

Mass Balance

Enabler of drop in solutions for circular raw materials into chemical processes



Miriam Bechtle¹, Birgit Himmelreich¹, Peter Hawighorst², Claudia Kroll², Jan Henke²

¹ Covestro Deutschland AG, Corporate Sustainability

² Meo Carbon Solutions and ISCC

Motivation

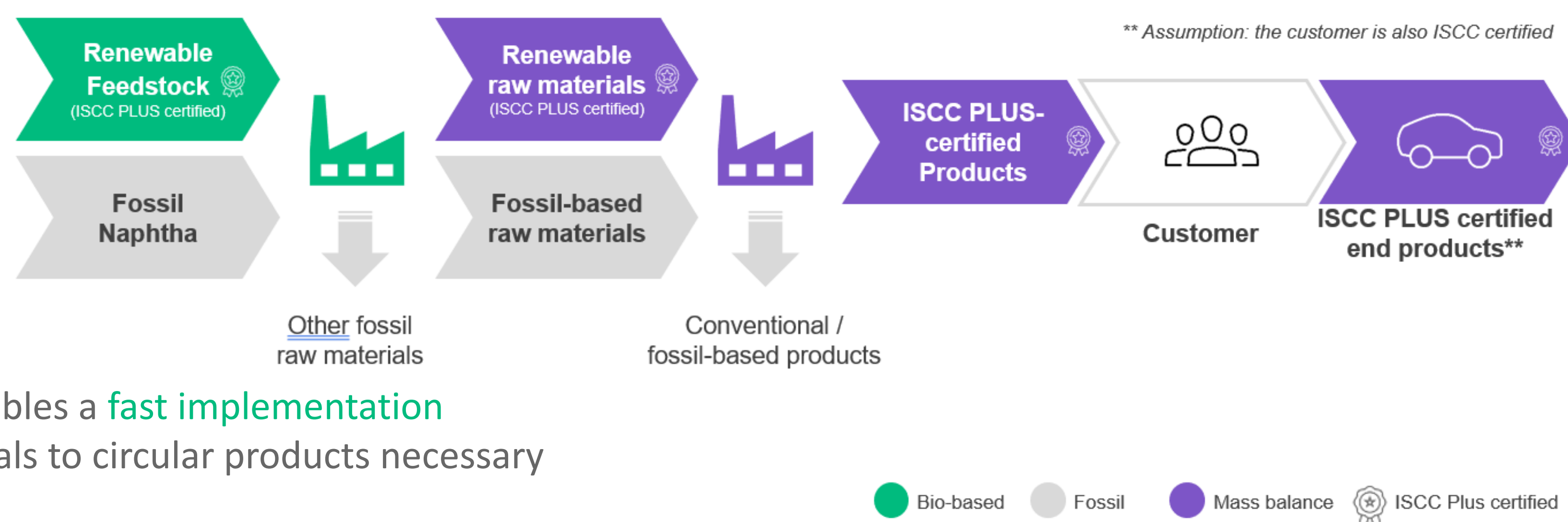
In light of the Green Deal the plastics market demands for products with a reduced carbon footprint.

Circular Economy is looking for raw materials in our supply chain that can be made from

- Bio-based feedstocks
- Feedstockbased on waste streams
- Carbon dioxide

Goal of the substitution

- Less usage of fossil resources
- Less waste
- Reduction of environmental impact (e.g. carbon footprint)



- Using existing assets to ramp-up volumes of circular products enables a fast implementation
- Transparent Methodology for allocation of renewable raw materials to circular products necessary
- Mass Balance Approach offers certified system

Conversion factor

In ISCC document 204 (Mass balance calculation methodology) the conversion factor is defined as

