformer produces hydrogen (the only process at the refinery, besides additional plants, like steam-reforming, which produces hydrogen). The output products of both processes - the isomerization and the catalytic reforming - are blended to premium or regular gasoline at the gasoline blending system, while naphtha is sold as feedstock to the chemical downstream industry.

Kerosene is often 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 processed at the hydrofiner to desulfurize diesel and light fuel oil. The desulfurized products are fed to the middle distillate blender. The residue from the atmospheric distillation is fed to the vacuum distillation to produce light vacuum gas oil, vacuum gas oil (wax distillate) and vacuum residue.

At some refineries, a portion of the atmospheric residue is processed at the visbreaking unit (mild thermal cracking). Small amounts of atmospheric residue 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, is further processes at the hydrofiner (hydro treatment), is desulfurized, and sent to the middle distillate blender.

Some of the vacuum distillate yield, which has been taken from the middle trays of the vacuum distillation, is processed at the base oil production unit to produce base oils and further lubricants and waxes (paraffins).

However, most of the vacuum distillate is fed either to a catalytic cracker, such as a Fluid Catalytic Cracking (FCC) - sometimes first desulfurized - or a hydrocracker, where the feeds are converted into shorter chains by molecule restructuring (cracking). 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.

Butylene of the FCC is further used together with external supplied methanol or (bio-)ethanol to produce Methyl-Tertiary-Butyl-Ether (MTBE) respectively Ethyl-Tertiary-Butyl-Ether (ETBE), a product used as octane booster. The naphtha of the FCC must be treated in a special desulfurization process to reduce its high sulfur content.

The vacuum residues are processed in a coking process, which produces again, gases, gasoline, middle distillates and heavy fuel oil. An additional product is petroleum coke, which is typically purified and sold as a product. The vacuum residue, like some of the atmospheric residue, is also used as feed for the visbreaking unit, which also produces gases, naphtha, middle distillates and heavy fuel oil.

The hydrogen sulfides of all hydrotreatment (desulfurization) units are converted to elemental sulfur at the sulfur recovery unit (Claus process).

Refineries require heat, steam and electricity for its operation. This energy is most often produced onsite at a refinery power plant and incinerators using refinery fuels such as refinery gas, light fuel oil, heavy fuel oil (residual oil), petrol coke and sometimes LPG, and smaller amounts of the energy is produced using purchased natural gas or steam and/or electricity is directly purchased from external sources outside the refinery boundary.

A simplified flow chart of a refinery is shown below in Figure 1. The arrangement of these processes varies among different refineries and few, if any, employ all of these processes.

