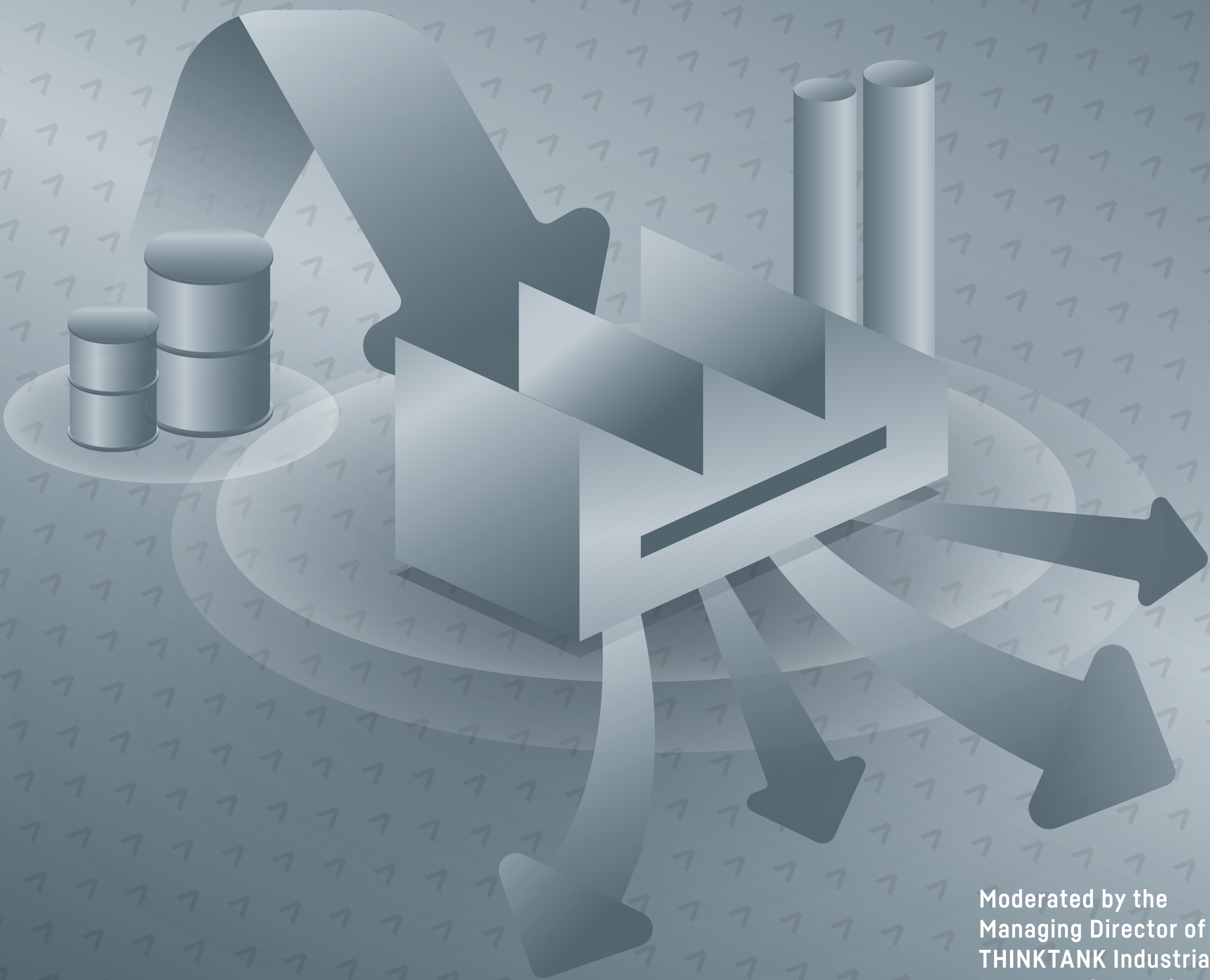
THINK TANK FOR INDUSTRIAL RESOURCE STRATEGIES

Corporate Forum Chemical Recycling (CFCR)

MASS BALANCING FOR CHEMICAL RECYCLING



Moderated by the Managing Director of THINKTANK Industrial Resource Strategies

Explanations on field of action 3

"Use of specific and flexible mass balance processes" of the paper "Fields of action of politics for the raw material turnaround and the transformation to a circular economy by means of chemical recycling in Germany".

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Summary

To achieve the social goal of climate neutrality and reduce dependence on imports, non-fossil carbon sources are needed for the chemical industry. The recycling of plastic waste makes an important contribution to this. In addition to mechanical recycling, chemical recycling can also provide products from plastic waste for this cycle, which until now have been incinerated and thus removed from the carbon cycle.

When chemically recycled products (oils and gases) are added as feedstock to a chemical company's petrochemical process (e.g. a steam cracker), they are mixed with conventional fossil feedstock, i.e. feedstock derived from crude oil or natural gas. And this mixing of recycled and fossil feedstocks necessitates a mass balance process. **To be able to use the existing infrastructure of the chemical industry for a circular economy for plastic waste and thus also to replace fossil raw materials and close the carbon cycle, the mass balance approach "Fuel-Use-Excluded"** will be needed for the foreseeable future. The alternative mass balance approaches "Polymer-only" or "Proportional Allocation" result in too low recycled fractions for the end products to induce consumers to make purchasing decisions that form the economic basis for the use of the large-scale chemical infrastructure. This is also in line with the legal recycling definition in the EU Waste Framework Directive.

