ENABLING A CIRCULAR ECONOMY FOR CHEMICALS WITH THE MASS BALANCE APPROACH

A WHITE PAPER FROM CO.PROJECT MASS BALANCE

ELLEN MACARTHUR FOUNDATION

CE100

TABLE OF CONTENTS

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EXECUTIVE SUMMARY

Realising a circular economy for products and major materials could seem complex but achievable. By contrast, retrieving the tens of thousands of compounds currently used as additives, paints, adhesives etc. and isolating them for recycling seems out of reach. Yet solutions that make economic sense exist. To fully unlock the circular economy potential of the chemical sector, a new approach is needed. This paper explores how a mass balance method offers a workable set of rules to ensure the traceability of recycled feedstock into new products.

The chemical industry uses a small set of raw materials or feedstocks to produce tens of thousands of products, many of them at 'world scale' plants operating at very high efficiency. They are the backbone of the chemical industry, which has over $2.5 trillion in investments worldwide. So far, however, the industry has been much less proficient at getting back the non-consumable products it produces once they have been used and feeding them back into production. Current recycling rates of major chemical products are very low (e.g. 9% worldwide for plastics) and to enable a circular economy there is an urgent need to find ways to loop them back into the production system.

Since chemicals are often used in complex combinations, discrete cycles are only possible in some cases (e.g. glass, metals, some plastics). Moreover, when products move through the economy, there will often be additional mixing and contamination, making it practically and economically infeasible to separate them even if they are physically and chemically distinguishable. Breaking such substances down into simpler chemicals, to be used as feedstock for new products, can be the best option.

Using chemical processes to bring mixed, diluted or low-volume substances back into the value chain presents an opportunity but also has inherent constraints. The opportunity in such 'chemical recycling' technologies - in contrast to mechanical ones - is that they generate virgin-grade feedstock. However, these processes need to plug into the existing chemical infrastructure in order not to be prohibitively costly from an investment point of view. Therefore, recycled feedstock will not exist in physically separate flows from other raw materials, with all materials needing to be blended in the chemical manufacturing complex. This means it is not possible to physically track where a recycled feedstock ends up.

Mass balance accounting is one of several well-known chain of custody approaches which have been designed to trace the flow of materials through a complex value chain. It is used in a number of established programmes related to sustainable and/or responsible sourcing, such as the Forest Stewardship Council (FSC) and Better Cotton Initiative (BCI). It is in principle well suited to address the challenges facing chemical recycling when trying to track the flow of recycled feedstock around chemical industry plants. The mass balance approach provides a set of rules for how to allocate the recycled content to different products to be able to claim and market the content as 'recycled'. To a chemicals manufacturer, recycled feedstock is just another raw material that enters the production system. Inside, it will blend with, and be converted to, many other things, but the amount of recycled content leaving the production plant equals the amount entering it (within the physical and chemical constraints of conversion efficiency and losses).

For the mass balance approach to work and be widely applicable, it is crucial that the basis for calculation and allocation rules are generally applicable and robust. Because compounds are of different value to the chemical process even if their atomic content is the same, mass balance accounting cannot be based on mass alone (except in some special cases). Instead, this paper proposes using chemical value-related properties, e. g. the 'lower heating value' (LHV) as the basis for the calculation. A common set of allocation rules enables a flexible and versatile market for a large range of recycled feedstock, so for the accounting to work well at a global level, allocation rules and use guidelines need to be agreed internationally.

A mass balance approach to enable the sale of certified recycled products at virgin-grade quality could be very valuable to all users of materials and chemicals in the value chain. The demand for recycled materials from downstream customers is crucial to drive the development of chemically recycled materials. Furthermore, increasing shares of recycled content in products is one of the key ways for a business to transition to a circular economy approach.

It is crucial that the claim of 'recycled content' is easy to understand for the end user, highlighting the importance of high-quality communication of the mass balance approach. It is especially important to be clear about the difference between chemically (mass balanced) recycled material and mechanically recycled material, and to demonstrate that chemical recycling is not a replacement, but a complement to mechanical recycling. To be able to make credible claims and be fairly compared to competitors and peers, a common, standardised protocol would be needed to pass recycled content along the value chain.

Standardising a mass balance approach for recycled chemicals can be achieved using a well-established methodology. A practical way forward could be to use a parallel consensus/non-consensus process for developing requirements and certifying performance in real marketplace applications while a higher level discussion on international standards takes place.

By publishing this white paper, the project stakeholders propose a standards development frame for a mass balance approach. They see a mass balance approach with clear and pre-defined rules as a key way to facilitate and encourage the use of recycled raw materials in the production of new products using a mass balance approach with pre-defined rules. One or more standards could be developed within the frame. The next key step in this process would be to increase the number of stakeholders working on standards development to broaden and harmonise how is applied in the market.

1. INTRODUCTION – WHY MASS BALANCE APPROACH?

1.1 CHEMISTRY AND THE CIRCULAR ECONOMY

To realise the ambitious proposition of a circular economy, we need to find ways to circulate all kinds of materials and substances. After all, in a circular economy the concept of waste does not exist, which means that it is not enough to prevent high-value, large-volume assets and materials (like cars, steel and buildings) from dissipating into lower-value things: the same principles must apply to the countless number of compounds incorporated in all of our materials, (like those giving objects colour, those imparting surface finishes of smoothness or roughness, and additives used to extend product lifetimes).

Seeking to create an economy that is regenerative by design is relatively intuitive in some familiar cases. Instead of selling a car, for example, a manufacturer can choose to sell mobility as a service while designing the vehicle to optimise repair, disassembly, remanufacture and recycling of parts and materials. Though it must involve a complex network of processes and stakeholders, it is not that difficult to envision how such a system might work, component by component and supplier by supplier, or to trace the flow of the goods and services.

Chemicals, on the other hand, are a different story. While discrete material flows can be devised for products made of metals, concrete, wood etc. (or combination of them), chemicals are commonly present in small quantities as additives to other materials, adding to a challenging complexity of many after-use material streams. Extracting and isolating such small quantities from other materials would be very resource-demanding and often turn out intrinsically unsustainable. Since tens of thousands different chemicals are in commercial use, it is clearly infeasible to design a system in which each can be recycled separately.

Yet, chemicals play a vital role in the modern economy, and it is therefore crucial to find a way to circulate them to truly transition towards a circular economy. The challenge lies in understanding where separate (or ‘closed-loop’) reuse or recycling of a material or chemical makes sense from a value capture point of view (for example reuse models for plastic packaging or chemical leasing of solvents or lubricants), and where collection and reprocessing of mixed material flows need to be considered. To unlock the potential for a circular economy for chemicals, it is clear that a new approach is needed to deal with such cases.

This project deals with what such an approach might look like. We know from even basic textbook chemistry that all molecules can be made or broken up by (re)combining their basic building blocks as long as a chemical pathway is provided together with an appropriate amount of energy. In other words, all chemicals can be broken down to simpler building blocks and made into the same or different chemicals again, even if they are heavily mixed or contaminated. This insight forms the basis for ‘feedstock recycling’, where a mix of components are broken down into simpler but common building blocks, which can then be fed into a chemical process to make new products.

However, once a material or chemical is recycled into simpler building blocks, it cannot be distinguished from identical building blocks of other origins, making the traceability of recycled feedstock a key challenge. Even if we manage to break down a mix of chemicals into simpler building blocks that can be fed into a chemicals plant, we cannot know for sure which products coming out in the other end contain the recycled content, and which do not.

That is why the ‘mass balance’ approach presented in this paper is a key tool in order to make recycling of chemicals work at scale, to enable the customers of the chemical industry to use recycled chemicals and therefore to contribute to the transition towards a circular economy.

1.2 PRINCIPLES OF PRODUCTION IN THE CHEMICAL INDUSTRY

Chemistry is the science of transforming one substance into another substance. Therefore, it is at work everywhere around us, in each and every living organism and in every corner of the universe. The chemical industry exploits the properties of atoms and molecules, together with the laws of thermodynamics, to make the myriads of compounds and materials that sustain modern living. Using a relatively small number of building blocks or 'platform chemicals' as junctions in a complex production network, the chemical industry has optimized to convert raw materials to the enormous diversity of materials we use today.

An example of a typical building block is illustrated in Figure 1. Mono-ethylene glycol (MEG) is a simple molecule that can be obtained from several raw materials (e.g., petroleum, natural gas, coal or biomass) and ends up being used in or being a precursor for many different products that are used in a variety of applications.[1]

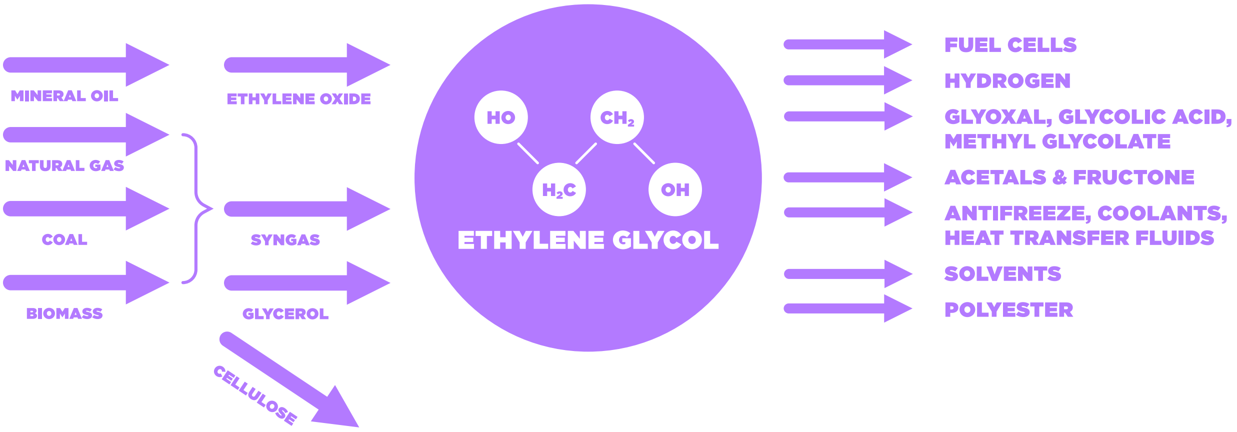

Figure 1. Ethylene glycol is an example for a key platform chemical

Throughout the industrial history, platform chemicals have come to originate from a small number of basic raw materials such as oil, natural gas, and (some) biomass due to their abundance and versatility in chemical processing. The few raw materials are converted in 'world scale' plants in vast quantities (millions of tons) to the building blocks that are used by the thousands of chemical plants that make (in Europe alone) about 20,000 different products. These products, in turn feed more than 20,000 companies in Europe, ranging from big businesses to lean start-ups.

Even if they do not belong to the same company, different chemical plants are often directly linked to each other, either physically through pipelines or through rail-, road- or water-bound logistics chains (logistical systems are a form of inter-connectedness). This enables by-products from one chemical process to be the starting material for another downstream chemical plant. Such interconnectedness contributes to the industry's efficiency and is – in principle – a good starting point to enable an increasing use of recycled feedstock.