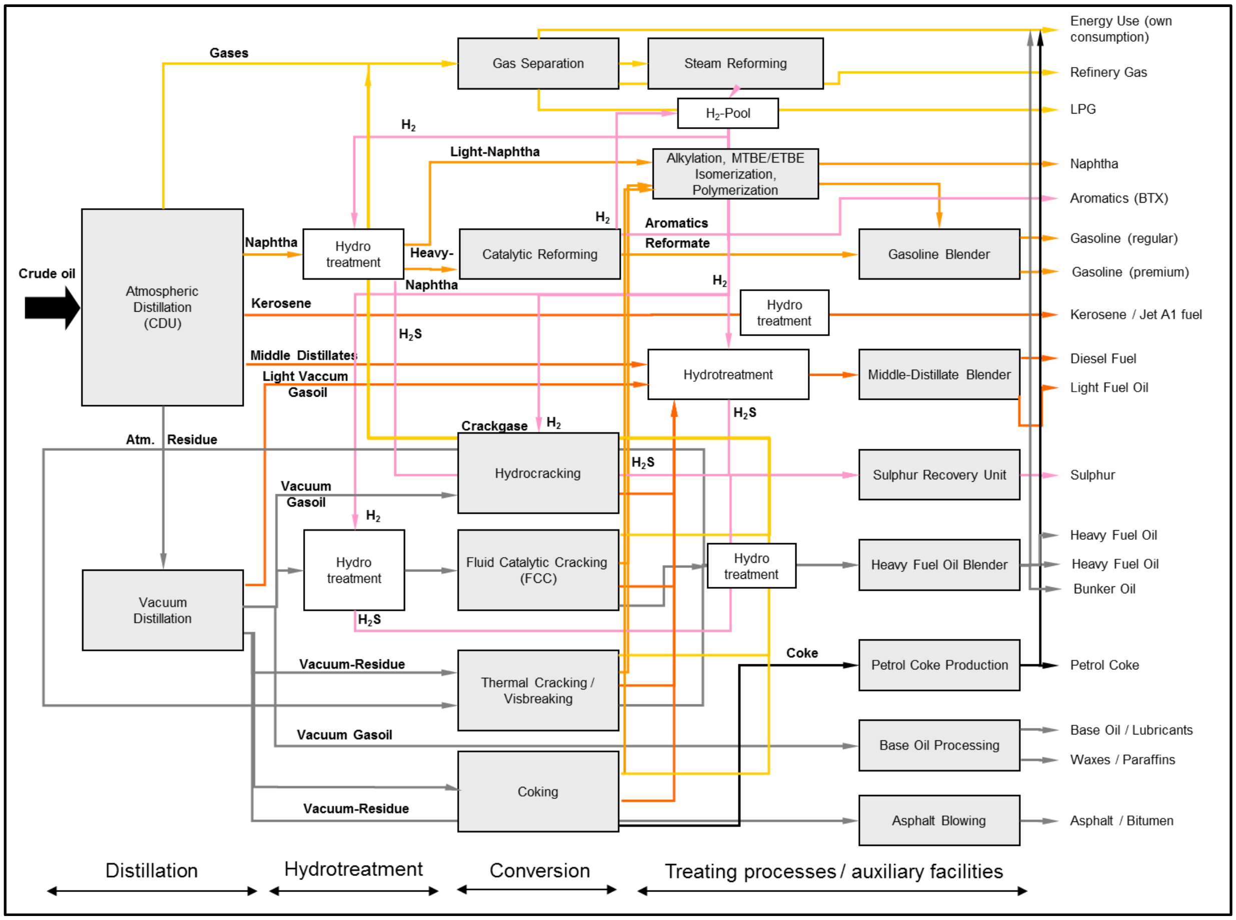

Figure 1: Simplified Flow Chart of a Refinery

The GaBi LCA Refinery Model

Modelling Approach

Due to the interlinkages within a refinery, all refinery products and all processes within the refinery must be considered when analyzing the environmental performance of refinery products.

The “GaBi LCA Refinery Model” is a generic, parameterized LCA model which describes the conversion of crude oil into finished refinery products. The model follows an attributional modelling approach, i.e. analyzing an average liter of diesel, gasoline, etc. produced, instead of looking on marginal changes to the system if the gasoline or diesel production is in-/decreased (consequential modelling).

Generic means, the model provides a suite of different refinery processes which can be turned on/off and parametrized means the model is fully adjustable to adapt the model to different input properties, outputs slates and fuel specs, and refinery operations schemas, etc. The following key parameters can be adjusted, among others:

- Crude oil and refinery product output slates
- Crude oil and refinery product properties (such as density, sulfur content)
- Layout and sequence of different distillation, conversion and upgrading processes
- Energy consumption (thermal energy, electricity) of each process
- Energy supply (onsite produced/purchased, and used energy carriers and fuels)

In consequence, the “GaBi LCA Refinery Model” can be used to either analyze specific or a country-average refinery and delivers average environmental inventories of refinery products. All GaBi background datasets on refinery products represent country averages, i.e. are using averaged parameters.

System Boundary

The “GaBi LCA Refinery Model” considers crude oil and other feedstock inputs (quantity of other feedstocks depend on the refinery or country under consideration).

Natural gas is either used at a steam reforming process to produce hydrogen or is used as fuel at the refinery power plant. Most refineries have an electricity grid connection and purchases either electricity for the daily operation, use the connection as a backup or even sell electricity to the grid. All is handled by the model. Methanol and (Bio-) ethanol is used to produce MTBE / ETBE, and water is used for producing steam, as a cooling absorbent or for washing purposes. Model outputs include in addition to the finished refinery products, mainly emissions and wastewater. Hydrogen is considered as special, since in some refineries, hydrogen is produced (and sold), while other refineries purchase hydrogen. Anyway, the “GaBi LCA Refinery Model” can handle both ways.

The main material and energy in- and outputs of the “GaBi LCA Refinery Model” are shown in the following graph.