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Summary

The application of the "Fuel-Use-Excluded" approach with the focus on plastics from household and commercial waste that are difficult to recycle, and not the classic packaging waste, increases the recycling rate to a high degree:

- acceptance for chemical recycling,
- bringing new material to be processed that is 'from recycled feedstock', then this is additive to the fossil system, and that additional amount should be given a protected allocation through the system
- the investment by companies in the expansion of existing chemical recycling processes and in new technologies for recycling such plastics and rubber products,
- the willingness of the chemical industry to pay the extra price for the recycled gases and oils; combined with the certainty of finding customers for them who can and must use these substances in the long term,
- the willingness of the chemical industry to adapt its infrastructure in the long term to use as much of the recycled feedstock as possible in the future, along with the possibility of bringing the accounting process closer to that of mechanical recycling.

The "Fuel-Use-Excluded" approach is the only approach that is practically comprehensible and at the same time economical for the large-scale chemical industry. It is ensured via existing standards such as ISO 22095 or certification procedures such as that of ISCC (International Sustainability and Carbon Certification):

- that no more recycled feedstock is allocated than entered the system,
- that the share used as fuel is first deducted from the balance for recycled products and the remaining recycled shares can be allocated mathematically according to a certified mass balance procedure to flexibly selected products whose customers are already willing or legally required to pay the surcharge for circularity and the reduction of fossil raw materials.

This approach is thus best in line with the goals of a comprehensive circular economy.

1. Introduction

In August 2023, the Corporate Forum Chemical Recycling (CFCR) ("Unternehmerforum Chemisches Recycling" (UFCR)), an association of representatives from the entire industrial value chain, published the "Policy fields of action for the raw material turnaround and the transformation to a circular economy by means of chemical recycling in Germany". The points for advancing the implementation of chemical recycling on an industrial scale in Germany are set out in 9 key points.

In field of action 3 "Use of specific and flexible mass balance procedures" it is stated that the "fuel-use excluded mass balance approach" is necessary as a regulatory framework for chemical recycling and should be recognised under the condition of a identifiable external certification. With this approach, chemically recycled feedstocks are first replacing fossil feedstocks and second are attributed to the target products, excluding energy and process-related losses.

In this paper, this field of action is explored in greater depth, and it is explained why mass balances for products of chemical recycling from plastic waste are necessary and why an economically stable use of the existing infrastructure of the chemical industry can only be ensured by applying the "fuel-use-excluded" approach. For this purpose, an overview of the currently discussed mass balance procedures and their approaches is given, and these are evaluated with regard to their feasibility.

2. Mass flow and mass balance – differences and fields of application

2.1 Volume flow

In mechanical recycling, we generally speak of mapping a **quantity flow** to document the whereabouts of collected waste physically and in terms of the balance sheet. For example, the use of granulates in products can be tracked through sorting, mechanical processing, and refining. With the presentation of the quantity flow, the collected quantity of a waste from a collection point to the sorting plant can be proven by measuring the delivered weight. Even if the waste is then mixed with the same waste of the same type (e.g. household packaging waste) from other locations and regions, after sorting it can be determined by weight how many specific or mixed plastics, paper and other materials and residues were sorted out.

For plastic waste, for example, this means that when a specific bale (e.g. a polyethylene bale) is loaded at a recycling plant, it can be determined by weight how much of this sorted, specific plastic (polyethylene) has been sent to a recycler. The recycler in turn processes these delivered quantities and produces a granulate. In the process, additives are added, and residues are produced. The recycler then passes the granulate on to a producer as 100% recyclate, who then decides whether his own plastic product is to be produced from 100% of the recycled plastic or from a mixture with conventional plastic made from crude oil. This allows the content of recycled plastic to be precisely determined. Furthermore, it can be shown in the accounts over the entire chain from collection to use in the product how much recycled plastic of a specific material, from the totality of the collected and sorted, has gone into a product. This approach has been implemented in mechanical recycling so far.

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The same approach can be analogously illustrated to produce a recycled plastic granulate for a product produced by chemical recycling – from plastic waste to, for example, a chemical recycled oil. The parties involved must also document what and how much they have collected, sorted themselves or handed over to a sorting company (household, commercial or industrial waste). The sorting company, in turn, shows which fractions it has sorted out, what it has sent for incineration and what it has handed over to a processing company. The processing company – in this case the chemical recycler – also records the quantities of its incoming material and waste. As a further waste handler in the process chain, he sorts and checks the delivered material, creates an overview of his waste quantity and documents how much oil, gas and residues he produces and what quantity of recycled products he has handed over to the chemical industry. These processes are legally anchored in the Closed Substance Cycle Waste Management Act, the Packaging Act and the Commercial Waste Ordinance. In addition, there are further implementation regulations by the LAGA (Bund/Länder Arbeitsgemeinschaft Abfall.

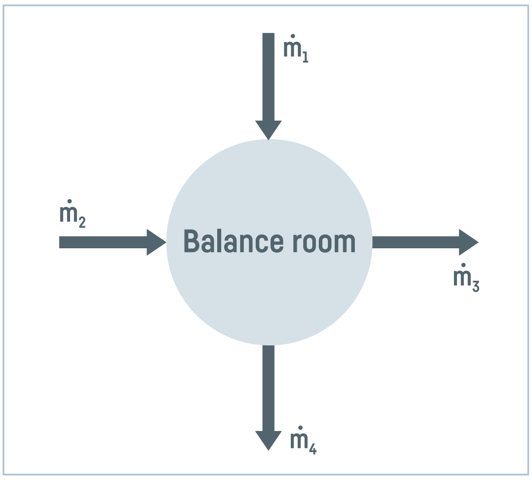
IMPORTANT:
This accounting and weight recording of the accruing waste quantities, the sorting and processing up to the incineration or generation of a product are mandatory and precede any further processing. The declaration of the "end of waste" of a waste requires the presentation of the origin and the processing steps – regardless of whether a mechanical or chemical recycling process is carried out.