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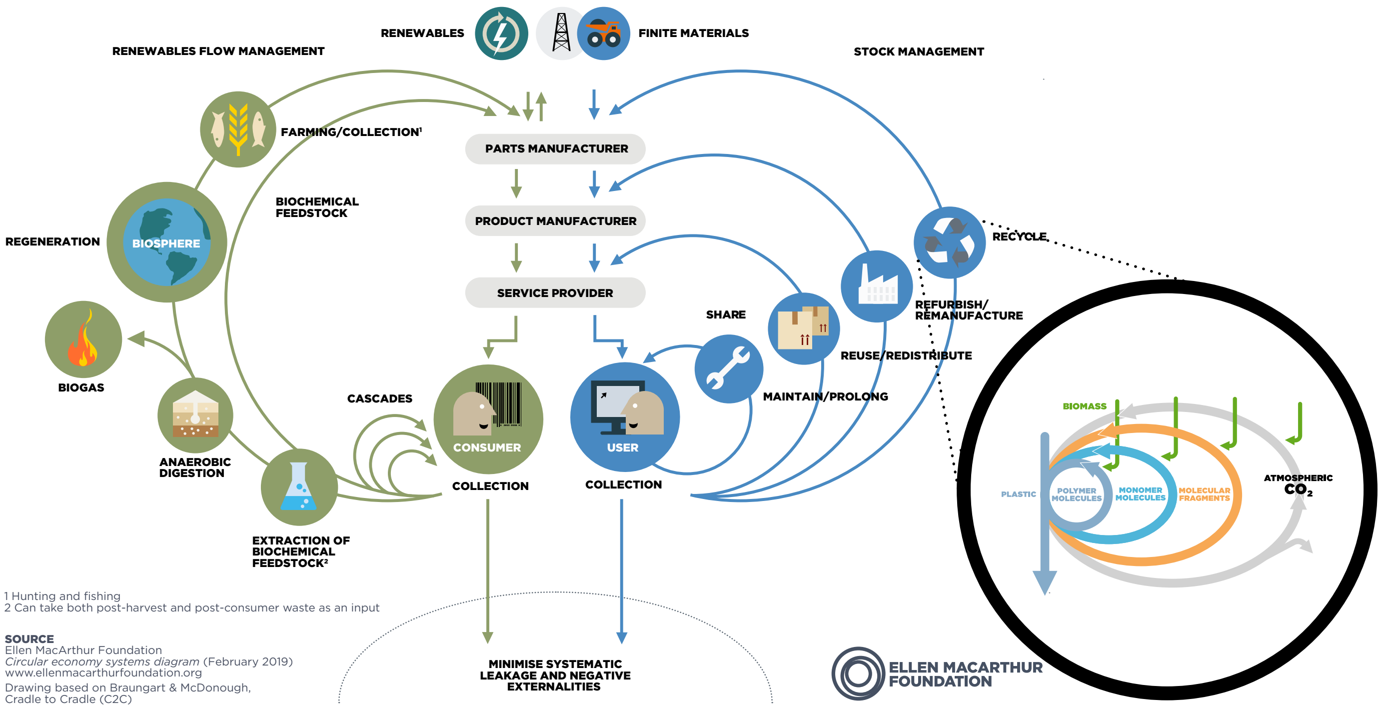
[1] It is important to consider that chemical recycling can be achieved by different recycling loops. In favourable cases, whole molecules can be recycled. In other cases, a complete break-down of the to-be-recycled materials mix to petrochemicals is needed. For instance, polyamides and polyesters can often be recycled without having to go through the process of breaking them down to a petrochemical feedstock first.

As mentioned above, the few basic raw materials can come from a renewable source (e.g. biomass) but also a recycled feedstock. After all, the materials share the same constituting atoms. Since chemical industry is very asset heavy – the global chemical industry has invested EUR >2.7 trillions in assets over the past 20 years – it would be desirable to use this existing infrastructure to scale up the use or renewable and recyclable feedstock, as opposed to developing new infrastructure.

1.3 RECYCLING CHEMICALS AND MIXED MATERIALS



1 Hunting and fishing
2 Can take both post-harvest and post-consumer waste as an input

SOURCE
Ellen MacArthur Foundation
Circular economy systems diagram (February 2019)
www.ellenmacarthurfoundation.org
Drawing based on Braungart & McDonough, Cradle to Cradle (C2C)

Figure 2. The circular economy system diagram (edited for the purpose of this white paper)

In the transition to a circular economy, all industries need to become better at getting what was once produced back into circular material loops (Figure 2). The inner loops, such as reuse (with or without repair), refurbishing or remanufacturing, preserve more value, but are not possible for numerous products and materials. When inner loops are not feasible, different recycling loops, most typically mechanical recycling, can be used to get materials back in use. Mechanical recycling is suitable and a good solution for many materials such as metals, glass and some plastics – especially in Europe where the recycling infrastructure is relatively well established and can achieve high-level separation. However, for more complex materials and substances, mechanical recycling has limitations as it depends on physically sorting different materials to achieve high quality and therefore utility of the recyclate.

Many substances are used in combination with others, like chemical additives and plastic composites, and are therefore not easily separable from each other. This leads to impurities in the recycled material if using the mechanical recycling route, and therefore limits material quality in further usage. Moreover, when products move through the value chain, there is additional mixing and contamination of materials, making it economically unfeasible to separate many materials even if they are physically and chemically distinguishable.

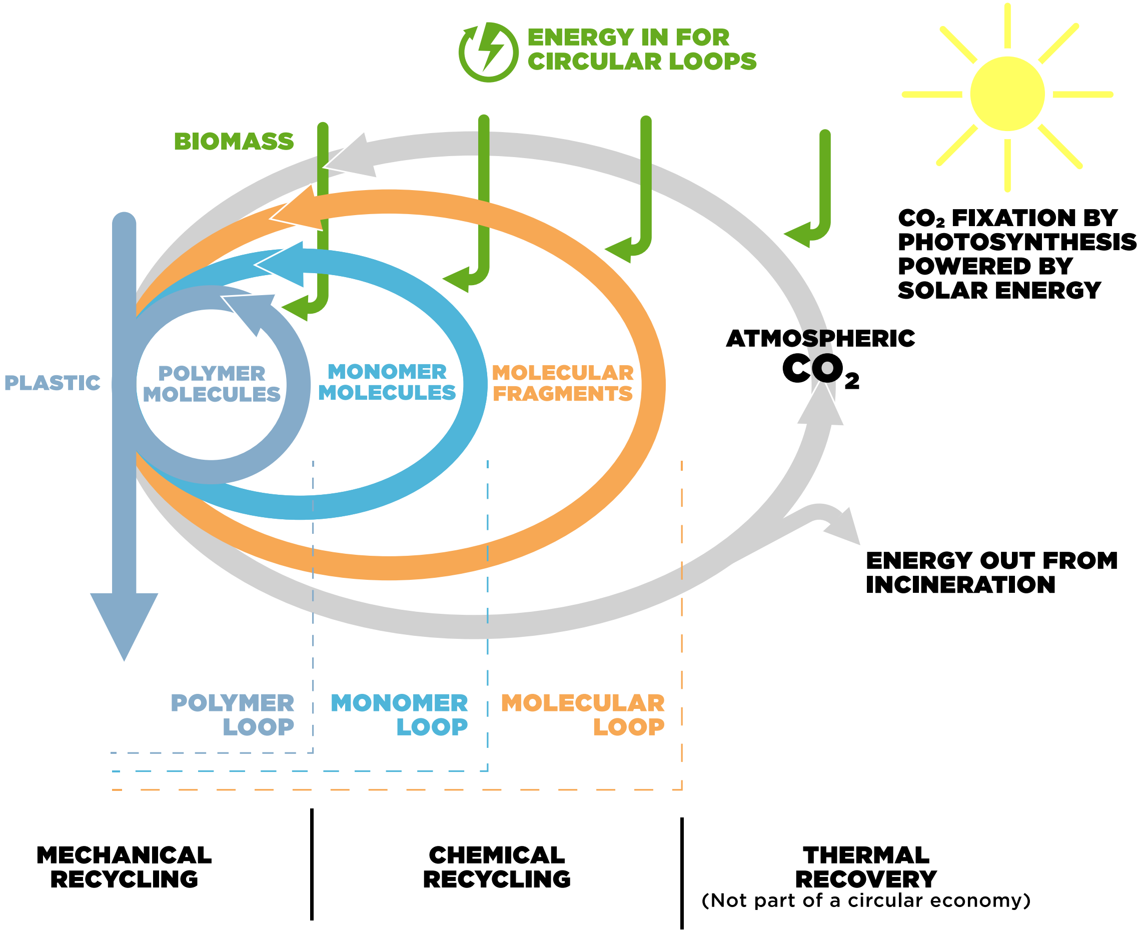


Figure 3. The composition of waste (plastics in this example) determines which recycling loop option is technically and economically feasible or preferred. Simplified: The more mixed and worn the plastic waste is, the more to the right the most-suited loop reaches. NB: Thermal recovery of non-renewable materials is not in line with the principles of circular economy and not in scope of this paper.

Due to the limitations of collection systems and mechanical recycling, the recycling rates of major chemical and plastic products are very low (e.g. 9% worldwide for plastics). There is thus an urgent need to find ways to loop them back into the production systems and move towards a resource efficient circular model.

The prospect of using chemical processes to get mixed, diluted or low-volume materials back into the value chain is an opportunity worth exploring. ‘Chemical recycling’ (Figure 3) provides a new pathway to take low-grade, mixed substances into the recycling loop and to break them down to simpler building blocks that are used as feedstock to make new materials and chemicals of virgin-grade quality.[2] This makes chemical recycling a valuable complement to mechanical recycling, as described further in section 3.1.

As noted above, the most efficient way to introduce chemically recycled feedstock to manufacturing is to feed it into existing chemical asset networks to make the recycling economically feasible. Therefore, when envisioning a general chemical recycling system, it means that the recycled feedstock will be blended with other raw materials in the chemical manufacturing complex. In continuous chemical processes, it is impossible to physically track different feedstocks, which are mixed already in molecular level in the process. To be able to properly follow and account for the right amounts of recycled substance, a robust chain of custody method is needed.

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[2] This paper does not aim at describing different chemical recycling technologies in detail. For reference, the reader is referred to other published material, e.g. European Commission, A circular economy for plastics – Insights from research and innovation to inform policy and funding decisions, (2019); Closed Loop Partners, Accelerating Circular Supply Chains for Plastics (2019)

1.4 CHAIN OF CUSTODY MODELS

‘Chain of custody’ models have been designed in various industrial settings to create transparency and trust throughout the value chain regarding properties of goods and materials that are otherwise hard to distinguish between samples. Such properties include origin, production practices, and raw material composition. This enables end users or customers to choose a more sustainable solution without having the ability to control each aspect themselves, by knowing the proportion of a desired component in a determined supply.

There are four chain of custody models, described in Table 1 and illustrated in Figure 4. Their common objective is to guarantee solid bookkeeping and to corroborate a link between in-going content (e.g. ‘sustainable’, ‘recycled’ or ‘organic’ by some definition) and the finally out-going product. They differ in the very nature of said link, whether it is physical or administrative, the set of rules for balancing, and the objective possibility to keep materials streams segregated or not.

The identity preservation model is only applicable in case the desired goods or components can be identified individually (e.g. food appellation d’origine contrôlée). In cases where separate origins cannot be identified in an aggregate, but where the goods are themselves equivalent within the defined standard (e.g. certified organic food), the segregation model applies. In the segregation model, materials from different sources can be mixed within a common category, but material categories are kept physically separate (I.e. organic versus non-organic).