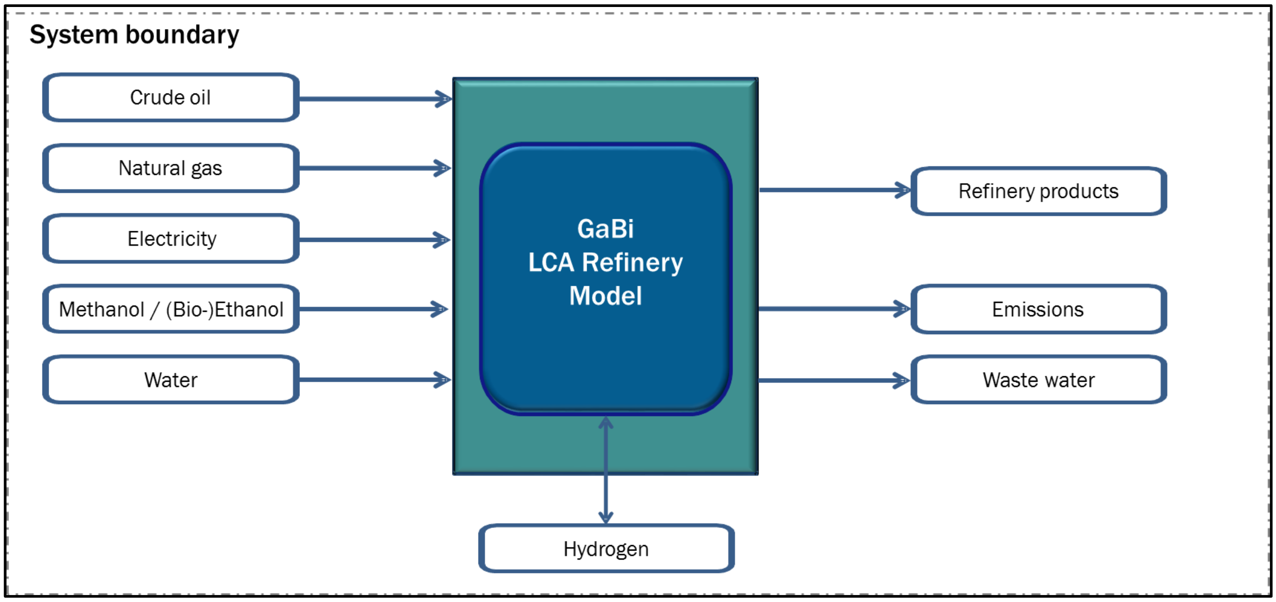

Figure 2: System Boundary – Considered In- and Outputs

Model Outline

The “GaBi LCA Refinery Model” is based on a detailed mass balance. The mass balance of the whole refinery is developed by considering the crude oil input, other feedstocks, the refinery output spectrum, as well as the processing capacities of each unit process (including its utilization) and the process unit output shares. The mass balance of the “GaBi LCA Refinery Model” is shown in Figure 3.

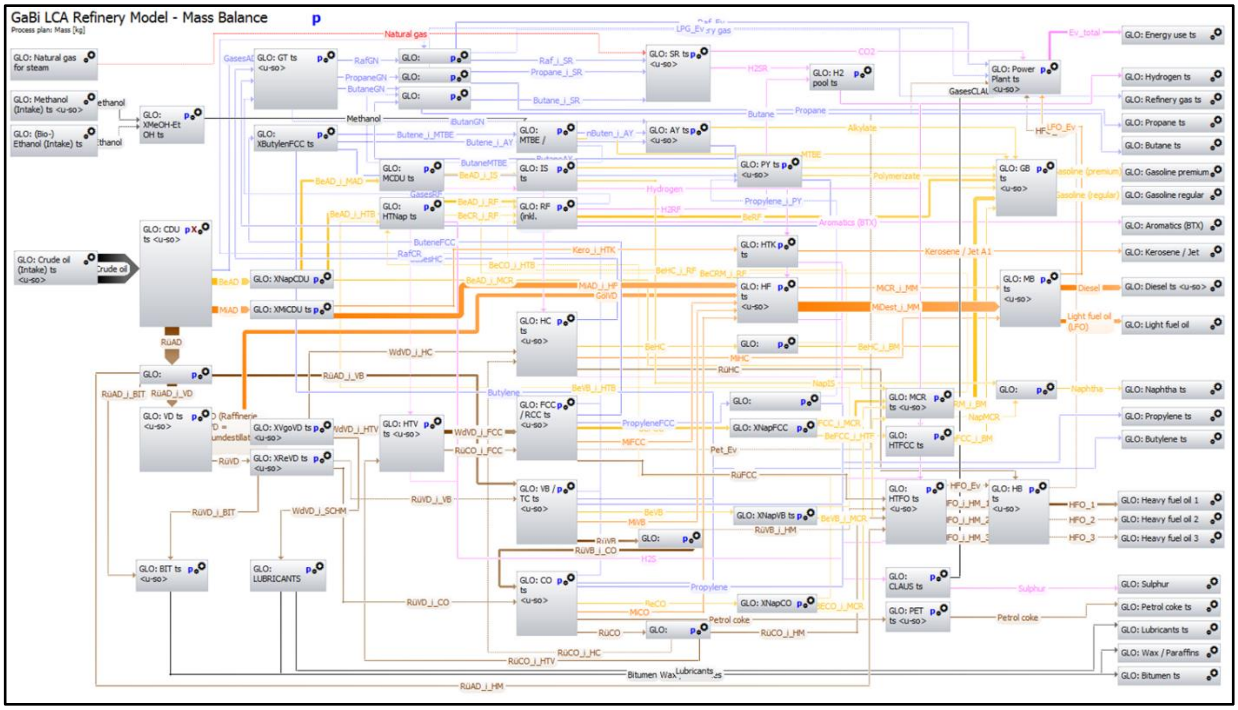

Figure 3: Screenshot of the “GaBi LCA Refinery Model” – Mass balance (Sankey diagram)

As the mass balance of the hydrocarbons is modelled thorough the refinery, the sulfur balance is modelled as well following an average distribution pattern. Thereby, the sulfur content of each hydrotreatment unit input is known, and by knowing the feedstock type (VGO, naphtha, FCC gasoline, diesel, etc.), and the output spec, i.e. sulfur limit in product, the amount of hydrogen needed at the desulphurization units is calculated. In this way, the hydrogen demand of the whole refinery is calculated.