The chemical recycler is also registered as a waste-treating company and has been certified according to the principles of the Ordinance on Specialised Waste Management Companies (Entsorgerfachbetriebsverordnung) based on the §56 of the Closed Substance Cycle Waste Management Act (Kreislaufwirtschaftsgesetz) and the Ordinance on Waste Disposal Records (NachwV). Accordingly, he is obliged to keep a volume flow and must keep his books from the receipt of the waste to the production of the product and the delivery of the product to a customer and to provide the authorities with all the evidence required to prove the treatment of the waste up to the production of the product. This already starts with the application for the authorisation of the enterprise according to the 4th BImSchV[1] , which creates the basis for the "recovery and disposal of waste and other materials" with Annex 1 No. 8.

[1] Fourth Ordinance for the Implementation of the Federal Immission Control Act (Ordinance on Installations Requiring a Permit – 4th BImSchV

2.1 Massenbilanz

In a closed system, the consideration of mass is trivial: since no mass can cross the system boundary, the mass in the system always remains constant. In an open system, however, mass can be exchanged with the environment. These mass flows with the environment are recorded by the **mass balance**.[2] For this purpose, the balance area with its balance boundaries, at which the recording of the mass flows takes place, must be defined.



The upstream process step of chemical recycling is not part of the mass balance process, neither with the process (treatment of waste) nor with the manufactured and stored product (oels or gases). Recycled products are produced from (plastic) waste (analogous to plastic granulate, for example oils), which are able to replace fossil raw materials. They are therefore considered 100% recycled products and are part of the mass flow procedure in terms of weight and accounting.

Only in the next step, with the transfer of these recycled products to a petrochemical process, for example, is the balance area formed for mass balancing. When the recycled products (oils and gases) are added as feedstock to the downstream petrochemical process (e.g. a steam cracker) of a chemical company, they are mixed with conventional fossil feedstocks, i.e. feedstocks obtained from crude oil or natural gas. And it is this mixing of circular and conventional fossil feedstocks that makes a mass balance process necessary. The petrochemical process forms the balance area under consideration.

Mass balancing is already used in many areas to calculate the input and output of complete production processes. It enables traceable, credible information on the end products and allows consumers to make informed purchasing decisions. Mass balance is already used in many areas, e.g. for renewable energies (green electricity) and biofuels, but also for fair trade chocolate and sustainable forestry (FSC®).

[2] According to Wikipedia

For example, “Deutsche Bahn” buys a quota of fossil-generated electricity and electricity from renewable energies. The railway decides whether to allocate 100% green electricity from renewable energies to the ICE (as long as the purchased quota is sufficient) and fossil-derived electricity to the other trains. It goes without saying that the trains travel over the same routes and draw the same electricity from the line. The allocation is made solely on the basis of the balance sheet. An analogous approach is also used for the mass balance.

The aim is to implement the scaling of sustainable solutions – such as the recycling of plastics – quickly and efficiently by using existing infrastructures. In the production process that follows chemical plastics recycling, the mass balance approach is the decisive instrument for integrating the chemically recycled products obtained into the existing infrastructure of the chemical industry (petrochemical processes) and directly replacing fossil raw materials. In these petrochemical processes, several hundreds of thousands to millions of tonnes of conventional fossil materials are used per year in large-scale plants such as steam crackers. Only this order of magnitude allows the chemical industry to operate economically. The available quantities of chemically recycled products from plastic waste cover only a fraction of the required quantities. Separate operation of a petrochemical plant with exclusively recycled feedstock is not economically feasible today. A mixture of different carbon sources from fossil, and in future increasingly from renewable and non-fossil sources, is still necessary for the chemical industry.

With the mass balancing approaches, the quantities of recycled products used can be specifically allocated to individual products from the petrochemical process. This is particularly necessary for product areas that require plastics in virgin material quality, which until now could only be achieved with fossil-derived plastics. These include requirements for performance, hygiene or safety, such as those for medical packaging, food packaging, safety-relevant automotive parts or building materials.

The mass balance is at the same time a model for securely tracing product chains (chain of custody), in which input and output are monitored at every step of the production process and checked and certified by third parties. This is crucial to ensure credibility and transparency of the associated information on the use of recycled products and to prevent greenwashing. Independent certification organisations such as ISCC or REDcert already audit the use of bio-based and recycled plastics on the basis of established standards (e.g. ISO 22095), so that clear information can be provided on the end products. The mass balance calculations audited using these methods provide information on recycled content in end products where it is technically impossible to measure the proportion of recycled material directly.

3. Approaches of Mass balancing

3.1 Petrochemical Process

In one of the common petrochemical processes, for example, refined crude oil is used as a starting product (naphtha) to produce a variety of intermediate products. For this purpose, so-called steam crackers are used, which break down (crack) the larger molecules into smaller molecules by means of steam. With the help of the steam cracker, it is possible to control the process so that certain end products are produced preferentially. This means that there are several ways to operate a cracker.

What does this mean for the processing of the chemically recycled feedstock and the petrochemical processes? Figures 1 and 2 illustrate two petrochemical processes using the example of steam crackers. Figure 1 shows the operation of a steam cracker for the preferential recovery of precursors for plastics production. Figure 2 shows the operation of a steam cracker for the preferential extraction of precursors for plastics production as well as for other products and fuels. Depending on the entrepreneurial decision and process operation, different proportions of the product flows can be specifically adapted.

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In the steam cracker, 100 t of a mixture of chemical recycled oil and naphtha from conventional fossil sources are used as feedstock.[3] In the case of the preferential extraction of precursors for plastics production, these are extracted (Figure 1):

> 29 t Precursor for polymer 1
> 16 t precursor for polymer 2
> 28 t precursor for other products (such as pharmaceutical products), of which for other polymers 12 t (5 t + 7 t)
> 11 t fuels and combustibles
> 16 t for process energy and loss.

The conservation of mass in the mass balance is fulfilled: Input: 10 + 90 = 100 and Output: 29 29 + 16 + 28 + 11 + 15 + 1 = 100

The share of feedstock used for plastics production in this case is 57 % in total (box).