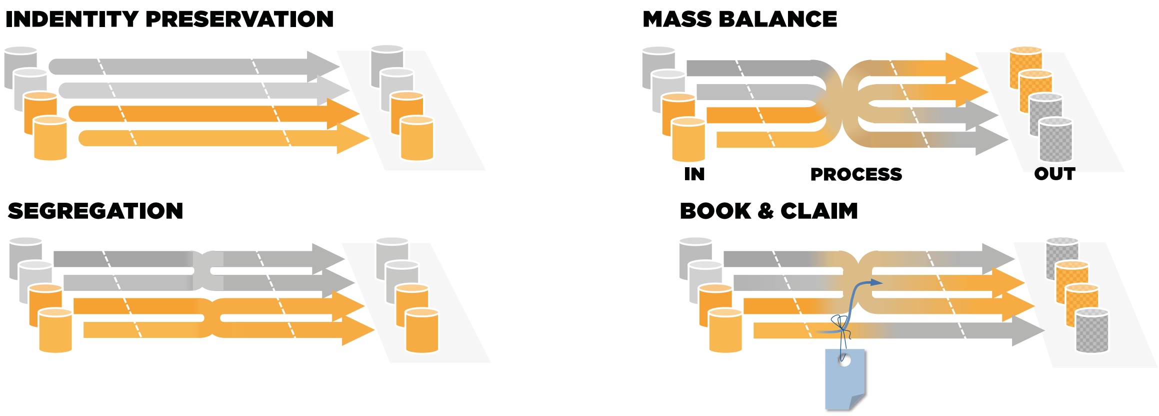

Figure 4. Four types of chain of custody models

In other cases, however, the volumes or values of goods or materials from the desired sources are too low to be shipped, stored or processed separately, or the technical processes do not allow to differentiate. Then, the **mass balance** chain of custody is designed to track the total amount of the content in scope (e.g. sustainably sourced wood fibre) through the production system and ensure an appropriate allocation of this content to the finished goods based on auditable bookkeeping. Property conservation principle is set to ensure that the total certified output does not exceed its original input and take into account the appropriate conversion losses and production / assembly ratios.

A **book and claim** model can be applied when there is no physical connection between the final product and the certified supply. An illustrative example is renewable electricity, where power is traded on a spot market irrespective of where the energy has been produced, and the certified ‘green’ electricity purchased by the end user is likely to be produced somewhere else.

Table 1. Chain of custody (COC) models[3]

Model	Principle	Example
Identity preservation	It is possible to physically track the product to its desired origin, ensuring unique traceability and physical separation of products from other sources along the supply chain.	Buying food from a single certified farm.
Segregation	Consists in the aggregation of volumes of products of identical origin or produced according to the same standards in one stock item.	Buying food from a trader that exclusively handles identically certified supplies
Mass balance	Considering the output, no physical or chemical difference exists between in-scope and out-of-scope. It involves balancing volume reconciliation to ensure the exact account of volumes of in- and out-of-scope source is maintained along the supply chain, provided that the volume or the ratio of sustainable material integrated is reflected in the product produced and sold to customers. This model requires that a reconciliation period is defined (e.g. a month, a year).	Buying a certain percentage of a supply from certified origin. Applies to, e.g., sustainable forestry, recycled, bio-based or renewable materials, aluminium, organic cotton
Book and claim – certificate trading	The certified product / component is completely disconnected from the certification data. The certified product evolves in separate flows from the certified supply. Credits or certificates are issued at the beginning of the supply chain by an independent body reflecting the sustainable content of supplies. The intended outcome is that outputs from one supply chain is associated with total credit claims corresponding to the certified input.	Buying renewable energy certificates offsetting GHG emission by equivalent agroforestry CO2 capture certificates.

For credibility, all chain of custody models need standardization and preferably an independent third-party certification scheme. To this end, allocation rules need to be defined and a certification process set up, including what types of claims can be made and what branding can be used. Company claims on product chain of custody should be made according to ISO 14020 standards series on environmental declaration, and all relevant national regulations applicable to product environmental declaration and certification. In that case, regulation would define the protocol and requirement for certifying product / supplies and define the claim to be made regarding product as well as the criteria for selecting certified third parties as certification organisations.

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[3] Chain of custody models and definitions – ISEAL Alliance September 2016 www.isealalliance.org/sites/default/files/resource/2017-11/ISEAL_Chain_of_Custody_Models_Guidance_September_2016.pdf (accessed January 7th 2018)

With a common standard, chain of custody systems can then be voluntarily verified or certified by third-party bodies to ensure reliability and trust along the supply chain and ensure that claims are not misleading. Choice of third-party verification depends on the use of chain of custody models and the type of claim the producer wants to make regarding the products themselves or regarding the global material flows in their supply chains. At company level the chain of custody information and relevant supplies certificates can, for example, be reviewed by auditors during a CSR report verification process.

Table 2. Product categories, voluntary labels and traceability models[4]

Product	Label Certification Organization System	Traceability Model Allowed[5]				Year of introduction
		Identity Preserved	Segregation	Mass Balance	Book and Claim	
Palm oil	RSPO	**X**	x	x	**X**	2004
Soy	RTRS		x	**X**	**X**	2006
	ProTerra	x	**X**			2012
Sugar	Fair Trade	x	**X**	x		1997
	Bonsucro		x	**X**	**X**	2006
Cotton	Fair Trade	x	**X**			1997
	Better Cotton Initiative		**X**	**X**		2005
Marine Fish	MSC		**X**			1997
	This Fish	**X**				2010
Aquaculture Fish	ASC		**X**			2011
Timber	FSC	x	**X**	x		1993
	PEFC	x	x	**X**		1999
Biofuels EU Market	15 Different Schemes	x	x	**X**		2009
(non) GMO Crops	EU		**X**			1997/2004

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[3] MOL, A. P. J. & OOSTERVEER, P. 2015. Certification of Markets, Markets of Certificates: Tracing Sustainability in Global Agro-Food Value Chains. Sustainability, 7, 12258., doi:10.3390/su70912258

[4] A capital and bold X means used for the major share of the market; small x means less often used;

Product	Label Certification Organization System	Traceability Model Allowed[5]				Year of introduction
		Identity Preserved	Segregation	Mass Balance	Book and Claim	
Biofuels	RSB	x	x	**x**		2007
Agricultural Products	FOAM	x	**x**			1972
	Rainforest Alliance	x	**x**	**x**		1987
	Organic Label US and EU		**x**			1990/1991
Tea	Fair Trade	x	**x**	x		1997
	UTZ	**x**	**x**			2002
	Ethical Tea Partnership		**x**			2009
Cocoa	Fair Trade	x	**x**	x		1997
	UTZ	x	**x**	**x**		2002
Coffee	Fair Trade	x	**x**			1997 (1988)
	UTZ	x	**x**			2002
	4C Association	x	**x**	x		2006
Meat	GRSB	**x**	**x**			2016

As seen in Table 1 and Table 2, several chain of custody systems have been created and achieved wide application, especially in the areas of farming practices (FairTrade, various organic labels), forestry (FSC), fishing (MSC) and renewable energy (green electricity certificates). Given the way in which recycled basic chemicals are expected to be mixed with other feedstocks in chemical plants (as described in sections 1.2 and 1.3), the mass balance approach appears the best suited to account for their allocation in new products.

With a common standard, chain of custody systems can then be voluntarily verified or certified by third-party bodies to ensure reliability and trust along the supply chain and ensure that claims are not misleading. Choice of third-party verification depends on the use of mass balance and the type of claim the producer wants to make regarding the products themselves or regarding the global material flows in their supply chains. At company level the chain of custody information and relevant supplies certificates can, for example, be reviewed by auditors during a CSR report verification process.

Historically, chain of custody systems have been developed for organic farming, fair trade and sustainable food production. In 2015, Arthur P. J. Mol and Peter Oosterveer published an extensive inventory of existing Chain of custody systems in Agro-Food sector and the principles they are based on (see Table 2).

2. HOW WOULD A MASS BALANCE APPROACH FOR CHEMICALS WORK IN PRACTICE?

2.1 RECYCLED MATERIALS AS AN ADDITIONAL FEEDSTOCK IN THE CHEMICAL PRODUCTION

As described in Chapter 1, the use of recycled materials as a source of feedstock is an excellent opportunity to decouple value creation from the consumption of fossil resources. To a chemical manufacturer, a recycled feedstock is just another raw material that enters production. Co-feeding both recycled and virgin feedstock into the same network of chemical production plants offers a pragmatic way to enable the chemical industry to transition towards a circular economy, as well as being an enabler for other industries. By feeding into existing and continuously running steam crackers or synthesis gas (a.k.a syngas – a mix of carbon monoxide and hydrogen) plants, the full scope of chemical value chains can be accessed, and the same end products can be manufactured on the very same quality level with minimal upfront investment.

It is indeed viable to harvest the synergies of the existing chemicals assets and infrastructures for innovative and sustainable feedstocks as it has been shown with bio-based feedstock. Here, the bio-feedstock is mixed with conventional fossil-based feedstock at the very beginning of the production chain and then allocated to selected products through a precise accounting method. Customers of ‘biomass-balanced products’ contribute to reducing CO2e emissions and save fossil resources (detailed description in VCI 2017[6]). The same rationale holds true for recycled feedstocks. Balancing enables precise accounting of the amount of recycled materials used in the production plants and traceability on how these are allocated to products-to-be-sold (Figure 5).

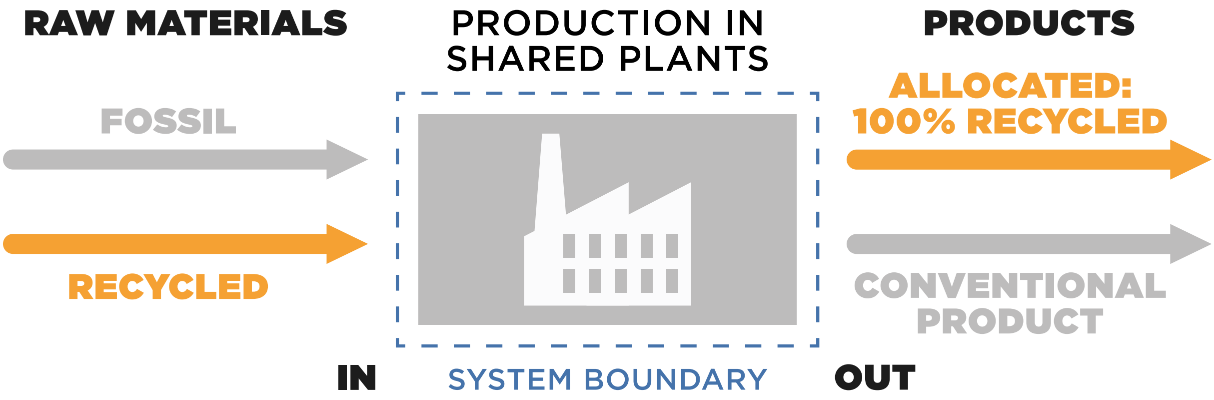

Figure 5. Co-feeding: Recycled materials and fossil-based raw materials are used in parallel, as physically mixed feedstock in existing production assets. Yield and cost advantages of established fossil-based production routes are immediately accessible for recycled materials.