The heat, steam and electricity demand of each unit process is quantified. Note, that some unit processes do not need heat, steam or electricity. If so, these inputs are set to zero or if the unit process is even delivering heat due to its exothermic nature, the model can handle it by using negative values, which are than credited to the process and hence its outputs. Anyway, based on the thermal energy and electricity input values, the energy balance of the refinery is calculated.

Certain amounts of produced fuels are fed to the refinery power plant to convert the fuel into heat, steam and/or electricity. At the “GaBi LCA Refinery Model”, the fuels used at the power plant can be determined. Either refinery fuels, such as refinery gas, LPG, LFO, HFO can be used or purchased fuels from external sources such as natural gas. The power plant conversion efficiencies can be determined as well. In addition, the share between onsite produced electricity and purchased electricity can also be adjusted.

The “GaBi LCA Refinery Model” calculates the allocation factors for each refinery product dependent on the individual way through the refinery and allows the attribution of the total refinery emissions from the commonly used power plant (bubble) to the different products. For more details on the allocation method applied, see section 0.

The use of catalysts as well as consumption of fuel additives are not considered in the model.

Please note, that the “GaBi LCA Refinery Model” is a model that calculates the environmental impact of refinery products. Even the models calculate its results based on the underlying mass balance and considers things like energy balance as well as hydrogen balance, the model is not a classical LP model, simulating operation pattern or optimizing the outcome towards certain criteria. It is a Life Cycle Assessment model quantifying the environmental footprint of a certain static state, in practice mostly an annual average of the refineries of a specific country.

Functional Unit

The “GaBi LCA Refinery Model” itself refers to 1 kg of crude oil input. I.e. all mass flows (intermediates / products) within the refinery model are quantitatively related to the input.

However, to have comparability among different products within a refinery or across several refineries, all finished products are re-scaled to 1 kg of the corresponding product, e.g. 1 kg of diesel and 1 kg of gasoline.

The overview of the “GaBi LCA Refinery Model” is shown in Figure 4.