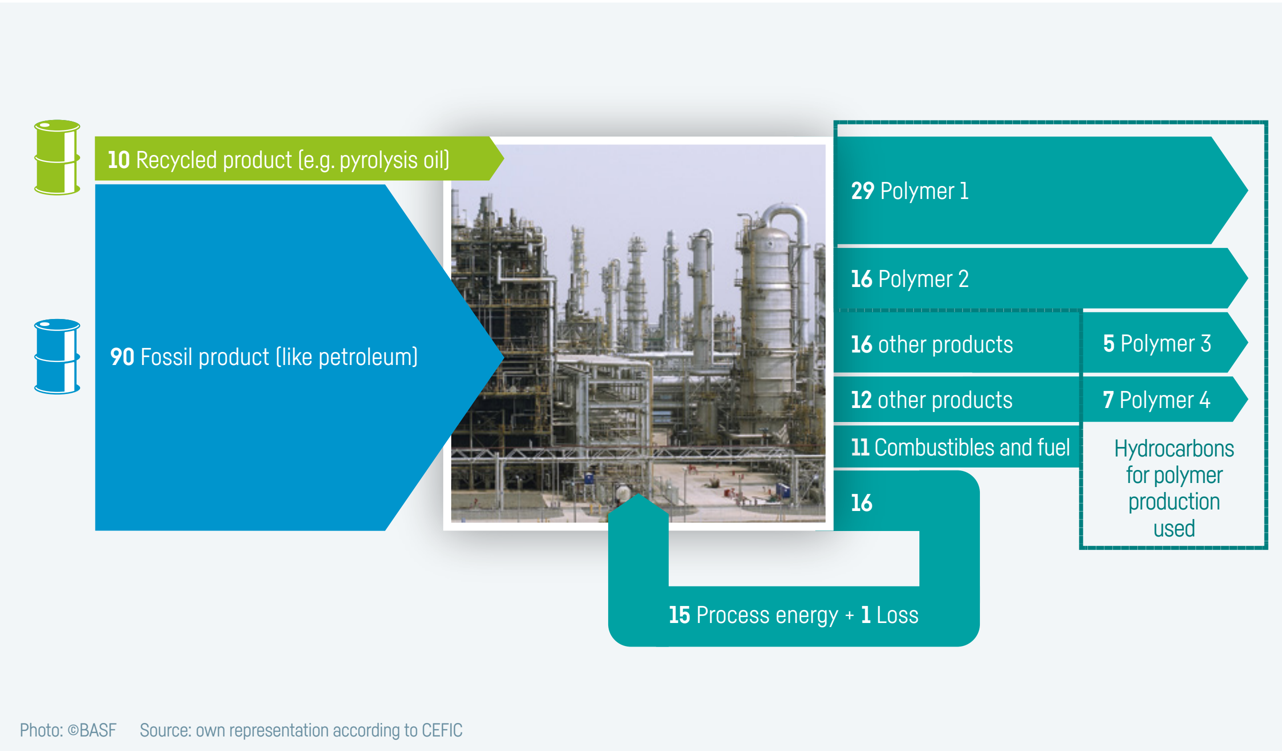

Figure 1: Volume flows of a steam cracker, which is preferably operated for the extraction of precursors for plastics production.

[3] This example calculation works with the distribution of 100 tonnes of feedstock. As explained above, the operation of a common steam cracker runs with hundreds of thousands of tonnes of feedstocks.

In the case of preferential extraction of other products and fuels in addition to pre-products for plastic production are obtained from it (Figure 2):

- 10 t precursor for polymer 1,
- 10 t precursor for polymer 2,
- 30 t of precursor for other products (such as pharmaceutical products),
- 40 t of fuels and
- 10 t for process energy and loss

The conservation of mass in the mass balance is fulfilled: Input: 10 + 90 = 100 and Output: 10 + 10 + 30 + 40 + 10 = 100.

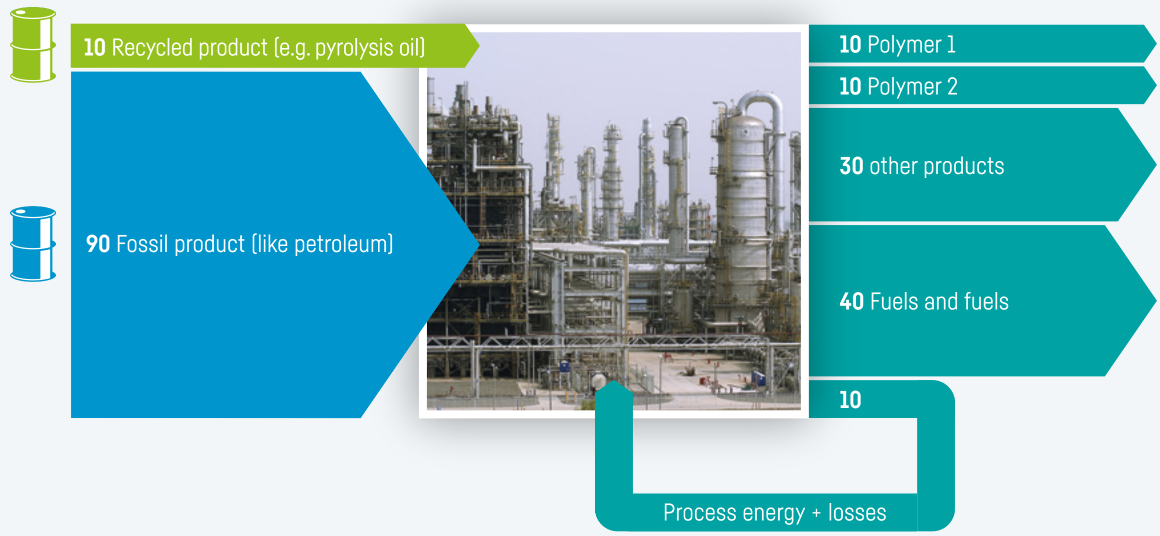

Photo: ©BASF Source: own representation according to DOW

Figure 2: Volume flows of a steam cracker that is operated preferentially for the extraction of other products and fuels in addition to precursors of plastics production

The decisive question now is to which end products the 10 % chemically recycled output products are assigned.[4]

[4] In the following exemplary allocations, we stick to the somewhat simpler case of the steam cracker with fewer plastic precursors.

