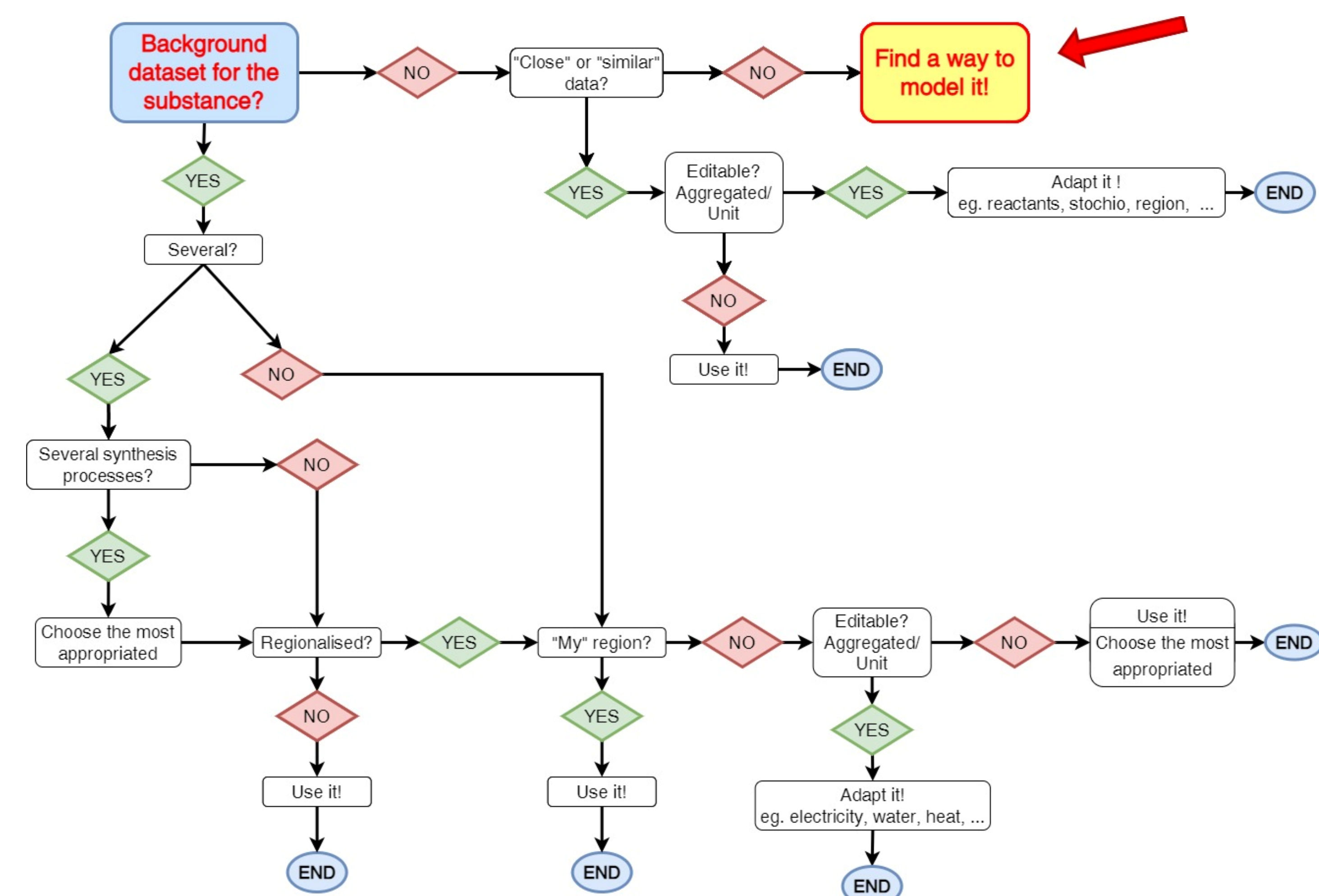
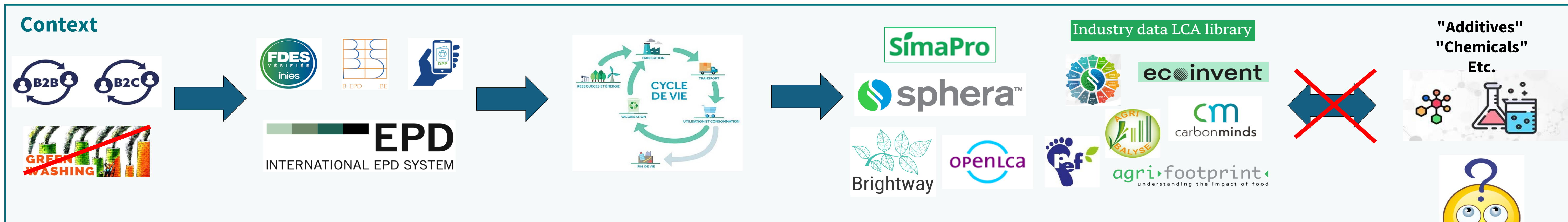
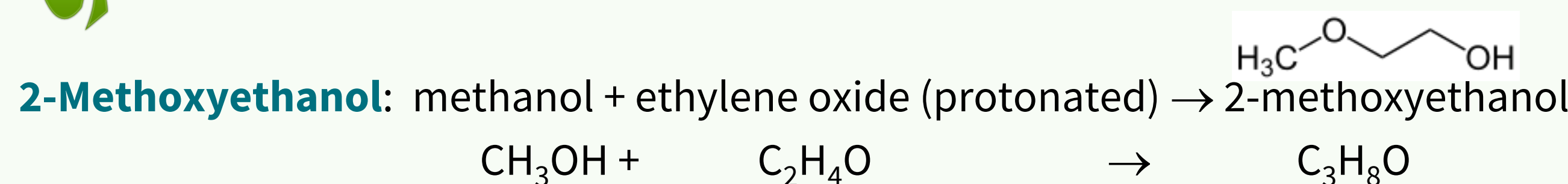