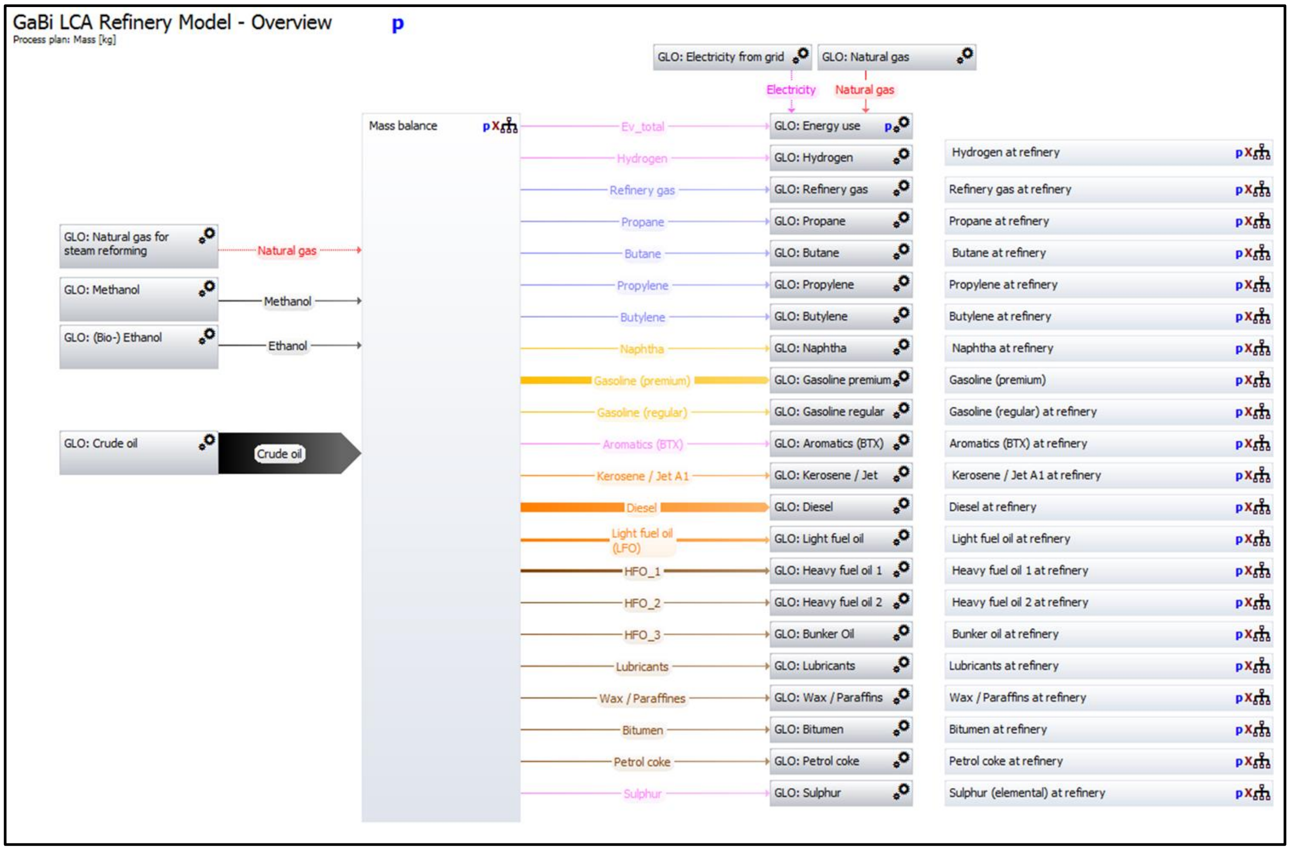

Figure 4: Screenshot of the “GaBi LCA Refinery Model” – Overview (Sankey diagram)

Allocation

Almost all refinery units (processes) are multi-output processes. Multi-output processes produce two or more products simultaneously. The challenge is to allocate the environmental burden associated with the operation of the process to its products. ISO standards 14040/44 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.” As nearly each single refinery unit process is a multi-output process, a suitable allocation method needs to be defined.

Each refinery process handles a hydrocarbon feedstock and consumes a certain amount of heat, steam (both grouped to “thermal energy” in the following), and electricity. At the “GaBi LCA Refinery Model”, steam is converted from kg to MJ by using a factor of 3.05 (MJ/kg). In case of the atmospheric distillation the hydrocarbon feedstock is crude oil, while all other refinery units process intermediate feedstocks, which are basically also derived from crude oil (with a few exceptions, like ethanol used for ETBE production).

The environmental burdens associated with the supply of crude oil, e.g. upstream emissions and energy consumption at the refinery, e.g. emissions from the thermal energy and electricity generation must be allocated to the different refinery products.

At the “GaBi LCA Refinery Model” the environmental burden of each process unit is allocated to its products and each product is followed individually through the refinery (backpack principle), i.e. the allocation is done at the refinery unit level (allocation to intermediate products) and is based on prorated allocations reflecting the physical I/O relationships (mass and energy yields). The actual distribution of the emissions is done by using allocation factors. Thereby, the sum of the allocated emissions to the refinery products are equal to the emissions before allocation.

Furthermore, all emissions released at the refinery (from heat, steam, and electricity production, individual processes and emissions due to losses) are considered as bubble and are allocated to the refinery products on a unit process level. This approach is validated to be suitable by the fact that nearly all emissions (>95%) are released by the energy supply and, in particular, by the on-site power plant / incineration processes. Exception are losses or VOC emissions from storage tanks.

In conclusion, the environmental burdens of the following items must be allocated to the refinery products. These include:

- The emissions of the refinery (representing all refinery emissions, including the power plant itself, converting plants, decentralized boilers, storage, diffuse losses)
- The environmental impacts of the crude oil supply (i.e. the upstream impacts)
- The environmental impacts of purchased electricity from the grid (i.e. electricity purchased which is used in addition to the one produced at the refinery power plant)
- The environmental impacts of the natural gas supply (if natural gas is purchased)
- The environmental impacts of the methanol/ ethanol supply (if MTBE/ETBE is produced)
- The environmental impacts of the hydrogen supply (if hydrogen is purchased).

The emissions caused by the refinery, by the electricity from grid, and natural gas supply are allocated the products following a mass allocation. The impacts related to the crude oil supply are allocated by energy content to the products. Environmental impacts from methanol/ethanol and hydrogen supply are assigned directly to the applicable products, e.g. methanol / ethanol supply emissions to the produced gasoline, hydrogen to the desulfurized products, like diesel, gasoline, etc.

In the following, the choice of the allocation method is described and explained by using examples.

Allocation of Crude Oil

Processing crude oil determines emissions in the crude oil supply chain, including crude oil production & processing as well as and crude oil transport to the refinery. These emissions must be allocated (attributed) to each refinery product.