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[6] VCI (2017) The use of renewable raw materials in the chemical industry, applying mass balance approaches. However, it is also possible to measure the exact amount of bio-based content by using the Carbon-14 method. This fact creates a challenge for using mass-balance approach to allocate bio-based content to products, since the actual (measurable) quantity is likely to be different from the allocated quantity. The debate on how to best solve such discrepancies is still ongoing. This paper addresses using the mass balance approach for recycling of chemicals and will not go deeper into how to best measure and claim bio-based content.

Consider the example of chemical recycling of plastics. Some polymers, such as polyesters and polyamides, can be converted back into their constituent monomers under favourable reaction conditions. However, such route is not available to other polymers such as polyethylene and polypropylene. These common plastics need to be broken down, e.g. in a pyrolysis process or via syngas, to molecular fragments and converted into a liquid mix of simple hydrocarbons. In both variants, energy-Intensive thermochemical processes need to be employed that use high temperature to convert the solid plastic materials to oily fluids. The latter may then be used to replace naphtha, e.g. by being co-fed to a steam cracker, and starting a versatile loop of chemical value creation - but now on a truly circular materials basis. (See Annex A for more details.)

2.2 BALANCING TO ALLOCATE 'RECYCLED CONTENT' TO SELECTED PRODUCTS

The idea of the mass balance approach is that recycled feedstock replaces an equivalent amount of virgin feedstock at the beginning of the value chain (input) to be allocated to the product (output) in such a manner that the input and output match. What happens in between is less relevant, as long as the balancing task can be met in a proven and reliable manner by considering a few boundary conditions in the calculation:

- Firstly, for each product (selected for 'allocation of recycled content') the exact amount of fossil feedstock necessary for its production needs to be determined, i.e. how many tons of feedstock are needed to produce one ton of output. Despite the complex nature of chemical production networks with different formulations, yields, and losses, this is common practice for conventional fossil feedstocks.
- Secondly, it needs to be determined what amount of recycled feedstock can replace a certain amount of fossil feedstock.
- Thirdly, for proper balancing, the system boundaries in space and time need to be defined, i.e. the set of production assets and the time period where the recycled feedstock booked in and the recycled content of the products booked out need to match.

In principle, the system boundaries can be chosen in a broad range of ways, if stringent accounting is guaranteed. If the production systems are not interconnected, we would be talking about book and claim. Strict qualifying requirements are needed: The system boundary should cover an integrated chemical production system, with physically interconnected production plants at the same location, or plants at different locations which are temporally and physically interconnected by dedicated transportation systems e.g. pipelines, ships, trains or trucks. This can be within production sites of one company or within a group of companies, even in different countries. Many value chains intrinsically build on intermediate chemicals that are produced outside the defined system boundary, e.g. sourced from competing chemical companies. The system boundary should include all assets needed to convert the recycled feedstock into the selected product (Figure 6) and, preferably, they should not contain separate chemical production systems that are not physically interconnected.

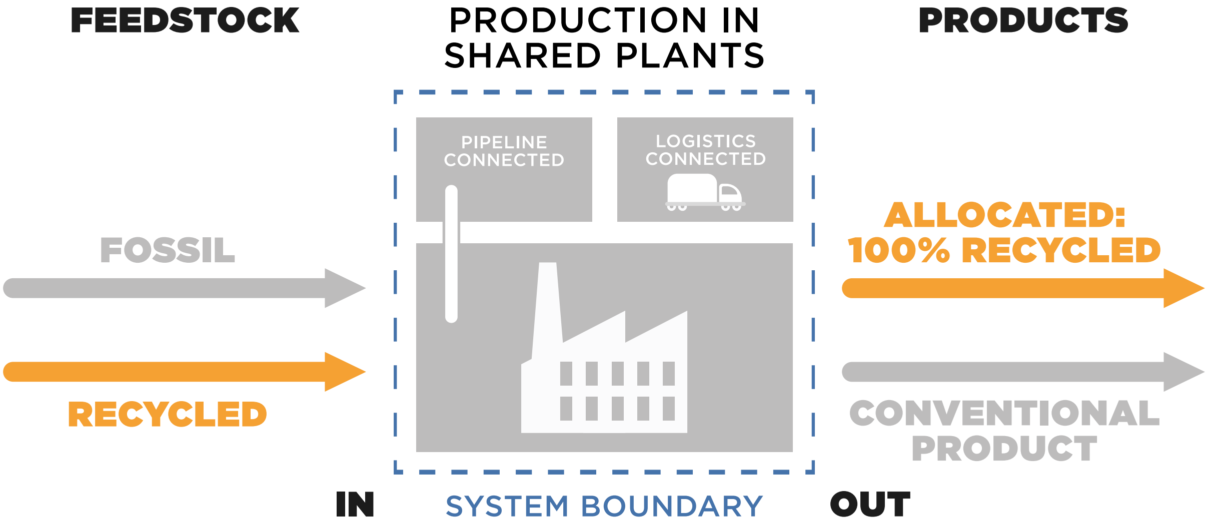

Figure 6. The system boundary can comprise various elements of an integrated chemical production system with potential physical substance stream between the recycled feedstock and the selected product including multi-site transfer in global manufacturing supply chains.

The system boundaries need to contain a defined booking period, i.e. the time span in which all materials streams with the attributed quality (incoming as well as outgoing) are reconciled. For most purposes, an annual balancing is pragmatic and sufficient. Only raw materials used as feedstock for the production - not as energy - should be considered for allocation in mass balancing[7].

2.3 ALLOCATION RULES IN MASS BALANCING

In the chemical production, the various raw materials reacting to end products have different values for the chemical synthesis. For the comparison of the varying materials a conversion factor, a kind of 'chemical value' is needed. There are different approaches to quantify and to compare the different feedstock sources: mass allocation, carbon counting, or the lower heating value (LHV) also known as net calorific value[8].

The composition of plastic waste and its deviation from both the to-be-replaced fossil feedstock and the targeted products introduce an accounting challenge in balancing: Fossil feedstock mainly consists of carbon and hydrogen atoms. Chemical products of whatever composition can be derived back to such petrochemical feedstocks. Many waste products in scope for chemical recycling, such as plastics, often can introduce additional chemical species that are 'ballast' and should not be counted as basis for recycling content. Examples are oxygen, nitrogen, chlorine-contents or inorganics like salts, mineral fillers, or glass fibres.

For a proper balancing, a reliable procedure is required that counts the to-be-recycled content and disregards the not recycled 'ballast'. If two raw materials with virtually identical compositions are compared, simple weighing is pragmatic and mass balancing is sufficient (e.g. comparing bio-methanol with fossil-based methanol). However, if raw materials differ in composition (e.g. comparing polyamide with glass-fibre reinforced polyamide) it may become necessary to determine the carbon content and to honour in tracking

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[7] However, the use of recycled feedstock as fuel replacement may qualify in other circular schemes for waste reduction or avoidance.

[8] For many energy consuming world scale reactions e.g. syngas production, LHV is a proxy for value. Hydrogen has a comparably high value as co-feed in the syngas process and can be evaluated by its LHV although it is a carbon-free intermediate. (This value would be misrepresented if one were to choose mass allocation or carbon counting as basis for calculation.) Reporting of feedstock in the chemical industry frequently is done in the unit of LHV to make it comparable.

only that materials fraction (polyamide) that is indeed to-be-recycled, e.g. by carbon counting. If the raw materials are even more mixed and contain variable fractions of carbon, hydrogen, oxygen and nitrogen, e.g. plastic waste containing polyolefins, polyester, polyamides, then methods that measure the net calorific value[9] would be needed to determine the ‘chemical value’ in the recycled feedstock[10]. Mass balancing requires the stringent application of feedstock characterization that reflects the to-be-recycled content and disregards diluting ballast. Figure 7 demonstrates how such allocation rules that overlook the ’chemical value’ of hydrogen or disregard the ’diluting effect’ of oxygen distort the balancing.

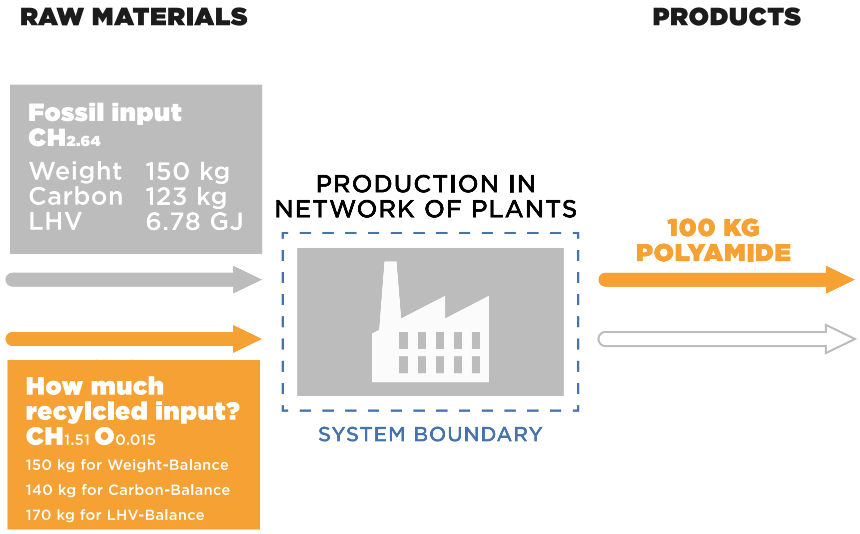

Figure 7. Comparison of different allocation procedures for the hypothetical production of polyamide based on mixed polyester plastic waste: When balancing on basis of LHV, 170 kg of recycled feedstock is needed to replace 150 kg of fossil raw materials. On basis of mass, while disregarding compositional differences, the very same 150 kg recyclate would be needed. And if only the carbon is counted, mere 140 kg recycled feed would be demanded.

The conclusion is clear - in extraordinary simple feedstock systems, where the composition of fossil and recycled feedstock and target products are virtually identical, mass allocation or carbon-counting can be an adequate balancing approach. Under such conditions, it yields almost identical allocation results as the more elaborated LHV method. However, if employed in a (probably real life) complex waste situation, simple weighing may turn out inadequate and eventually discredit an otherwise scientifically fair and robust balancing approach (see Annex A for more details). Consequently, mass allocation or carbon allocation should be used in special cases only. Counting based on carbon mal-estimates the role of all non-carbon intermediates in chemical synthesis such as hydrogen or amines. The calculation via LHV is then the pragmatically preferred option.

THE SPECIAL CASE OF QUALIFIED CREDIT TRANSFERS (QCT)

A widely held opinion is that unrestricted Book & Claim cannot be allowed, but there is no consensus on the reason for not allowing the Book & Claim chain of custody. Some consider it less transparent and therefore less reliable. Yet, it is believed that an important alternate chain of custody model is needed. Circular Economy will be significantly accelerated

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[9] The LHV is a well-established measure and can characterize hydrocarbon feeds from naphtha fractions over natural gas to coal, as well as renewable feedstock like bio-gas or sugar. It is also applicable to recycled feedstock despite its intrinsic compositional variability.

[10] For sake of clarity, if used battery materials should be recycled, the ‘chemical value’ for the recycled feedstock would need to reliably mirror the metal elements lithium, cobalt, and so forth

and expanded if mass balance accounting includes a chain of custody model under which recycled material credits can be administratively transferred within a predefined system boundary. Without the ability to transfer credits companies would face prohibitive challenges in shipping of materials (i.e. shipping essentially identical materials between sites) and the need for redundant assets that have no return on investment.