Life Cycle Assessment of chemicals out of the fields commonly represented in general databases

Dr Ir Sylvie Gros Lambert, Prof Angélique Léonard
With the collaboration of Ir Sabela Teixeira Taboada
Liège Université (ULiège - Belgique) - s.gros Lambert@uliege.be



It exists a very close background dataset



ecoinvent: Methyl-3-methoxypropionate: synthesis: methanol + methyl acrylate
 ⇒ Replacement of the methyl acrylate by the ethylene oxide

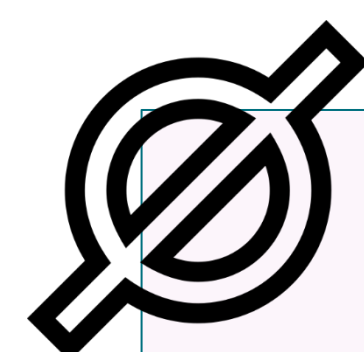
- Adaptation of quantities: stoichiometry
- Energy consumption (electricity, heat): kept as they are



It exists a very close background dataset

"Soude/soda" / Natural sodium carbonate: Na_2CO_3 ; ecoinvent: only Solvay process
 But ...
USLCl: Soda ash including trona as natural resource
 ⇒ Used as a basic reference

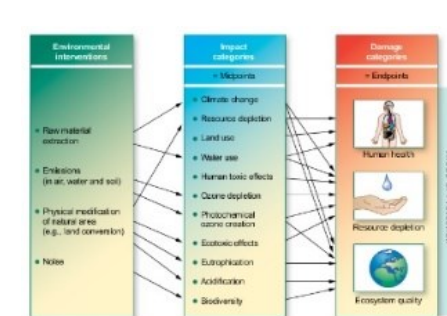
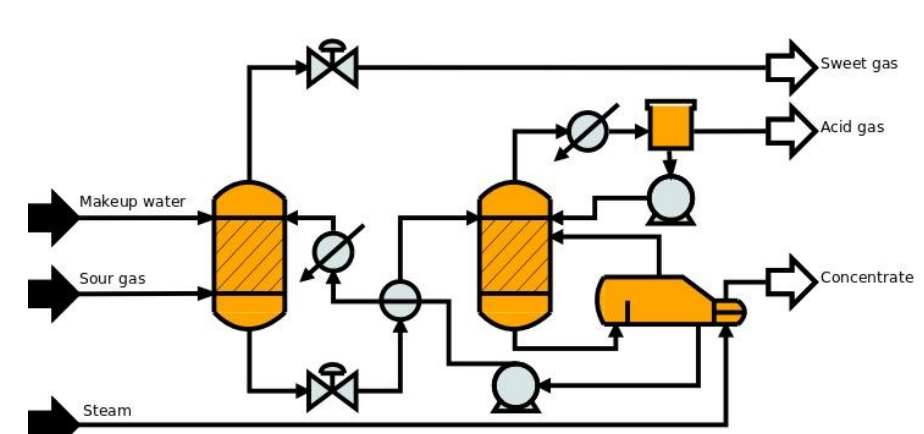
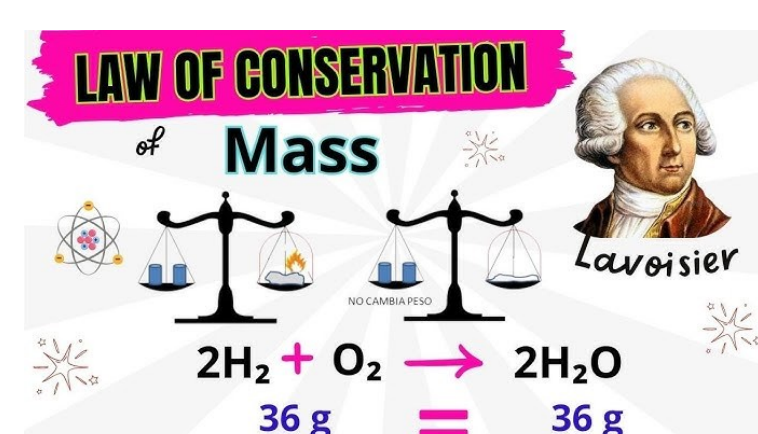
- Adaptation of US background data with European data
- Adaptation of energy sources (bituminous coal → natural gas)



No "proxy" available ...
 ⇒ **Creation of the model**

Synthesis + Production

- Reaction:** stoichiometry : $a\text{A} + b\text{B} \rightarrow c\text{C} + d\text{D}$
 Yield? coproducts? (⇒ allocations?)
- Process:**
 - Energy : electricity, heat
 - Emissions, waste
 - Others ...