3.2 Mass balance- Approaches

When selecting a mass balance approach, the objective that is being pursued is decisive. Mass balancing itself is a purely mathematical allocation of flows within the balance area – independent of the physically real situation. The sum of the input and output mass flows must be identical. In principle, there are two different approaches to allocation for a mixture of substances used (Figure 3):

A Rolling Average: the end products have the same pro rata composition as the initial mixture.

B Credit Method: the available shares of the individual components of the initial products are allocated to the end products by calculation. The maintenance of mass must be guaranteed.

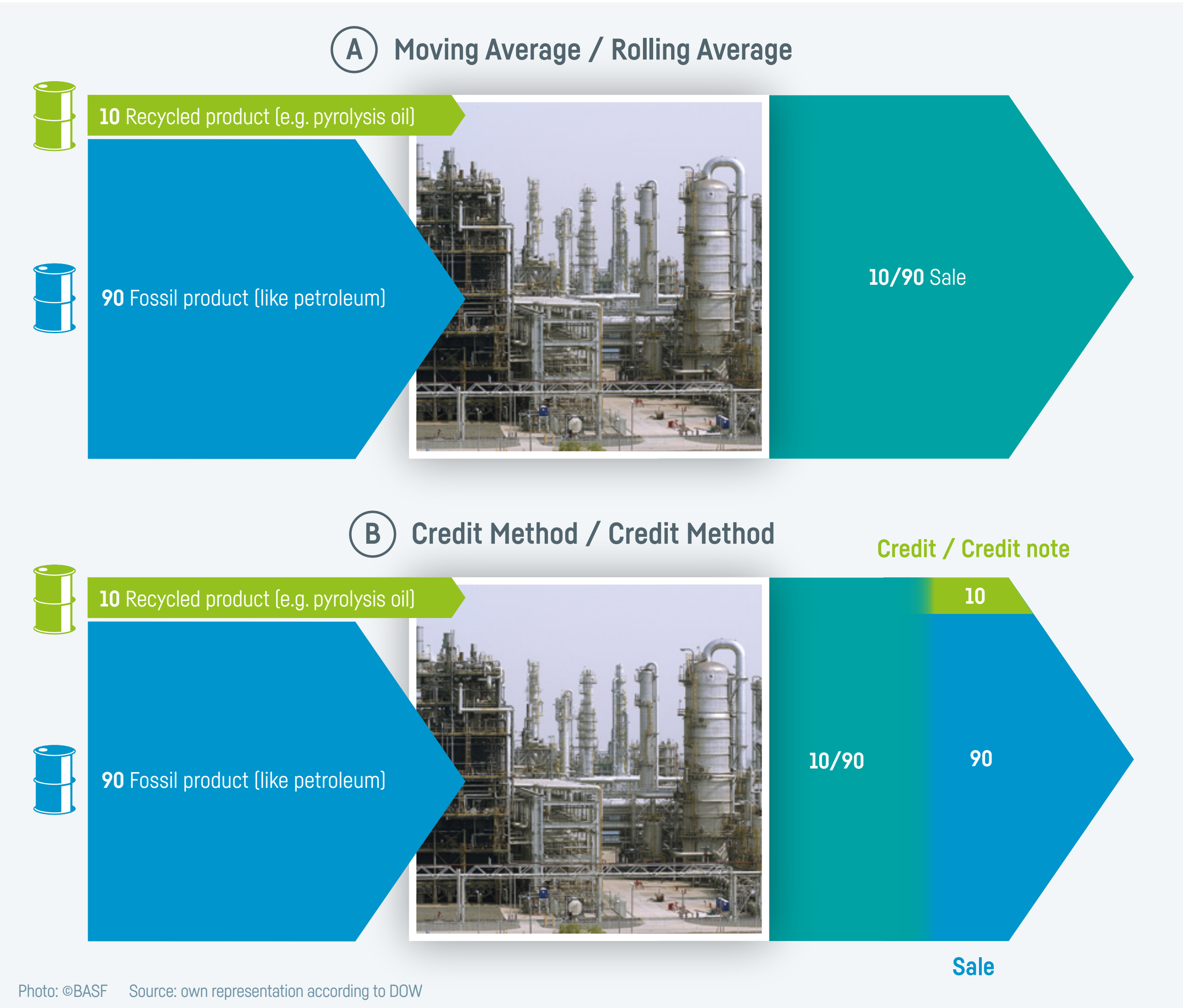

Figure 3: Methods of mass balancing

Case A "Moving Average / Rolling Average

Proportional approach[5]

Regarding the parallel use of recycled and non-recycled feedstocks, this means that the same pro rata of recycled (green) and non-recycled fossil (blue) feedstocks (pro rata to the proportion in the feed mixture) is allocated for all products formed.

In a petrochemical process in the chemical industry, all product groups would receive the same, currently very low proportion of recycled material, regardless of what they are further processed into. For the above example of a steam cracker with an input of 100 t (Figure 4)

> 10 t chemically recycled products (such as pyrolysis oil) and
> 90 t fossil petroleum product (naphtha)

this means that all material flows of end products of the plant are in turn assigned exactly 10 % recycled material content:

> 10 t precursor for polymer 1, with 9 t fossil and 1 t recycled material content,
> 10 t precursor for polymer 2, with 9 t fossil and 1 t recycled material content,
> 30 t precursor for other products (such as pharmaceutical products), with 27 t fossil and 3 t recycled material content,
> 40 t of fuels, with 36 t of fossil and 4 t of recycled material,
> 10 t for process energy and loss, with 9 t fossil and 1 t recycled output product.