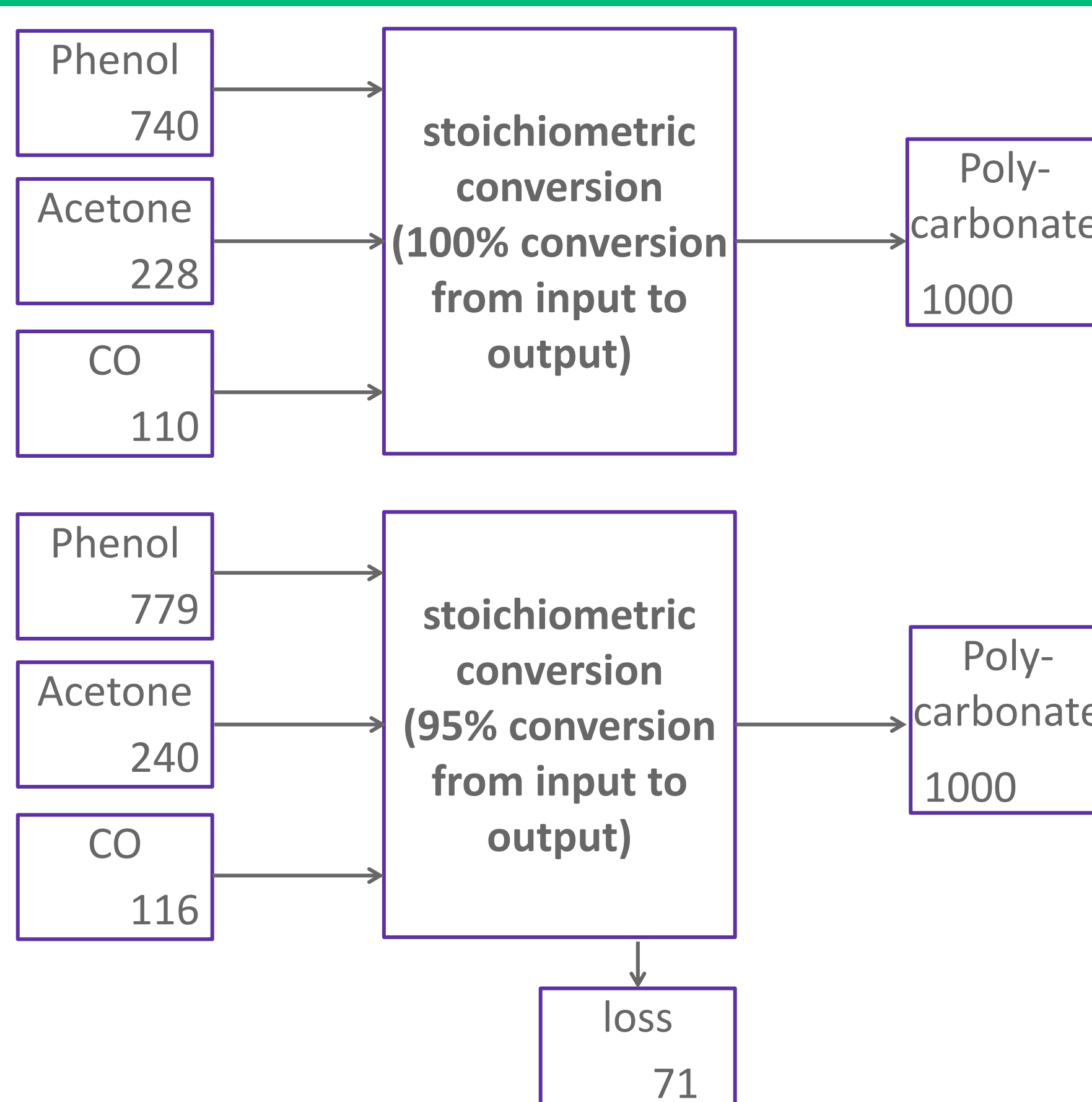
$$C(\%) = \frac{A_o}{A_i} \cdot 100$$

C: Conversion factor

A_i: Amount of process input material

A_o: Amount of output yielded by the internal process based on input

Chemical reactions often have several input and output components. Usually only one (sometimes two) output component is of commercial interest. But due to the chemical reaction the other output components are coupled to the formation of the component of interest.



In addition, the synthesis of chemical components are often multi-step reaction networks, with different yields according to the different input components. According to the ISCC PLUS guideline the production process at one site is described as a black box. The conversion factor is a description of how efficient the input material is converted to the output material. In chemical reactions the ratio of the different inputs is not equally distributed among all the different input streams and the input streams cannot be mixed arbitrarily. The ratio is defined for 1 kg of output material, so increasing one input stream while decreasing another one will not necessarily lead to the same amount of output material.