It exists an EPD for a product / a scientific paper with results
 → **without available inventory data**
 ⇒ Same method / same characterisation factors: EN15804+A2, EF 3.x

- Use of results as is
- Creation of pseudo-substances corresponding to categories
- Input from nature, emissions to air/water/soil, waste, ...
- Addition of CF = 1 for these pseudo-substances in the methods



Synthesis? → Research tools, bibliography, patents, AI, ...



Production: Generic background dataset ecoinvent

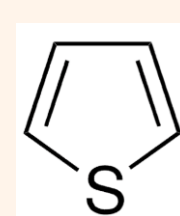
Used for *Chemical, chemical production, (in)organic*

⇒ **Most relevant proxy in the absence of primary data**

- Electricity: eg.** Calculated based on literature data published by the GENDORF Chemical Park. The factory produced an average of 2462760 tonnes of chemical substances (including intermediates) per year in the years 2015-2019. The average consumption of electricity in the years 2015-2019 was 982796751 kWh per year. This equals **0.39906 kWh/kg chemical produced**.
- Heat: eg.** Calculated based on literature data published by the GENDORF Chemical Park. The factory produced an average of 2462760 tonnes of chemical substances (including intermediates) per year in the years 2015-2019. The average consumption of natural gas in the years 2015-2019 was 4645920000 MJ per year. This equals **1.8865 MJ/kg chemical produced**.