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[5] The proportional approach is not mentioned directly in the ISO 22095 standard, but was derived from the rolling average method for multi-output processes described there.

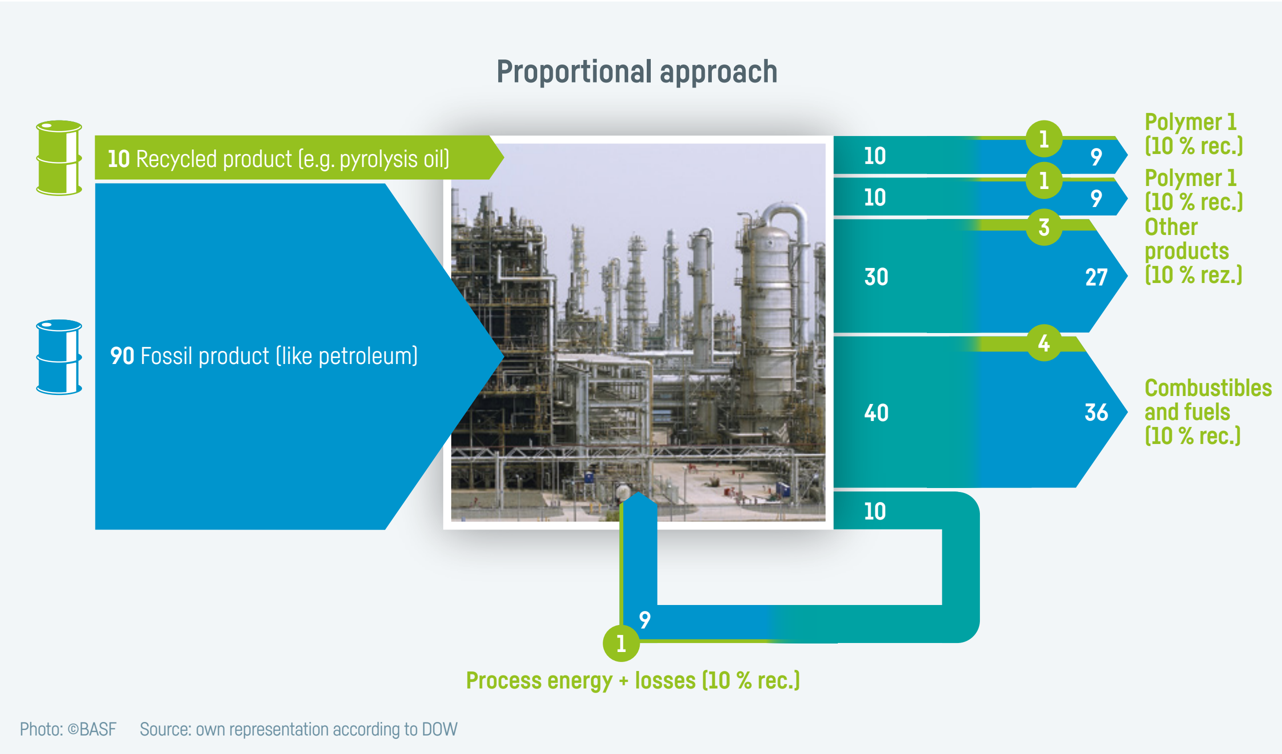

Figure 4: Volume flows and allocations for the "Moving Average/Rolling Average" method with the "Proportional Approach

Since only polymer 1 with a share of recycled source product is relevant for the market, this means in practice that out of 10 t of recycled product, only 1 t can in fact be economically utilised. The other 9 t "disappear unrecognised" in products that are not relevant for the market and for which there will be no demand for recycled products. If only 10% of the recycled feedstock is available for the marketing of high-quality recycled products, it is not possible to operate a petrochemical process economically. The existing infrastructure of the chemical industry can thus not be used for the circular economy.

It must be considered that the processes in the cracker are much more complex than shown in this simple illustration, that the recycled products are not identical but show variances within the permissible specification and that a time offset in production must also be taken into account. In this respect, this is also a mathematical approach since molecules of the recycled material are not exactly 10% each in the final products of the steam cracker.

Case B "Credit Method" / Credit Method

Two different approaches to allocation can be distinguished for this method. Here, one must abandon the idea that a "molecule-sharp" tracing of source materials through the complex chemical processes to individual end products is possible.

Polymer-only / Polymers-only approach

With this process approach, only the recycled quantities of end products of the steam cracker that lead to new plastics (polymers) in terms of process technology may be allocated. The approach is analogous to case A "Moving / Rolling average". However, the proportion of the recycled feedstock that would flow into intermediate products of plastics production (here polymers 1 and 2) is now mentally allocated to the desired market-relevant target product (here polymer 1).

For the above example of a steam cracker with an input of 100 t

> 10 t chemically recycled products (such as pyrolysis oil) and
> 90 t fossil petroleum product (naphtha)

this means that the material flows of the two precursors for polymers 1 and 2 totalling 2 t can be allocated to the market-relevant polymer 1. Accordingly, polymer 2 is not allocated any recycled material (Figure 5):

> 10 t precursor for polymer 1, with 8 t fossil and 2 t recycled feedstock,
> 10 t precursor for polymer 2, with 10 t fossil and 0 t recycled feedstock,
> 30 t precursor for other products (such as pharmaceuticals), with 27 t fossil and 3 t recycled feedstock,
> 40 t of fuels, with 36 t of fossil and 4 t of recycled material,
> 10 t for process energy and loss, with 9 t fossil and 1 t recycled material content.