Alternative approach: Specific Consumption factor and sustainable share

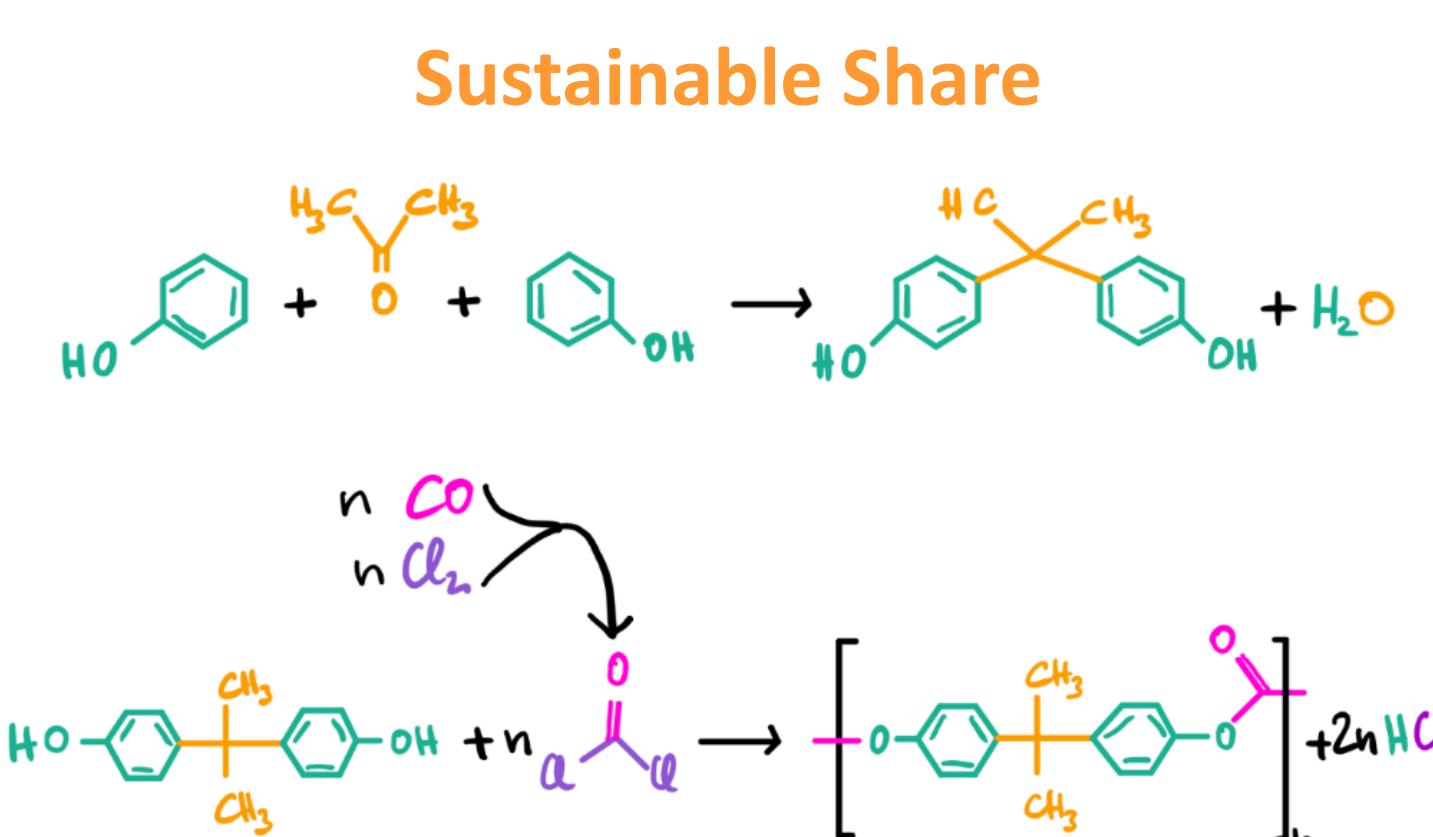
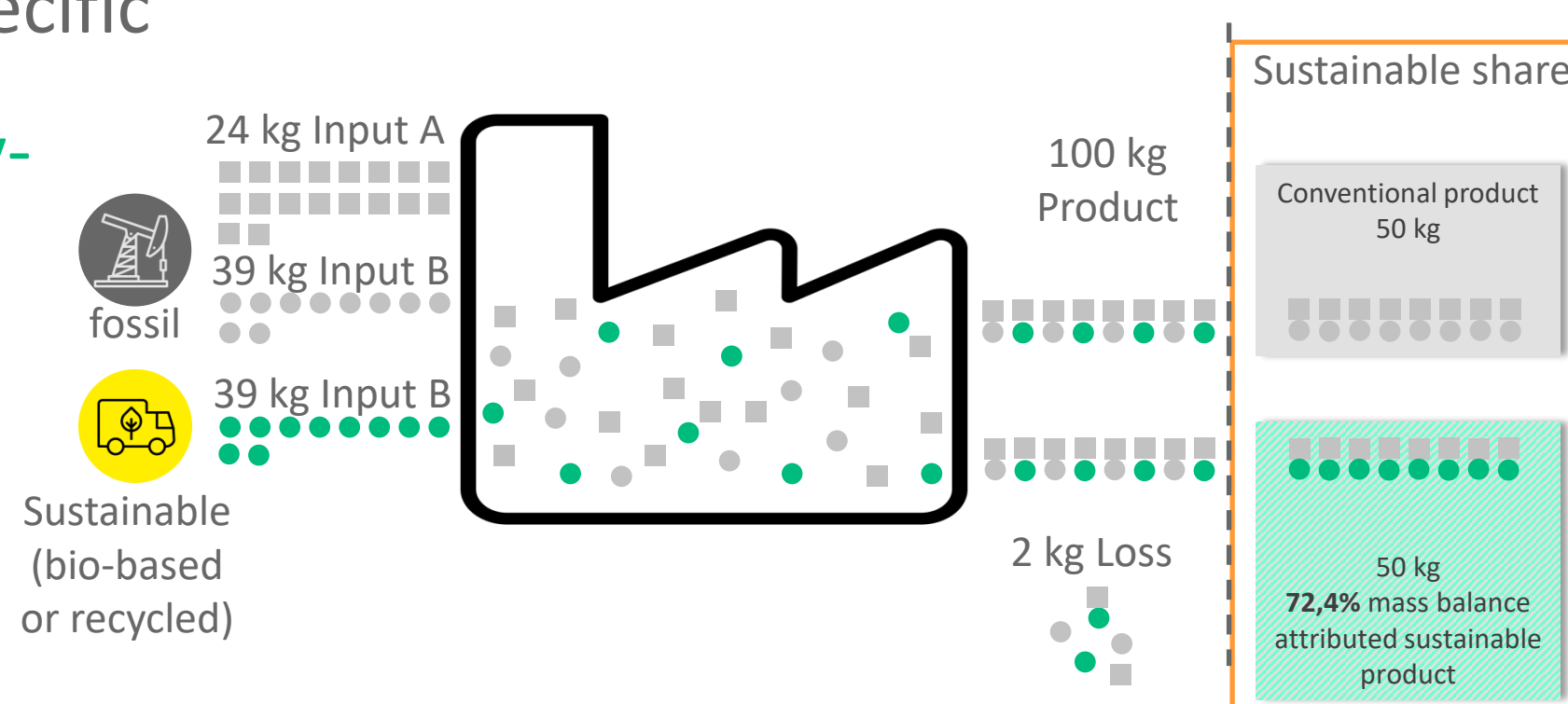
Specific consumption factors, which reflect, how much input material (including all material losses due to chemical reaction or process inefficiencies) needs to be used to produce a specific amount of the desired component, are more accurate in terms of raw material consumption than overall conversion factors.

Different yields are considered in this approach and the specific consumption factors are independent of the question, if by-products are counted as loss or output.

Phenol	Bisphenol A	Polycarbonate
870 kg	1000 kg	900 kg
0,78		1

Chemistry: Input A + Input B → product

Consumption:	24 kg	78 kg	100 kg
Consumption factor:	0,24	0,78	1



Sustainable share is the contribution of the individual raw material to the final product molecular weight

Raw material	Phenol	Acetone	CO	Chlorine
Sustainable share in Polycarbonate	72,4	16,5	11,0	0

Conclusion

The Mass Balance approach is a versatile method to track the chain of custody of sustainable raw materials along the value chain. For chemical processes with complex material flow networks it is more complicated to determine the consumed amount of raw material than for petrochemical processes with only a few similar input streams. Indicating the sustainable share of the certified product illustrates the chemical connectivity of the mass balanced substitution of one or several input materials. Using a specific consumption factor instead of an overall conversion factor is an alternative and for chemical reaction processes a sound method to calculate the needed amount of certified input for a certain amount of certified mass balanced output. Life cycle assessments ensure the reduced environmental impact of our mass-balanced products.