Qualified credit transfers between sites may help to accelerate the transition to a Circular Economy and while at the same time prevent unintended consequences or incentivise unsustainable practices. For example, without the ability to transfer qualified credits between sites some companies might want to ship materials between distant sites in order to expand a mass balance system boundary.   Shipping just to expand the system boundaries would require additional transportation, it might also require constructing redundant storage and manufacturing assets all of which would incur additional unnecessary environmental impacts. This is illustrated in Figure 6b.

Specific limits to the expansion of the system boundary need to be developed within a multi-stakeholder standard development process and may include requirements such as: 1) in the absence of physical connectivity, credits may only be transferred for materials that both have been fairly assessed for their respective chemical value, e.g. by the LHV method, 2) each site must be included in a pooled mass balance system and be certified under the same certification system; 3) the sites must have management control by the same company; etc.

The option for credit transfers between sites under strict qualifying conditions is available in existing “mass balance” certification systems (derived from the biofuel certification) for all industries, not just chemicals. QCT may thus be discerned from unrestricted Book & Claim.

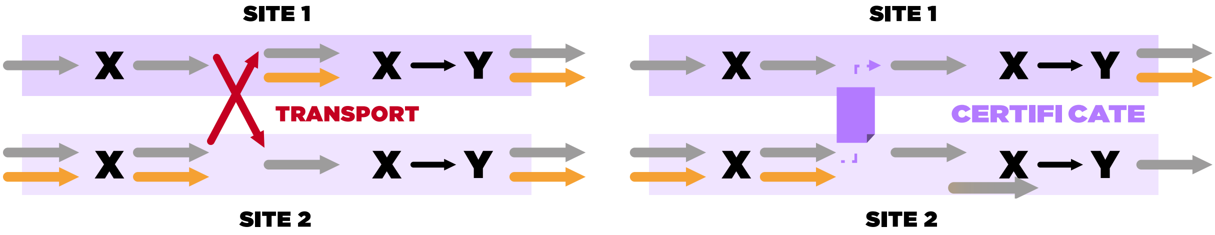

Figure 8. Material balance accounting may include options for qualified credit transfer between same-company sites for same-materials in order to eliminate administrative barriers to the adoption of a circular economy. This allows companies to economically use existing assets to maximize the use of recycled of materials without wasteful shipping or requirement to build redundant assets. Multi-stakeholder standardization is needed to determine acceptable qualifying conditions.

2.4 PRACTICAL DESCRIPTION ON ALLOCATION RULES

In simple cases, where “same kind of”[11] recycled twins are available (e.g. recyclate PE/PP/PET to replace virgin PE/PP/PET) a mass-on-mass balance is easy to understand and there is only a need to agree on the eligible geographic flexibility of Feed-In-Point vs. the site of production, i. e. system boundary for of the recyclate-claimed[12] product.

Rule 1: mass-on-mass balance is possible with “same kind of” recycled chemicals.

Rule 2: System boundary must be defined. Mass balance can be made across different sites of the same company (even in neighbouring countries).

More frequently, chemicals and polymers are made from several other chemical intermediates from a production network. They can also always be manufactured according to a mass balance method. Rule 1 applies when the “same kind of” recycled chemical or polymer or ALL “same kind of” intermediates are available: this is very unlikely! Therefore, more allocation rules are needed:

Rule 3: The feedstock demand of chemicals and polymers can be analysed and expressed in RMUs[13] considering all intermediates. The RMU demand reflects the petrochemical origin of all chemicals: oil & gas.

Rule 4: To enable a flexible and versatile market for a large range of recycled feedstock and to work well at an international level, RMUs should reflect the chemical value, and a 100% compensation (mass balance) should be attempted within the system boundary.

Rule 5: The system boundary comprises the chemical production network of a company.

EXAMPLE: 1 TON OF POLYAMIDE WITH RECYCLATE CLAIM

Option A: 1 ton recycled twin “same kind of” polyamide is used within system boundary.

Option B: Value analysis of 1 ton of polyamide shows feedstock requirement corresponding to 67.8 GJ. Recycled feedstock (e. g. MxP oil) quality available: 40 GJ/tonne: need to feed in 1.7 ton of recycled feedstock within system boundary for 100% recyclate claim.

[11] Criteria to define “same kind of” are nevertheless required

[12] Product with recyclate content*   Footnote: *applying a mass balance

[13] RMU = raw material unit

3. NEEDS AND CONSIDERATIONS FROM ACROSS THE VALUE CHAIN

This chapter reflects the opportunities and challenges emerging from applying a mass balance approach throughout the value chain as it could be a key enabler for implementing a circular economy for mixed feedstocks. It promises to reconcile the demand for quality products that meet the highest consumer expectations (with regard to product safety, appearance, and performance) with the societal expectations to minimize waste and maximize efficient use of resources. By creating the very same product molecules, in the very same processes and in the very same assets as for virgin products this can be expected to be achievable.

However, it needs to be clearly understood that for realizing such upsides, societal efforts and energy is needed. For public acceptance its needs to be ensured that the need for additional energy does not conflict with other environmental targets, e.g. for reduction of greenhouse gas emissions. Consequently, all parties along the circular value chains need to be encouraged to preferably employ energy from renewable sources, not undermining the benefits of mass balance by undesired detrimental impacts be it social or environmental.

3.1 PLASTICS – A GOOD PLACE TO START?

The key opportunity for the mass balance approach to be applied at scale lies in the increasing focus of key actors to consciously move towards recycled, sustainable and circular resources, especially in the application of incorporating recycled plastics into products. This is evident from the growing number of voluntary participants to the New Plastics Economy Global Commitment[14]. Similar initiatives are present, among other, at the European Union level (European Strategy for Plastics in 2018) and the French Circular Economy Roadmap with 50 measures with the first measure being “use more secondary raw materials in products”.

Provided the right conditions in terms of traceability, validation and acceptance are met, the mass balance approach could be among the key levers to meet the challenge of increasing recycled content and making plastic pollution a thing of the past. Mechanical recycling can be limited today in terms of:

- Challenges to meet the technical requirement in new applications, such as specific colours or mechanical properties;
- Lack of traceability on origin and content of waste materials, including potential presence of legacy chemicals;
- Regulatory constraints to use mechanically recycled plastics in several applications, e.g. food contact packaging

In light of these limitations, a mass balance approach can be a key enabler since it enables virgin-grade plastic to be derived from recycled feedstock.

Besides being able to include more recycled content in products, the main advantage for the downstream converter industry is that because the recycled material is chemically identical to virgin material, the technical properties and any approvals of the feedstock are unchanged, and no adaptation of downstream production processes to the different recycled feedstock is necessary. As a result, the product put on the market, using mass balanced feedstock should have the same technical properties than products made of virgin raw material without additional design approval and quality control.

Nevertheless, some points of attention need to be addressed to ensure customer’s acceptance of the mass balance concept. Customers need to understand the real added value behind the concept in order to make an informed choice and compare competing peers. A customer faces many ‘green’ offers on the market, from physically recycled plastics

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[14] newplasticseconomy.org/projects/global-commitment

to bio-sourced plastics and he needs simple and clear explanations about their environmental benefits and impacts. This is why it is essential to develop a robust standard as well as be precise regarding claims for customers.

3.2 SUGGESTED RULES OF THE GAME

Based on these considerations, this section proposes a set of ‘rules’ for applying mass balance to chemical production from recycled feedstock, with the ultimate goal to guide the development of a standardized protocol:

- An international standard, such as ISO, needs to be set up for recycled feedstock mass balance definition, calculation and consolidation methodology. Provisions need to be taken to provide evidence that the secondary raw material obtained by chemical recycling according to a mass balance approach is produced in an environmentally and socially responsible manner, and does not (re) introduce hazardous substances to the value chain
- This standard must be recognized, preferably worldwide, as contributing to the fulfilment of product- and application-specific recycling targets. Regulatory frameworks need to be set up to ensure this approach can be established in the markets. Description of claims needs to be clear, simple, understandable and unique when using mass balance approach. Especially it should always be clear: mass balance is based on tangible input of recycled feedstock in material flows and should not be assimilated as offset credit trades or unrestricted book and claim chain of custody. In the absence of physical connectivity, qualified credit transfers between site material balances of a company are acceptable under strict conditions established by multi-stakeholder certification systems.
- The environmental and societal benefits should also be transparent to the customer, e.g. underpinned with reliable lifecycle analyses.
- Claim for customer is core for the credibility of the approach. Each market / company must be free to embed the mass balance approach at a corporate or a finished product level in compliance with ISO 14020 standard series on environmental declaration and applicable regulations in case certification for the product is needed besides the raw material mass balance certification from supplier.
- Considering the potential need for consolidation of volumes of different mass balanced feedstocks in manufactured products, extended chains of custody programs covering feedstocks as well as product certification and claims rely on adequate allocation procedures. In case several recycled feedstocks are integrated in one product, manufacturers will have to consolidate volumes from different suppliers and different chains of custody programmes.

From the technical viewpoint, the mass balance approach enables the integration of recycled (as well as renewable) materials in the existing production plants and value chains, to scale up their use and mitigate resource scarcity. Still, the environmental and climate impact of chemical recycling needs to be monitored closely as the technologies scale up to commercial level, to ensure the pathway is indeed a sustainable alternative with respect to GHG emissions and other life-cycle impacts[15].

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[15] At the time of writing this white paper, this point has not yet been robustly proven.

4. A PRIMER FOR STANDARDIZING THE MASS BALANCE APPROACH

4.1 WHAT ARE STANDARDS AND WHY ARE THEY NEEDED?

Standards are written documents that typically normalize an agreed set of rules for products, processes or services. Once developed and issued, they enable the accurate measurement of attributes, an agreed level of quality or safety, and can promote inter-operability or a common understanding of results. Their development can be initiated at several different organizational levels including global, country or company level (Table 3). Which organization initiates the development process depends on the standardization level and includes governmental bodies, accredited standards organizations, or innovators seeking diffusion.

Table 3. Different levels of standards involve different initiators.

Level	Initiator	Example	Application
Global	Government or country	The International Electrotechnical Commission: IEC 62368-1:2018 ISO International Standards organisation	Standard for defining the safety of electrical and electronic equipment within the field of audio, video, information and communication technology
Regional	EU member states through national mirror committees or EU Commission mandate.	CEN - European committee for normalisation	Organisation establishing voluntary Standards applying in European Union. They are sometimes supporting Directive implementation in the context of harmonised regulations. EC 715/2007 : European Emissions Standard for defining the acceptable limits for exhaust emissions of new vehicles sold
Country	Accredited standards organization. National mirror committee of international standards.	ANSI, BSI, NEN, AFNOR, AENOR, JIS...	National standards development. Can integrate Regional / International standards in National collection thanks to mutual recognition agreements.
Organization	Innovators	Microsoft, Intel, IBM: USB port	Universal Serial Bus (USB) for improving interface between personal computers and peripheral devices

The mass-balance approach for chemical recycling introduced within this paper is an example of an innovation for which diffusion can be accelerated and enlarged through the development of standards. Standards would act in four main ways:

- Increase participation as standards can signal market stability, fairness and known requirements for access.
- Streamline auditing as standards can specify measurement boundaries and information requirements.
- Demonstrate compliance as standards can clarify adhesion to a set of mandatory or voluntary levels of performance
- Build trust by informing customers and consumers about performance within a given context and removing uncertainty, thereby helping them make informed purchasing decisions.