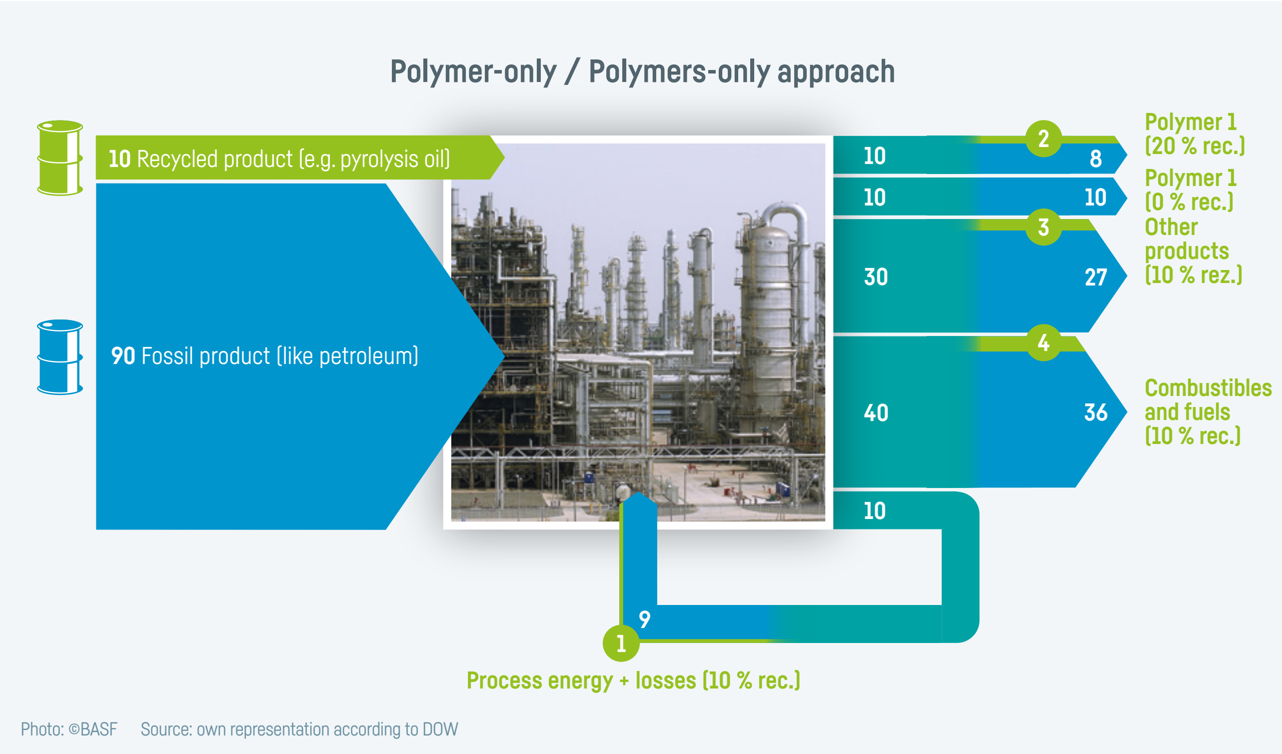

Figure 5: Volume flows and allocations for the "Kreditmethode / Credit Method" with the "Nur-Polymer / Polymers-Only Approach

The mass balance opens up again accordingly:

- fossil share: 8 + 10 + 27 + 36 + 9 = 90 (blue)
- recycled share: 2 + 0 + 3 + 4 + 1 = 10 (green)

This means that in this case 2 t can be allocated and used for the market-relevant polymer 1 – i.e. up to 20 % of the recycled starting products used in the steam cracker. But even here, with only 20 % of the 10 t of recycled source product usable, high losses are associated with the target product and economic operation is not possible.

Fuel-use-excluded approach / Fuel-use-excluded approach

According to the definition of the VCI/PED, which the UFCR endorses, "chemical processes fulfil the processes for the recycling definition whenever the resulting products are used for new materials (material substitution). In this case, they are "chemical recycling processes". If the resulting products are used as fuel, the processes are not chemical recycling processes"[6].

If this approach is applied to the petrochemical process, all material flows can be used for the allocation to the desired chemically recycled end products, except for the quantities required to produce fuels and for process operation.

In the specific case, this means that the most interesting polymer 1 for the market is allocated the entire quantity except for the parts of the recycled source product of the cracker used as fuel and resulting from process energy and loss. Consequently, no other products, be it polymer 2 or other products, are left with the possibility to market recycled fractions (Figure 6).