The crude oil consumption COi,Process (expressed in mass), required for the production of product i, (product i defined by its mass mi and its net calorific value of NCVi) of a certain unit process is calculated proportionately to mass, mi, and its ratio of its net calorific value NCVi and the average net calorific value, NCVavg, of all products produced in this unit process. The mass, mi, is calculated with the weight percentage, mpi, of the total mass of all products produced within this unit process.

$$CO_{i,Process} = \frac{\mathrm{m_i}}{\sum_{\mathrm{n=1}}^{\mathrm{i}} \mathrm{m_i}} \cdot m_{Crude\ Oil} \cdot \frac{NCV_i}{NCV_{avg}} = \frac{m_{pi}}{100\%} \cdot m_{Crude\ Oil} \cdot \frac{NCV_i}{NCV_{avg}}$$

(1)

with:

$$NCV_{avg} = \sum_{n=1}^{i} \frac{m_{pi}}{100\%} \cdot NCV_i$$

(2)

Summarized, the crude oil consumption (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 or in other words, the crude oil consumption is allocated to the products according to its net calorific value (energy).

Allocation of Thermal Energy

The thermal energy consumption, ThEi,Process, needed for the production of product i, with mass, mi, of the unit process is calculated with the total energy consumption, ThEtot,Process:

$$ThE_{i,Process} = \frac{m_i}{\sum_{n=1}^{i} m_i} \cdot ThE_{tot,Process} = \frac{m_{pi}}{100\%} \cdot ThE_{tot,Process}$$

(3)

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

Summarized, the thermal energy is allocated to the products by mass.

Allocation of Electricity

The electricity consumption, $El_{i,Process}$, 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 consumption with the total consumption of electricity, $El_{tot,Process}$:

$$\mathrm{El_{i,Process}} = \frac{\mathrm{m_i}}{\sum_{\mathrm{n=1}}^{\mathrm{i}} \mathrm{m_i}} \cdot \mathrm{El_{tot,Process}} = \frac{\mathrm{m_{pi}}}{100\%} \cdot \mathrm{El_{tot,Process}}$$

(4)

Summarized, the electricity is allocated to the products by mass as well.

Allocation Example and Explanations

Figure 5 shows the allocation of the atmospheric distillation (example).

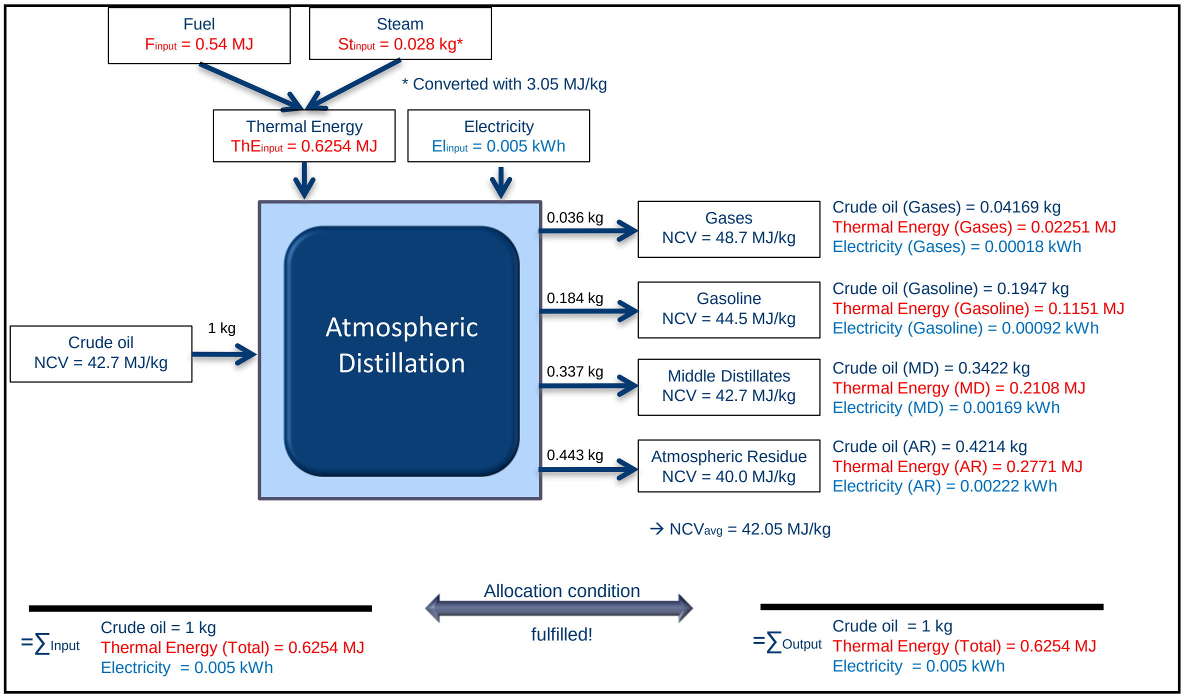

Figure 5: Allocation Example: Atmospheric Distillation

Explanation - Crude Oil Allocation

Figure 5 demonstrates that products with a higher net calorific value than the average (gases, naphtha, middle distillates), result in a higher amount of allocated crude oil 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 consumption. The atmospheric residue works contrary to those products with a high net calorific value. From 1 kg of crude oil input 0.443 kg atmospheric residue is produced, 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 is meaningful, 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 in operation, converting heavy fractions to lighter fractions, ultimately to products with a higher calorific value. Note, light products have often a higher market demand and market price as well. As previously mentioned, all products are considered to be main products (outputs) and are taken into account in allocation, but to obtain a certain quantity of lighter fractions require a significant effort.