In particular, uncertainty about the performance of recycled materials can be an important barrier to their uptake in the market. Standards stimulate demand by building trust that a recycled material is fit for purpose, which in turn stimulates supply. Uncertainty about the recognition of a given recycled material's contribution to a defined target can also constrain demand. Standards stimulate demand by making visible the recycled attributes and its qualifications for contribution to targets.

Considering the need to increase recycling of chemicals and complex materials – with plastics as a prominent example – and the advances in technology for doing so, it is an opportune time to explore a standard for mass-balance and recognize the benefits of standardization that can be delivered.

4.2 WHERE TO START

Standards for recycled content are already commonplace and serve as a good foundation for a mass balanced recycled content standard. However, there are unique requirements specific to the mass balance approach. Selected examples of such requirements might include:

- Consignments of material being used as co-feed must demonstrate that separable materials which are feasible to use in reuse or mechanical recycling have been removed from the material stream before entering the system.
- When materials enter the chemical recycling system the mass of material is transformed into credits using a stated unit conversion (e.g. LHV as proposed in Chapter 2). Units can be specific to the transformation within a given system. However, a system cannot use multiple credit units, only one credit unit is allowed in each system.
- Only materials going into (credit) and leaving (debit) a connected system of transformations and transport within a defined boundary can be included in a mass balance credit account.

This paper outlines several of the core principles to be used as the basis for standardization. By publishing this white paper, the project stakeholders have proposed a framework for developing a mass balance approach standard. TWhen coupled with inputs from other interested parties this could form the foundation of a national or international standard developed by an appropriate and accredited stakeholder.

It is to be noted that a formal standardization process initiated by NEN is ongoing in the field of Chain of Custody at the ISO Level ISO/PC 308 "Chain of Custody"[16]. Standardizing the criteria for mass balance approach could be addressed in the context of this working group. Recently, the ISO TC 323 "circular economy"[17] has been created to deal with the concepts, definitions, tools and metrics of the circular economy.

[16] www.iso.org/committee/6266669.html

[17] www.iso.org/committee/7203984.html

5. CONCLUSION & RECOMMENDATIONS

MAIN CONCLUSIONS

1. Chemical recycling is a needed complement to mechanical recycling to enable a circular economy, especially for avoiding that chemicals and materials that are hard to recycle are sent to landfill or energy recovery.
2. With a mass balance approach applied to interconnected chemical production networks, recycled and renewable feedstock can be transparently traced and allocated to select products.
3. A mass balance approach can accelerate the usage of recycled feedstock as a drop-in-solution for current mass production processes dominated by fossil feedstock.

RECOMMENDATIONS

1. In order to make chemical recycling a reality, it is essential that value is added and fairly shared among the recycling value chain participants.
2. A regulatory framework or widely accepted standards need to be prepared to ensure that chemical recycling is supported in the same manner as mechanical recycling (as a supplementary route for recycling). Certification may support a unified use of the mass balance approach.
3. Chemical recycling as an emerging recycling technology should be assessed in a life cycle perspective, in order to optimize/balance its economic, environmental and social impacts.
4. Mass balance allocated recycled content should be treated equivalent to directly allocated recycled content.

NEXT STEPS

This paper outlines several of the core principles to be used as the basis for standardising a mass balance approach. By publishing this white paper, the project stakeholders are proposing a frame for such a standardisation. They see a mass balance approach with clear and pre-defined rules as a key way to facilitate and encourage the use of recycled raw materials for the production of new products with recycled content.

There are several options to continue this work:

- Use white paper as a basis for the development of private standard by a private labelling company.
- Adapt this material to create a new voluntary standard within one of the existing national or preferably international standardization body technical committees.
- Support the creation of a mandate from governmental institutions to engage standardization in a harmonized standards system in the context of future circular economy regulation development.

These different approaches would ensure the continuity of this work and global recognition from the markets and/or institutions, from voluntary options, driven by market demand to regulated framework in principle widely implemented.

One or more standards could be developed committing to the frame. The next key step in this process would be to increase the number of stakeholders working on the standard development to broaden the consensus for how it should be applied in the market.

6. ANNEX A: TECHNICAL DEEP DIVE

USING MASS BALANCE APPROACHES TO INTEGRATE PLASTICS FEEDSTOCK RECYCLING IN THE CHEMICAL INDUSTRY

6.1 CONTEXT

The sorting plants of the recycling industry produce millions of tons of mixed plastics (**MxP**) that can hardly be recycled mechanically. Here is where the production network of the chemical industry offers **chemical recycling** as an important solution to extend mechanical recycling: **feed-in points** for MxP.

Leveraging the existing chemical manufacturing infrastructure comes with a number of advantages:

- Since **feed-in points are integrated** into an existing optimized network with fossil raw materials, they imply **economies of scale and high efficiency**, i.e. energy efficiency, high material yields (conversion factors), low production waste.
- Feed-in points are linked to mature **high-performance products** (plastics and other chemicals).
- Co-feeding MxP or derived oils leads to the **saving of fossil raw materials** and supports decoupling from these finite feedstocks.
- The co-feeding of MxP can be carried out similarly and concomitantly to the co-feeding of sustainable biomass in a mass balance approach described previously[18].

The challenge is to think beyond isolated mechanical recycling systems, towards global standardization and implementation of an efficient chemical recycling of MxP that we will call feedstock recycling in this paper[19]. Mechanical recycling is constrained by several factors, such as costs, type of waste collection schemes, the quality of the recycled products and their potential application. In particular, mechanical recycling may come with degradation of polymers and toxicity concerns. Yet, mechanical recycling is easy to understand, because one material, typically characterized by the primary polymer is replaced by its recycled twin (same primary polymer but not same formulation). Applying the same thinking to the chemical industry as a whole would translate into the unlikely future of developing about 20,000[20] recycling processes to cover 100% of the chemical industry (Figure A1).

In contrast, feedstock recycling means replacing an equivalent amount of feedstock for any of the 20,000 chemicals by recycling the same or another chemical with an equivalent feedstock value[21] within a predefined system boundary. It avoids developing about 20,000 recycling processes to cover 100% of the chemical industry. Feedstock recycling combined with effective mechanical recycling will incentivize recycling and waste collection without changing the technical quality of existing solutions to the benefit of sustainable development. Feedstock recycling in the chemical industry is about evaluating the raw material demand of any of more than 20,000 substances, replacing the fossil raw materials by renewable or recycled ones and then allocating (attributing) the physical use of the replaced feedstock origin to the chemical. Thus, balancing output with input can be always achieved. The method of feedstock recycling as an extension of mechanical recycling should be described transparently in an international standard. This would ensure a common dealing with the multi-faceted issue.

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[18] REDcert2 Scheme principles for the use of biomass-balanced products in the chemical industry www.redcert.org/images/SP_RC^2_Biomass-balanced_products_V1.0.pdf TÜV SÜD, Mass balance for the traceability of renewable raw materials CMS 71 Standard V 3.0/2017 www.tuev-sued.de/uploads/images/1495439928171722620209/zertifizierungsstandard-erneuerbare-rohstoffe.pdf

[19] An example of feedstock recycling has been described previously "Back to feedstock": CEFIC, European Chemistry for Growth, www.cefic.org/Documents/RESOURCES/Reports-and-Brochure/Energy-Roadmap-The%20Report-European-chemistry-for-growth.pdf, p 62.

[20] To date about 20.000 substances have been registered in Europe. They are relevant to the entire industry: echa.europa.eu/de/press/press-material/pr-for-reach-2018

[21] The "equivalent feedstock value" is the amount of feedstock taken from the usual basket of chemical feedstock: gas and the distillation products of crude oil: naphtha, LPG, butane etc.

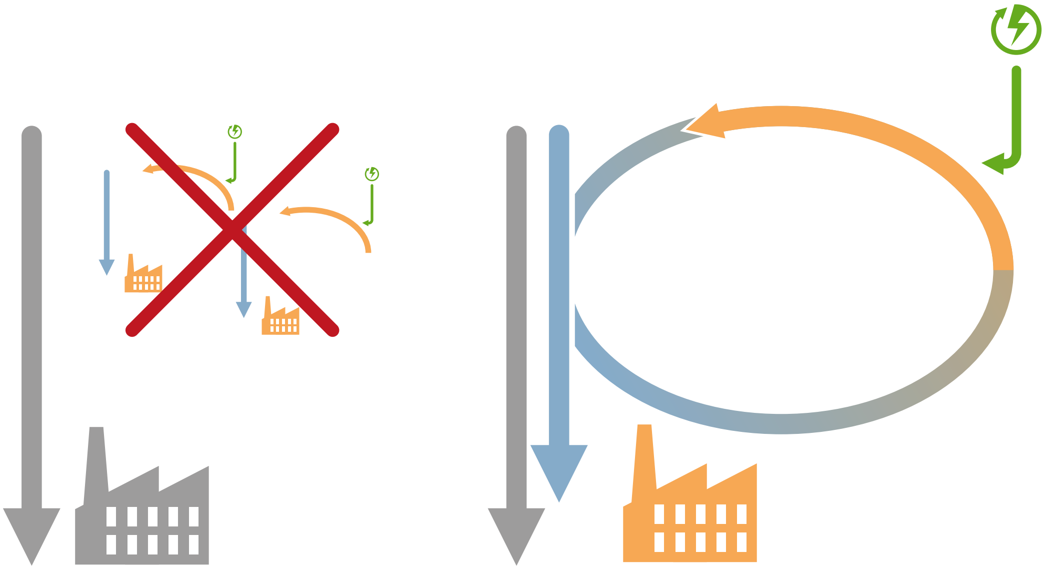

Figure A1. Avoiding a multitude of chemical loops by integrating chemical recycling into an efficient extended loop.

6.2 HOW IT WOULD WORK IN PRACTICE

VALUATION OF A RECYCLATE – QUANTITY AND QUALITY

Recyclate is to substitute conventional raw materials by co-feeding. The term 'raw material' has synonyms such as feedstock, input material, petrochemical or fossil resources. Here we define it to be the petrochemical material at the very beginning of the chemical value chain: crude oil, naphtha, methane gas etc. Its quantity can be expressed in 'tons' or some other measuring unit (see below). 'Raw material' (feedstock) does not encompass the energy (e.g. heat) sometimes needed to drive chemical processes. Energy is outside the scope of this paper. Inorganics, at present, are also out of scope (see further comments below).

Eligible feedstock should be something other than virgin and finite, i.e. a recyclate, waste based or bio-based. A standard including quality criteria for eligible feedstock from widely accepted international multi-stakeholder discussion should support the claims made (c.f. Chapter 4). Examples are legislation-based schemes or labels (e.g. RED, REDcert, ISCC, RSB). Quality criteria for eligible feedstock should be considered sustainable.

Eligible feedstock may come from a certified, accredited or registered auditing company according to above criteria. Certification is recommended because many feedstock properties are related to an environmental or social impact but cannot be detected by chemical analysis of the feedstock. Certification helps to support trust that the feedstock origin does not violate social and environmental criteria.

Greenhouse gas (GHG) savings should be calculated when comparing eligible feedstock with conventional fossil feedstock applying LCA methodology[22]. The circular economy is to be compared with the linear value chain. Any conversion steps required to make eligible feedstock fit-for-use in the process have to be included as well as the impact of incineration or landfill in the linear approach.