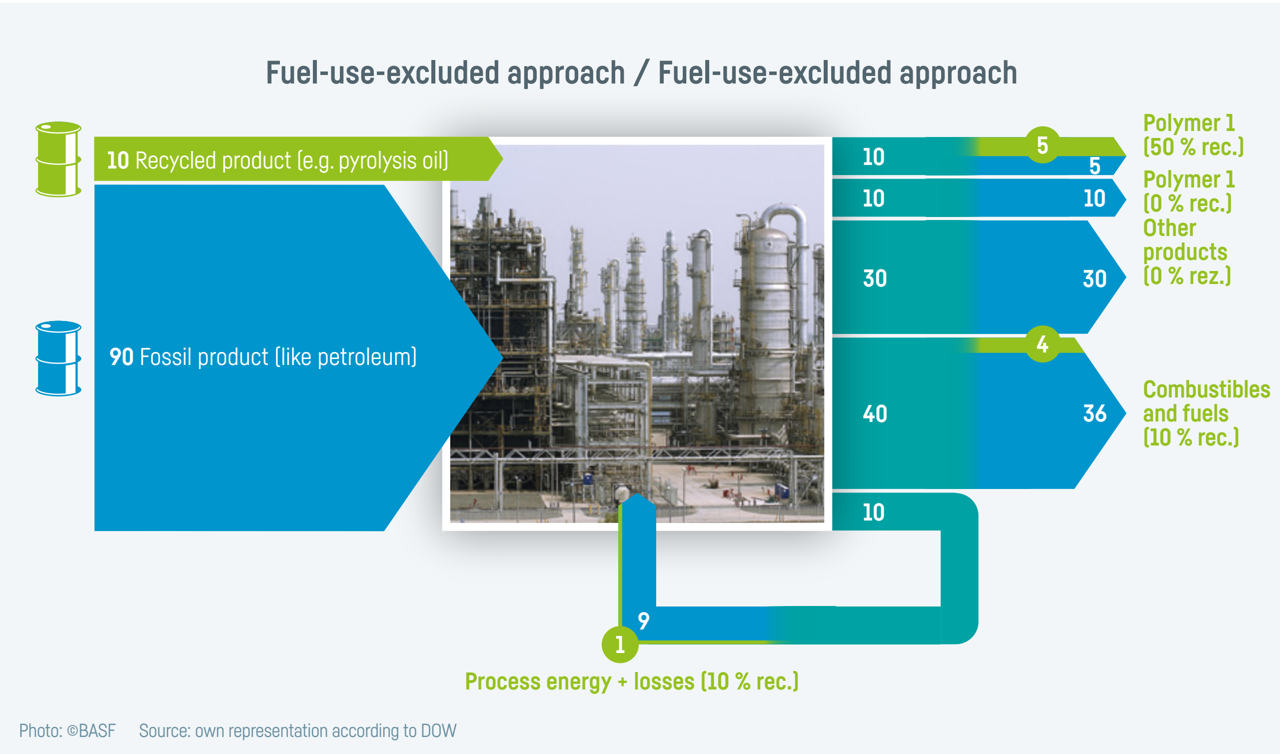

Figure 6: Volume flows and allocations for the "Credit Method" with the "Fuel-Use-Excluded Approach

[6] Source VCI/PED

For polymer 1, the allocated share of recycled feedstock increases:

- 10 t precursor for polymer 1, with 5 t fossil and 5 t recycled feedstock,
- 10 t precursor for polymer 2, with 10 t fossil feedstock,
- 30 t precursor for other products (such as pharmaceuticals), with 30 t fossil feedstock,
- 40 t of fuels, with 36 t of fossil and 4 t of recycled feedstock,
- 10 t for process energy and loss, with 9 t fossil and 1 t recycled feedstock.

The mass balance is back on track:

- fossil share: 5 + 10 + 30 + 36 + 9 = 90 (blue)
- recycled share: 5 + 0 + 0 + 4 + 1 = 10 (green)

This means that a total of 5 t and thus up to 50 % of the recycled output product can be allocated to the most market-relevant product of the steam cracker.

The method enables the chemical industry to quickly and scalable allocate significant recycled fractions, for example, to products for which the use of chemically recycled feedstock is required by law in the future, but for which mechanically recycled plastics cannot be used or are only available to a very limited extent for qualitative reasons (e.g. contact-sensitive or safety-related products). It ensures the economically stable financing of the entire chemical recycling process since the recycled input materials that are actually available can be allocated precisely to these products. This applies as long as the infrastructure processes a mixture of fossil and recycled feedstocks together.

4. Conclusion

To be able to use the existing infrastructure of the chemical industry for a circular economy for plastic waste and thus also to replace fossil raw materials and close the carbon cycle, the **mass balance approach "Fuel-Use-Excluded"** is now needed. Here, the total amount of recycled feedstock used, except for those used as fuels for energy, can be fully allocated as a recycled share to all or respectively selected end products.

This is also in line with the legal definition of recycling in the EU Waste Framework Directive. Since the large-scale production of plastics involves the parallel use of different fossil and recycled feedstocks and the simultaneous production of several different chemical precursors, a mass balance is necessary. For an economically viable expansion of the circular economy, the industry must be able to freely allocate the recycled share of the feedstock to those end products for which there is a sufficient market with a corresponding obligation and willingness to buy. The first legal market requirements have already been set by regulations such as the SUPD (Single Use Plastic Directive) and PPWR (Packaging and Packaging from Waste Regulation) and require these technical and economic solutions. The use of the fuel-use-excluded approach will enable the entire petrochemical production system to make its infrastructure available economically, to make the transition to a more circular economy and to initiate a system change.

At the same time, end products that also technically have shares of recycled feedstock in the production network, but which the market does not reward or legally prescribe, may only be declared as non-recycled (fossil). In this way, only those new circular feedstock products that actually and demonstrably enter the production system are allocated and marketed.

To ensure the complementarity of chemical recycling with mechanical recycling, labels of mass-balanced recycled content from chemical recycling in end markets should be linked to performance and control requirements that cannot be met by mechanical recycling processes on a large scale. This is the case, for example, for special plastic packaging and high-performance plastic components for the automotive and construction sectors, but also for sophisticated household and everyday products.

The UFCR advocates different labels for the information on the recycled content from physically separated and mass balance routes (mechanical and chemical recycling) to increase the transparency of the processes and thus credibility vis-à-vis consumers.[7] The mass balance also serves as proof of chemically recycled products in advertising statements (claims) to end consumers. For this purpose, the UFCR advocates a "label" for chemical recycling in parallel to mechanical recycling, as prescribed by the legislator, to exclude any possible consumer deception and greenwashing from the outset. On the contrary, such a label increases transparency and credibility with the end consumer and the associated consumer protection. The UFCR is currently working on a proposal for a consumer-oriented claim and label.

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[7] Corporate Forum Chemical Recycling (CFCR) – Political fields of action for the raw material turnaround and transformation into a circular economy by means of chemical recycling in Germany, Stuttgart, 2023

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