The allocation of the crude oil input by net calorific value can also be explained from a physical point of view. The energy content of refinery products represents basically a certain crude oil consumption and due to the predominant energetic applications of refinery products, these allocation approach attributed a corresponding crude oil consumption to the use.

The chosen allocation method is therefore providing a cause-oriented attribution of environmental impacts to its products. The physical parameter “net calorific value”” is used instead of the “market value", since most of the intermediate products are not treated on the market and hence, they simply don't have any market price. Anyway, due to an assumed correlation between market price and net calorific value (not linear and within limits), the conclusion of both allocation methods should come to similar results and conclusions.

Explanation - Thermal Energy Allocation

The first step to define an adequate allocation method is to clarify the purpose. In case of the refinery, the purpose of heat and steam (thermal energy) usage is to heat the different unit feedstocks to process temperature. The pre-heating phase is the primary energy consumer in most of the refinery unit processes.

Equation (5) describes the relationship between the heat, Qi, that flows into a system to increase its temperature by ∆T, which depends on the specific heat capacity of the medium, ci and its mass, mi. Many substances have a known heat capacity per unit mass.

$$Q\mathrm{i} = m\mathrm{i} \cdot c\mathrm{i} \cdot \Delta T$$

(5)

Since heavier fractions have higher specific heat capacities c compared with the lighter products, more energy is needed to heat them to the same temperature, and in addition higher temperatures are needed for heavier fractions, e.g. in distillation columns, to separate those fractions due to its higher boiling point. I.e. in a nutshell, the processing of higher fractions is more energy intensive.

Therefore, an allocation by mass is chosen for the consumed energy. An allocation based on "net calorific value," (as used for the crude oil consumption), would increase the environmental impact associated with the provision of lighter fractions. As a result, the chosen allocation by mass, avoids giving heavier products too much advantage compared with the allocation of net calorific value. The allocation is appropriate and cause-oriented.

Explanation - Electricity Allocation

The allocation by mass is used for the electricity consumption as well. The mass of the product is used for the allocation, not - as for the thermal energy consumption – due to the higher specific heat capacities 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.

In general, and independent of the chosen allocation method, 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 and in other words, the sum of allocated inputs and outputs to a process are equal to the sum of inputs and outputs before allocation. See Figure 4 at the bottom.

Allocation: Backpack Principle

To quantify and assess the crude oil and energy consumption that is essential to produce refinery products, the consideration of the atmospheric distillation alone, as described above, is not enough. Since most of the products pass a large number of processes within the refinery, all refinery processes must be considered, and material and energy efforts must be allocated to the final products. More complex products (which passes many unit processes), such as gasoline, have a high energy consumption (and therefore higher associated environmental impacts) compared with products which passes only a few refinery processes, such as straight-run diesel or vacuum residue which can be used directly as bitumen.

This requirement is achieved through the “Backpack Principle”. Each output (product / intermediate product) of a unit processes is assigned a “backpack” of allocated crude oil, thermal energy and electricity consumption. Thereby the backpack (allocated crude oil, thermal energy and electricity consumption of previous unit processes) of the input of the corresponding process and the thermal energy and electricity consumption of the corresponding process are allocated to the products / intermediate products and hence, the backpack continues to accumulate during the product journey through the refinery.

The formula for the allocation of the backpack’s content is the same as for the crude oil, thermal energy and electricity of the atmospheric distillation process as described above. In a respective backpack, a product carries a proportionate amount of the feedstock, as well as a proportionate amount that has been allocated in each unit process.

Note, crude oil is obviously only consumed in the atmospheric distillation, while thermal energy and electricity is also consumed in (all) other refinery unit processes.

Figure 6 outlines the backpack principle at the vacuum distillation, a subsequent process of the atmospheric distillation.