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[22] ISO 14040:2006 and ISO 14044:2006 standards for life cycle assessments and ISO 14045:2012 for eco-efficiency assessments.

From a practical perspective, the traceability of eligible feedstock within a predefined system boundary can be facilitated by conversion of the feedstock into standardized measuring units[23] at the feed-in point: **Raw Material Units (RMU)**. An RMU is traceable in established booking systems and it is an auditable measure of the recyclate fed into the production processes. Feedstock calculation of a product is about finding out how much fossil raw materials is needed per unit or per ton and to express it in a number of RMU. Regardless of whether two or twenty intermediates are required for the manufacture of a product, there is ONE[24] feedstock requirement in the end. This feedstock calculation is the first step for any manufacturer applying for a recycling claim[25] to a 'Recycling Allocated Product' (RAP).

Feedstock calculation of some of the 20,000 substances of the industry can be made public in a database. However, in many cases the exact number of RMUs per ton of product is a proprietary information of the manufacturer. It will be accessible to an auditor, but it should not be passed to the competitors as it implies the production cost structure.

VIRTUAL BASKET OF RAW MATERIALS

In the mass balance approach with renewables, recyclates, biomass and in feedstock recycling there is no need to replace dozens of intermediates required for the manufacture of a RAP by dozens of bio-based or recycled twins. It suffices to calculate the total feedstock demand of the RAP, and to introduce an equivalent amount of eligible feedstock (bio-based or recycled) or an intermediate or product somewhere within the system boundary connected to the production site of the RAP. This concept of a virtual basket of raw materials provides an essential element of flexibility to accelerate the uptake of recyclates and other new highlighted raw materials in an existing environment. The value of any recyclate input depends on the raw material savings at the feed-in point.

It is necessary to standardize what 'equivalent' means, because the feedstock demand of different intermediates may vary depending on their individual more or less efficient synthesis paths. The conversion unit "kilogram, kg" works smoothly in mechanical recycling when one intermediate is replaced by an identical renewable (bio-based or recycled) twin, but other conversion units may be preferable for feedstock recycling.

CONVERSION FACTORS

Of course, the quantity of the input (recycled) raw material can be expressed by a mass unit (kilogram, ton ...). Due to the heterogeneous nature of input recycled raw material, often containing worthless impurities, a measure reflecting the value of the input material is needed. Next to "mass" the "number of carbon atoms" or the "lower heating value" are candidates.

LOWER HEATING VALUE (LHV[26]) AS INDICATOR FOR 'CHEMICAL VALUE'

This is the preferred conversion unit for several reasons:

- The yield (hence value) of many raw materials in a basic chemical process such as the synthesis gas production essentially depends on the lower heating value of the input. For example, the amount of syngas per ton of gasified wood chips is much lower than per ton of petrochemical vacuum residue. Therefore, if one wants to replace 1 kg of vacuum

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[23] CMS 71 Standard r 3.0, Introduction www.tuev-sued.de/uploads/images/1495439928171722620209/zertifizierungsstandard-erneuerbare-rohstoffe.pdf

REDcert2 Standard v 1.0 Chapter 8.4, www.redcert.org/images/SP_RC²_Biomass-balanced_products_V1.0.pdf

[24] When there are multiple synthesis routes, it is common to take the average feedstock demand per ton of product in the system boundary.

[25] Market research shows that 100% (complete) claims are preferred by many customers over smaller percent numbers.

[26] Expressed in Joule (J) or tons of oil equivalent (toe); Synonym: net calorific value. 1 Kilogram of biomethane corresponds to 50 Megajoule. 1 Kilogram of naphtha corresponds to approximately 44 Megajoule.

residue, more than 2 kg of wood chips are required. This example shows that green washing is avoided.

- Hydrogen has a comparably high value as co-feed in the syngas process and can be evaluated by its LHV although it is a carbon-free intermediate.
- Renowned calculation methods such as LCA rely on the LHV.
- Reporting of feedstock in the chemical industry as a whole frequently is done in the unit of LHV[27] to make it comparable to the rest of the industry.
- Mixed recycled plastic (MxP) feedstock is commonly characterized by its LHV[28]
- From the perspective of many chemists any "resource savings" claim requires conversion units based on LHV.

CHEMICAL VALUATION METHOD. EXAMPLE: POLYAMIDE

The following example (polyamide) illustrates how the mass balance depends on the chemical valuation method (Figure A2). Assume that a manufacturer produces a polyamide product. A multitude of intermediates is required in the production of the polymer, and it is therefore unlikely that a manufacturer sets up a recycled twin process for each intermediate. Instead an analysis of the synthesis path of polyamide yields the quantity of petrochemical (fossil) raw materials, say 150 kg, and the average composition of the raw material is CH2,64 in our example. This quantity may be slightly different at the various manufacturers in the world.

In our example, to make the mass balance, recyclate raw materials are co-fed into cracker and syngas plants. We assume two recyclate feedstocks are (50%) co-fed in cracker and 50% co-fed in syngas plant. The average formula of the recyclate is CH1,51O0,015, typical for a recyclate mix. The formula is unlikely to be identical to the fossil feed (i.e. CH2,64) with respect to each of the relevant elements: C, H, N, O.... Therefore, a chemical valuation method to make the balance must be chosen. Shall the balance be in the number of carbon atoms replaced, shall it be weight, or LHV[29]? The method chosen should be made transparent, as the amount of recyclate needed depends on the method.

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[27] The annual feedstock demand of the European chemical industry is estimated to be about 2 EJ. Figure 2-8 in www.cefic.org/Documents/RESOURCES/Reports-and-Brochure/Energy-Roadmap-The%20Report-European-chemistry-for-growth.pdf#page=33

[28] Example: www.recycling-kontor.koeln/wp-content/uploads/2016/07/365-RKD-Produktspezifikation-Ersatzbrennstoff-Vorprodukt.pdf

[29] The LHV can be measured, or it can be approximated using a formula from de.wikipedia.org/wiki/Heizwert LHV = 32.8 x m(C) + 101.6 x m(H) + 6.3 x m(N) once the elemental composition of the raw material is known.

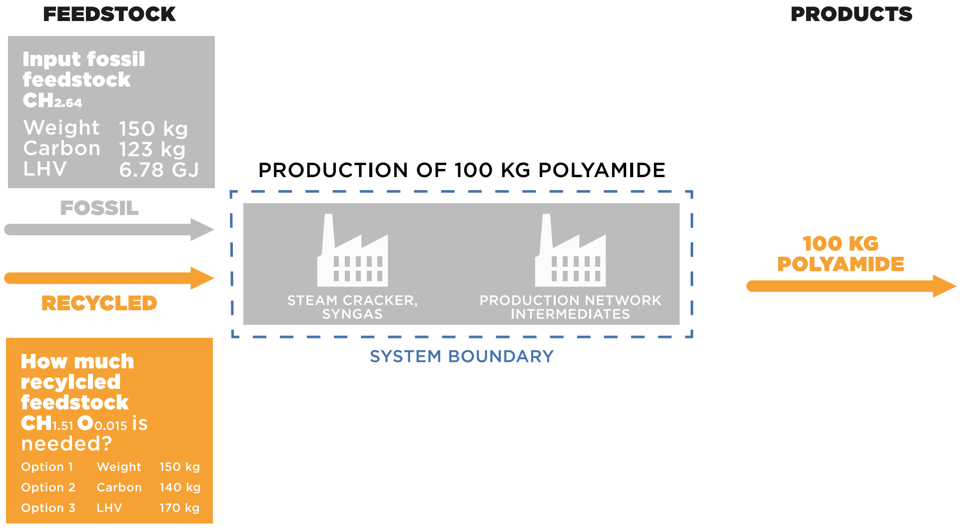

Figure A2. Chemical Valuation Methods, Example: Polyamide

IDEAS ON HOW TO MAKE A MASS BALANCE OF ORGANICS AND INORGANICS

The mass balance approach described above focuses on petrochemical (fossil) raw materials, essentially hydrocarbons. While a mass balance approach for inorganic chemicals– water, air, sulphur, aluminium, glass fibres, iron etc. – is out of scope for the present paper, some considerations follow below. Unlike organics the use of LHV as an RMU isn't generally useful for inorganics. RMUs can take on units other than joules or BTUs however. For inorganics a conversion to moles or mass of the element of interest might be used. For instance, when recovering an inorganic used in batteries, say manganese, the element of interest is the manganese, not manganese(III) oxide or manganese hydroxide which might be produced during recycling. By following the amount of manganese entering and leaving the system and ignoring the oxidation state of manganese the carrier of the electrochemical potential, the manganese, is properly accounted for. There may be other conversion systems used to produce RMUs of different units which will need to be explored for material systems other than organics. For any system RMUs of only a single unit (joule or mass for instance but not both) may need to be used to protect against double counting.

SYSTEM BOUNDARY

In a mass balance approach, there is no obligation to enforce co-feeding in exactly the same vessel. For example, it has been required that "mass balances shall be kept strictly site specific"[30]. Commonly, connectivity[31] of the entry point for recycled (eligible) and established material within one production site or connected sites is required. Connectivity between different sites is established by exchange of raw materials and/or intermediates which in turn are based on raw materials. The following criteria for connectivity are suggested:

- **Physical link** of recycled input material and "sustainable" product within a site or by pipeline between sites or by dedicated (regular) transportation between sites
- **Probability or chance of** recycled input molecules **reaching "sustainable" product**.

Within the system boundary RMUs can be allocated freely to any choice of products. The number of RMUs to be allocated depends on the specific raw material demand of the RAP. There may be an additional requirement to establish a "strictly site specific" mass balance (= balance of RMUs).

Within each system boundary balancing of RMUs is required to make the mass balance, and it is appropriate to define

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[30] ISCC PLUS, v 3.0, 9 August 2018

[31] A prior transparent consensus on the acceptable regional flexibility (scope) is desirable to avoid controversies.

a balancing period, e. g. of one calendar year. It is common to make the mass balance without allowing for a negative balance beyond three[32] months: eligible feedstock should be used before manufacture of a RAP.

DOUBLE COUNTING

Double counting can be prevented in the following way: “Standardized units”, RMUs are only generated at the feed-in point if the derivative from “waste plastic” is not marketed itself as recycled product. An auditor can examine the feed-in point, i.e. the process where the derivative from “waste plastic” is used physically, and he should request proof that the derivative from “waste plastic” is not sold for a second purpose. RMUs can then be transferred from the feed-in point to some other process within the connected system boundary.

RECYCLATE (ALLOCATED) CONCENTRATION

The concept of (allocated) concentration (or share) of a Recycling Allocated Product (RAP) is a tough issue. The definition and acceptance of the (allocated) concentration is needed for a level playing ground between the “real” concentration (can be measured by physical or chemical means) and the (allocated) concentration (describing the value chain impact) of a product with a 100% allocated property, RAP. A product with a (allocated) concentration is indistinguishable in its application technical properties compared to the conventional product. Yet, it carries a property, the value chain impact (sourcing and materially using recyclate in the value chain) that is verifiable by an auditor.

ADVOCACY

A recycling allocated product (RAP) made in the chemical industry is understood as a product which involves 100% allocated recyclate concentration. Its fossil feedstock demand has been compensated by an equivalent amount of recyclate in the value chain. When the focus of political action is on maximizing the quantity of recycled plastics both, mechanical and chemical recycling, closed and extended loop lead to desired and comparable results: offering rewards for using 100% mechanical recycled plastics or for a RAP based a plastic mixture (MxP) in the chemical value chain, rewards to the same impact.