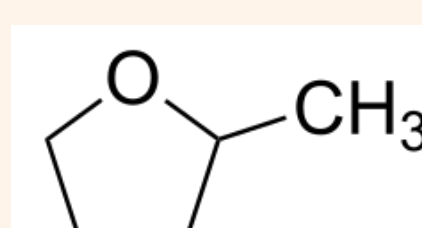
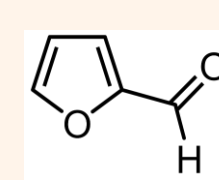
Thiophene $\text{C}_4\text{H}_4\text{S}$ (CAS 110-02-1)

- **Sources:** Brevet, ecoinvent
- **Reaction:**
 C_4H_6 (1,3-butadiene) + S → $\text{C}_4\text{H}_4\text{S}$ (thiophene) + H_2
- **Process:** ? → proxy ecoinvent : pyridine cf. heterocyclic
 - Yield, ratio butadiene/ sulphur
 - Energy (electricity, heat) kept as is + adaptation of the region
 - Emissions, waste: none



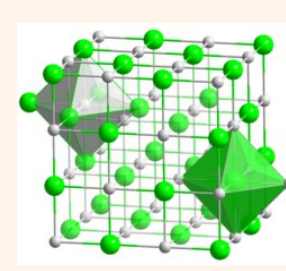
2-Methyltetrahydrofuran $\text{CH}_3\text{C}_4\text{H}_7\text{O}$ (CAS 96-47-9)

- Paper LCA MeTHF – **confidential inventory!**
<https://pubs.acs.org/doi/abs/10.1021/acssusresmt.4c00144>
- But precursor inventory : Furfural (+ H_2)
 → proxy with ratio as mentioned in the paper
- Furfural $\text{C}_5\text{H}_4\text{O}_2$ (CAS 98-01-1)**
 - **Sources:** paper, ecoinvent
 - **Synthesis** from corn
 - Inventory: in the supplementary data



Potassium iodide KI (CAS 7681-11-0)

- **Sources:** Ullman, ecoinvent
- **Reaction:**
 $\text{I}_2 + \text{SO}_2 + 4\text{KOH} \rightarrow 2\text{KI} + \text{K}_2\text{SO}_4 + 2\text{H}_2\text{O}$
- **Process:** ? → proxy ecoinvent
 - Methyl iodide, Potassium perchlorate
 - Coproducts: allocation (mass/economic)
 - Energy (electricity, heat): identical
 ⇒ kept as is + adaptation of the region



References

<https://onlinelibrary.wiley.com/doi/book/10.1002/14356007>
<https://www.wikipedia.org/>
<https://webbook.nist.gov/chemistry/>
<https://www.freepatentsonline.com/>
<https://scholar.google.be/>
<https://ecoquery.ecoinvent.org/>
 Similar approach: Huber, E., Bach, V., Holzapfel, P., Blizniukova, D., & Finkbeiner, M. (2022). An approach to determine missing life cycle inventory data for chemicals (RREM). Sustainability, 14(6), 3161 (Research – Reaction – Energy – Modelling).

<https://chatgpt.com/>
<https://claude.com/product/overview>
<https://researchrabbitapp.com/>
<https://www.google.com/>
<https://www.perplecity.ai/>
<https://www.opera.com/fr/features/aria>

<https://www.commport.com/digital-product-passport/>
<https://www.linkedin.com/pulse/rse-washing-greenwashing-que-se-cache-t-il-dere-dre-ces-jaurrey-uf0le/>
<https://support.simapro.com/s/article/How-to-use-external-LCIA-results-in-your-LCA-model>
https://fr.freepik.com/vecteurs-premium/tableau-chimie-dessine-main_4503937.htm
<https://www.sciencedirect.com/topics/chemical-engineering/flowsheet>
<https://pubs.acs.org/doi/10.1021/acssusresmt.4c00144>