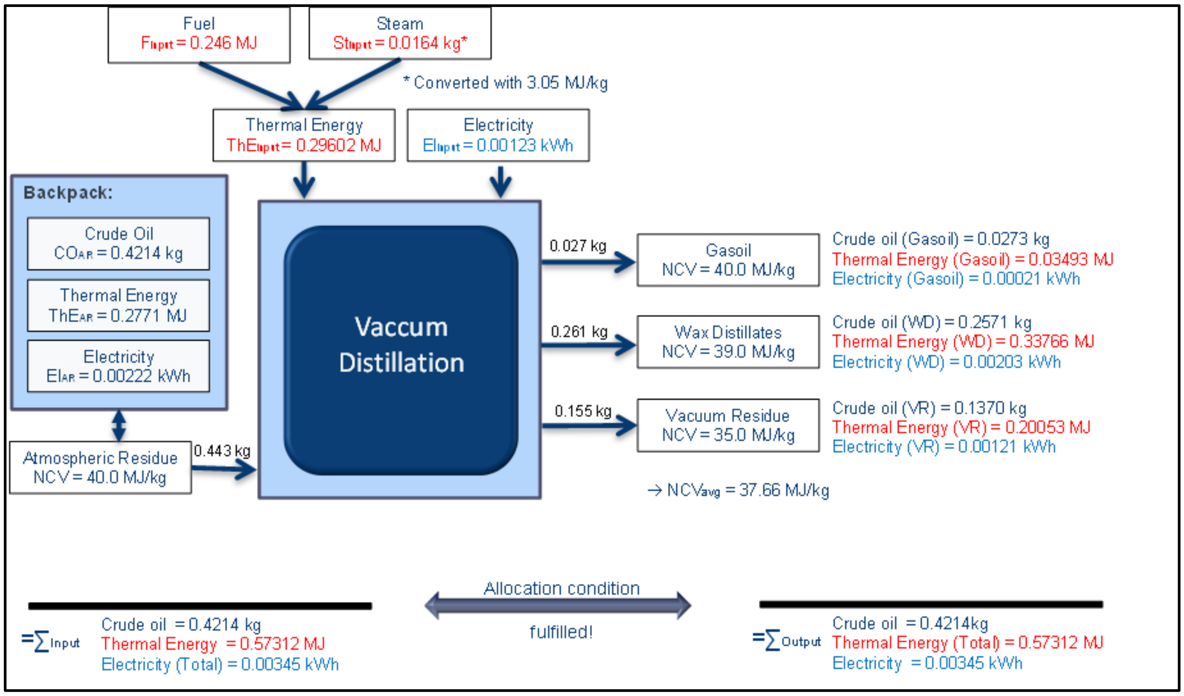

Figure 6: Allocation Example: Atmospheric Distillation

To the three products of the vacuum distillation unit (gas oil, wax distillates and vacuum residue) a share of:

- the crude oil (backpack of crude oil consumption accumulated at atmospheric distillation),
- thermal energy (backpack of thermal energy consumption accumulated at atmospheric distillation and thermal energy consumption of this process as well as,
- electricity (backpack of electricity consumption accumulated at atmospheric distillation and electricity consumption of this process,

are allocated.

The allocated crude oil consumption of subsequent process to the atmospheric distillation, i.e. at all "downstream processes" is re-distributed to the corresponding products. For the thermal energy and electricity consumption, the re-distribution also takes place, but in addition, the thermal energy and electricity consumption of the corresponding process is allocated to the products as well. Therefore, the thermal energy and electricity backpack increases according to the thermal energy and electricity required at the corresponding unit process.

For processes with two or more hydrocarbon inputs, the respective input fractions of the backpacks are summed-up.

In summary, all subsequent processes of the atmospheric distillation consist of five corresponding inputs: crude oil, thermal energy and electricity of the backpack, as well as thermal energy and electricity at each specific refinery unit process. Note, some unit process, do not need thermal energy / electricity to run the process (values set to zero) or are even delivering thermal energy due to its exothermic nature (negative value), which is credited.

Note, that there are significant differences in the thermal energy and electricity consumption of the different refinery unit processes. Also, the production route, i.e. the number of processes a product passes, to be sold as a finished product, is different from product to product. However, the backpack principle allows that each finished product is assigned the environmental impact shares of all processes it passed through the refinery and allows a cause-oriented attribution.

For example, a gasoline fraction derived from the atmospheric distillation, which is further processed in a gasoline desulfurization and catalytic reformer, has a smaller backpack than gasoline fractions produced via atmospheric distillation followed by vacuum distillation, vacuum distillate desulfurization, and FCC because more processes, and especially more important, more energy intensive process, are involved.

This detailed approach following a backpack principle contrasts with simple refinery models, at which the emissions of the whole plant are simply allocated among the final products by static factors (e.g. mass, energy content, market price). This simply allocation approaches do not reflect the complexity of a refinery and do not differentiate between production routes and such kind of allocations can't by classified as cause oriented.

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Abbreviations

ETBE	Ethyl-Tertiary- Butyl- Ether
FCC	Fluid Catalytic Cracking
HFO	Heavy Fuel Oil
ISO	International Organization for Standardization
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LFO	Light Fuel Oil
LPG	Liquefied Petroleum Gas
MTBE	Methyl-Tertiary- Butyl- Ether
NCV	Net Calorific Value (synonym for LHV = Lower Heating Value)
RON	Research Octane Number
VOC	Volatile Organic Compound