When a chemical manufacturer completely compensates the fossil feedstock demand of a product by an equivalent amount of recyclate by an allocation method in its production network such product should be clearly marked, and the product should qualify for rewards like mechanically recycled material.

Further downstream, producers may combine materials from mechanical and chemical recycling and even non-recycled sources.

PRODUCT NAME, RULES FOR SUSTAINABILITY CLAIM

Any product claim must be true. The dilemma is to describe a complex method truthfully and as concisely as possible without deceiving the end user[33], hopefully allowing for a positive emotion (e. g. bio) when the truth is good for the sustainable development of the world.

Political and legal support in defining an attractive yet adequately representative product name and claim may be the most helpful measure to drive recycled feedstock and eligible biomass into the chemical industry. Yet, other claims may be preferable to customers, e.g.:

- This RAP supports or involves recycling of eligible or advanced feedstock.
- Advanced product[34] involving recycling of advanced feedstock.

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[32] While allowing 3 months negative stocks is common this would be a topic for a standards committee to decide.

[33] DIN EN ISO 14021 provides some guidance on environmental labels and declarations

[34] rsb.org/wp-content/uploads/2018/12/18-12-11_RSB-STD-02-001-v2.0-RSB-Standard-for-Advanced-Products.pdf

- Product made with allocated recycled resources (PARR)
- RecycledMB product (recycling property allocated to products via mass balance).
- Product with recyclate content* Footnote: *applying a mass balance

VALUE CHAIN TRANSPARENCY

- To support trust in the method of applying the mass balance of eligible feedstock with the manufacture of RAP an enhanced level of transparency is recommended. RAP manufacturers should operate an internet website providing background information on the chain-of-custody from eligible feedstock all the way to the production site of the RAP.
- Raw materials: origin, reason for its eligibility, certificates, description of raw material input process, GHG savings compared to linear baseline, reference to LCA and critical review.
- Intermediates: Traceability and Scope, names of production sites and reason for being included in and connected to the scope. Examples of intermediates used for production of RAP and their valuation using conversion units, raw material standard units
- Products: List of RAPs offered to the market (identifiers, CAS), claims used
- Assurance, Audit reports, Certificates of auditing companies

6.3 REQUIREMENTS FOR DOWNSTREAM COMPANIES

Downstream companies that make combined products should prove that the use of mechanical and chemical recycling and even non-recycled sources requires only insignificantly more energy and thus saves fossil resources. Downstream companies have two options to carry out and claim the mass balance: A **weight-based** mass balance and a **resource-savings-based** mass balance[35]. Claims and communication of the combined products depend on the choice.

Transfer between system boundaries can be by mass, percent recycled (allocated) content by mass, of the transferred substance or material. If complex synthesis takes place at the next step, within a second system boundary, it is converted to RMUs and reconverted to RAP when leaving the system. In this way a unit process can be set up which can be scaled to large integrated systems of multiple smaller systems linked together.

Here we outline the weight-based mass balance: It determines the weight-proportion of input materials contained in the combined product. The balancing of input and output materials is carried out process-specifically. The balancing across different production units or sites is not permitted here. It is not necessary to convert materials into raw material units (RMUs). Only a production-based posting period is permitted for the process-related mass balance.

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[35] REDcert2 Scheme principles for the use of biomass-balanced products in the chemical industry, Chapter 8.9, www.redcert.org/images/SP_RC^{2}_Biomass-balanced_products_V1.0.pdf Resource-savings-based mass balance: The process-spanning balance determines which proportion of fossil raw materials (expressed as RMUs) is replaced by RMUs from recycled source along the entire value chain. To this purpose, the balance can be drawn up in the entire system boundary across several connected production units and sites. In contrast to the process-related mass balance, the balance here is based on RMUs. The conversion of all input materials into the unit RMUs is carried out by converting intermediate products into RMUs on the basis of the quantities of fossil raw materials required for the production of the respective input material. If there is no certified RMU value from the upstream supplier for this, the required raw material (RMU) quantity can be determined conservatively on the basis of processes described in the literature and implemented technologically. The balancing is carried out within the booking period, usually one year. A maximum balance overdraft period of three months is common.

7. ANNEX B: HOW TO DEVELOP A STANDARD

Standards development is typically a consensus process which brings together diverse stakeholders to develop normative requirements. The method and duration for agreeing the technical requirements varies by the nature or scope of the standard body (see Table B1 for indicative examples).

Standard type	Stakeholder Panel	Timeline (Indicative)
Technical Requirements	Technical author	1 month
Non-Consensus Third Party Standard	Technical Panel	6 months
Type 1 Ecolabel	Attempted consensus	1 – 3 years
National or International (CENELEC, ISO, ANSI, IEC)	Consensus based	1 – 5 years

Pursuing national or international standards development can be a lengthy process. However, some accredited standards development and certification bodies use a parallel consensus/non-consensus process for developing new requirements and certifying performance. This enables marketplace use while a formal standards development process is running, and has the advantage of gathering practical experience, which can be used to inform standards development. It is therefore possible to establish a preliminary accredited standard for mass balance whilst the approach is in its infancy. This can accelerate national and international standards development as the Mass Balance approach scales. Such an approach is shown in Figure B1.

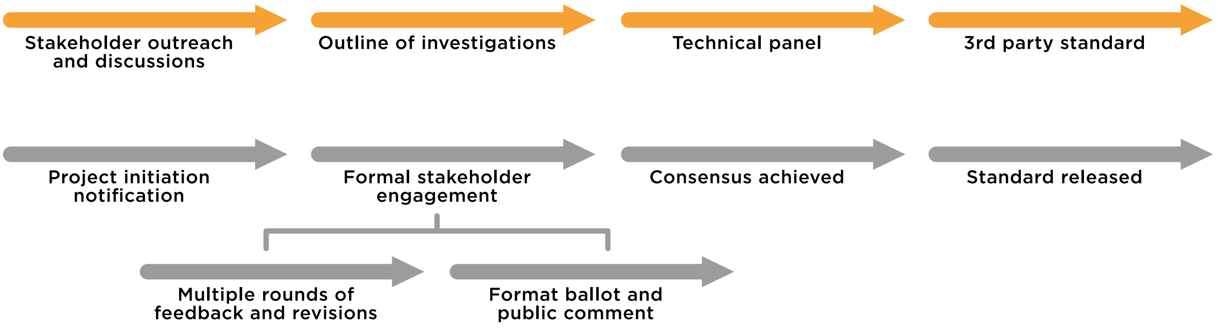

Figure B1. Parallel standards development approach

GLOSSARY

Booking period: A reconciliation of RMUs entering and leaving system boundary performed on an periodic basis (e.g. 1 year): it must be shown that enough inputs were available to produce the RAP claimed from RMUs leaving the system.

Chain-of-Custody: A system to document and verify the path taken by an eligible input material through all stages of transfer and production, to the final product. Here RMUs are transferred.

Equivalent feedstock value: Amount of feedstock taken from the usual basket of chemical feedstock: gas and the distillation products of crude oil: naphtha, LPG, butane etc. The lower heating value is taken as conversion unit for different feedstocks.

Feed-in point: A chemical process integrated to a chemical production network. A feed-in point is part of the system boundary.

Feedstock recycling: Conversion to monomer or production of new raw materials by changing the chemical structure of a material or substance through cracking, gasification or depolymerization, excluding energy recovery and incineration[36].

Mass Balance: A method to match output (i.e. products with recycled content) with input (i.e. quantity of recycled feedstock) within a predefined system boundary (see below) and within a given booking period (usually one year).

Mechanical Recycling: Processing of waste material into secondary raw material or products using mechanical unit operations only and without significantly changing the chemical structure of the material[37]. Examples include mechanical reprocessing of plastics and paper repulping.

RAP: Recycling Allocated Product (Mass Balance Product), a product which is a carrier of RMUs (raw material units) from a recycled, waste-based or bio-based source managed through a mass balance approach. A RAP might also be called "Product with Recycled Content" by applying a mass balance approach.

Chemically Recycled Content = Allocated Content: Percentage defined as mass of recycled material content / mass of finished product based on a mass allocation / credit system.

RMU: Raw Material Unit is the measuring unit for the quantity and value of recycled or bio-based feedstock as a substitution for fossil feedstock.

- RMUs are generated when recycled or bio-based feedstock is co-fed with fossil feedstock into a chemical production unit.
- RMUs must not be generated when the output of the chemical production unit is marketed as "recycled or bio-based"
- RMUs are stored in auditable booking systems.
- RMUs are consumed upon production of a RAP.
- Within a system boundary of connected sites and production units of a company and within the balancing period of one year the RMU balance must not turn negative.

Qualified Credit Transfer (QCT): The transfer of a quantity of recycle designation credit between RMU's for same type of materials between the mass balances of separate sites. Such a book keeping transfer Is only acceptable under a set of strict qualifying requirements.

System: A connected network of transformations and transport between transformations in which recycled, waste-based or bio-based material enters and is converted to a recycling allocated product.

System boundary: The point where materials flow into or out of the system. Materials are converted to credits when entering the system at a boundary and from credits to allocated mass when leaving the system at a boundary. Only materials which have an origin within the system boundary are eligible for recycled content credits from the credit system.

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[36] Definition from ISO 15270:2008

[37] Definition from ISO 15270:2008

ABOUT THE ELLEN MACARTHUR FOUNDATION

The Ellen MacArthur Foundation was launched in 2010 with the aim of accelerating the transition to the circular economy. Since its creation, the charity has emerged as a global thought leader, putting the circular economy on the agenda of decision-makers around the world. The charity's work focuses on seven key areas: insight and analysis; business; institutions, governments, and cities; systemic initiatives; circular design; learning; and communications.

With its Knowledge Partners (Arup, Dragon Rouge, IDEO, McKinsey & Company and SYSTEMIQ), the Foundation works to quantify the economic opportunity of a more circular model and to develop approaches for capturing its value. The Foundation collaborates with its Global Partners (Danone, Google, H&M Group, Intesa Sanpaolo, NIKE Inc., Philips, Renault, SC Johnson, Solvay, Unilever), Core Philanthropic Funders (SUN, MAVA, players of People's Postcode Lottery (GB)) and its CE100 network (businesses, universities, emerging innovators, governments, cities, affiliate organisations), to build capacity, explore collaboration opportunities and to develop circular business initiatives.

Further information:
ellenmacarthurfoundation.org
@circulareconomy

ABOUT THE CE100

The Circular Economy 100 is a pre-competitive innovation network of the Ellen MacArthur Foundation, established to enable organisations to develop new opportunities and realise their circular economy ambitions faster. It brings together corporates, governments and cities, academic institutions, emerging innovators and affiliates in a unique multi-stakeholder platform. Specially developed elements help members learn, build capacity, network and collaborate with key organisations around the circular economy.

ABOUT COLLABORATIVE PROJECTS (CO.PROJECTS)

Co.projects are opportunities for formal precompetitive collaboration between CE100 members. They are driven by members, for members and their focus can range from research initiatives to pilots and toolkits. Co.projects leverage the CE100 network with the aim of exploring opportunities and overcoming challenges which are commonly and collectively faced by organisations making the transition to a circular economy, and which organisations may not be able to address in isolation. making the transition to a circular economy, and which organisations may not be able to address in isolation.