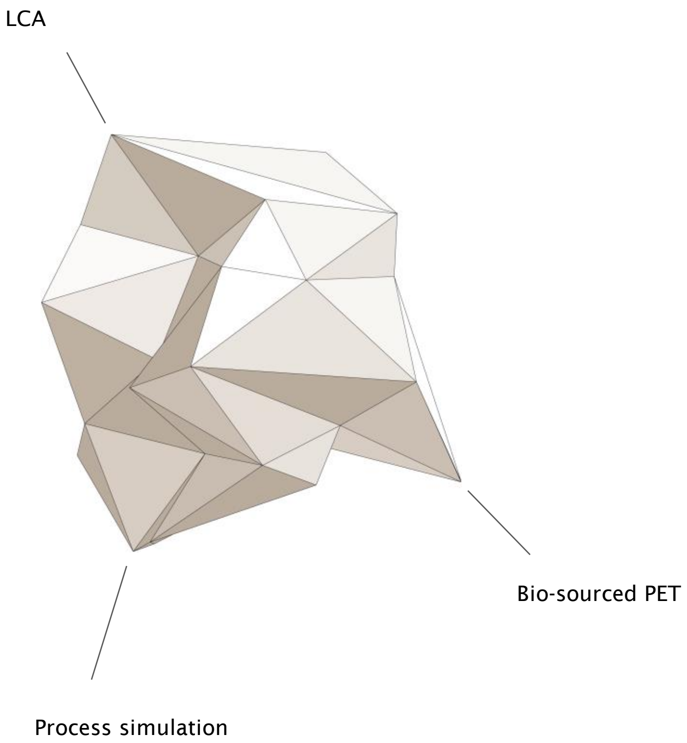
COUPLING PROCESS SIMULATIONS AND LIFE CYCLE ASSESSMENTS: THE USE CASE OF A BIO-SOURCED MATERIAL PRODUCTION PROCESS



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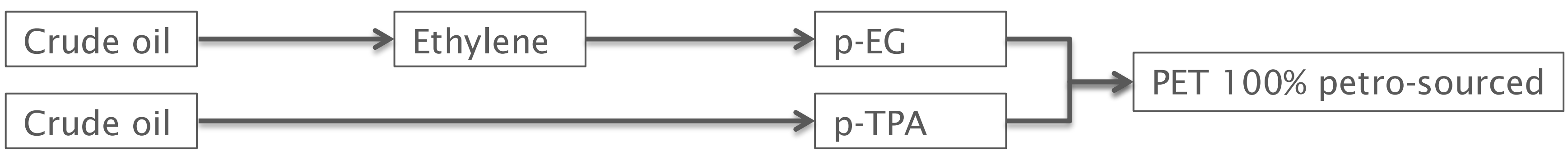
Altran Research

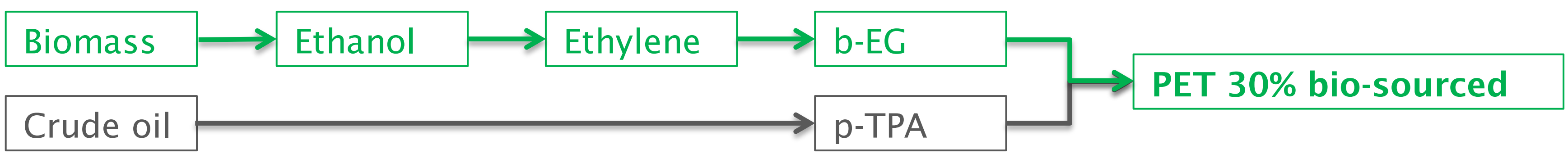
Is bio-sourced Polyethylene terephthalate (PET) a truly sustainable solution ?

PET is produced by polycondensation between ethylene glycol (EG) and terephthalic acid (TPA) : EG + TPA → PET

EG and **TPA** are usually petro-sourced :



EG can be bio-sourced from agricultural resource (sugar beet)



- We would like to compare the environmental efficiency of both processes.
- The bio-based materials sector is still emerging and it lacks a complete environmental database → We need to develop a methodology to assess the environmental performance of biomaterials.

Midpoint indicators will be considered to assess the sustainability of each pathway.

Midpoint indicators

Abiotic depletion	(kg_{eq} of Sb)
Acidification	(kg_{eq} of SO_2)
Eutrophication	(kg_{eq} of PO_4^{3-})
Global warming/GWP 100	(kg_{eq} of CO_2)
Ozone layer depletion	(kg_{eq} of CFC-11)
Human toxicity	(kg_{eq} of 1,4-DB)
Fresh water aquatic ecotoxicity	(kg_{eq} of 1,4-DB)
Marine aquatic	(kg_{eq} of 1,4-DB)
Terrestrial ecotoxicity	(kg_{eq} of 1,4-DB)
Photochemical oxidation	(kg_{eq} of C_2H_4)

CML2 (2000) ←

LCI

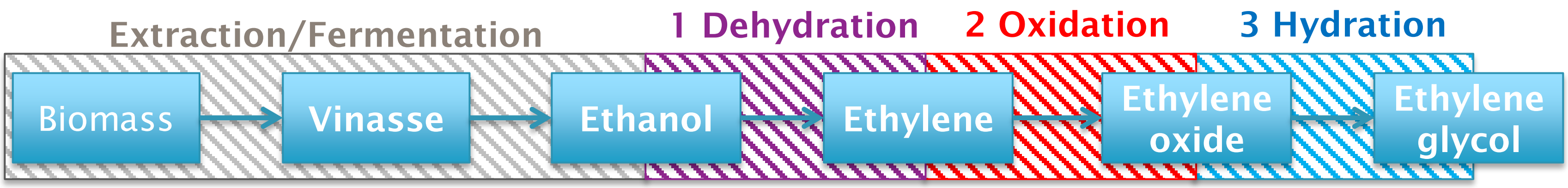
NO_x
CO_2
CH_4
C_2H_4
Naphtha
LPG
Coal
Natural gas
…

- Midpoint indicators are deduced from the inventory.
- We need to get accurate data for the Life Cycle Inventory (LCI).

Our method differs from classical Life Cycle Inventories (LCI) based on the Ecoinvent data.

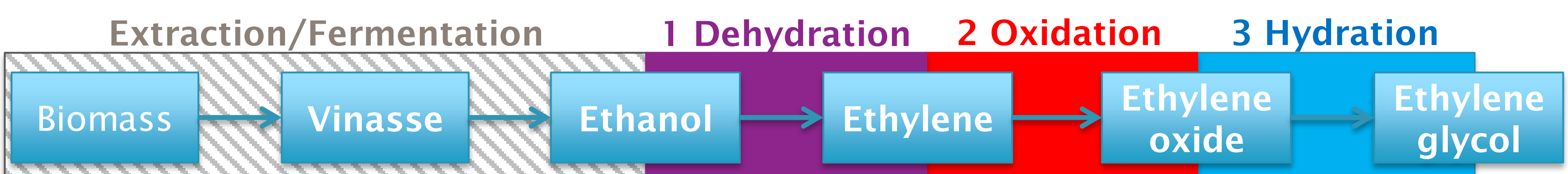
The classical assessment method : the REFERENCE

- Life cycle analysis using the Ecoinvent database.



Our method : the SIMULATED process

- Life cycle analysis coupled with process a simulating tool for the dehydration, oxidation and hydration steps.
- Purification steps and conversion rates are taken into account.
- Heat and matter are recovered and considered as “avoided products” by the system.



- For both : the functional unit is the production of 1kg of ethylene glycol.

We take into account the real conversion rates and required purity.

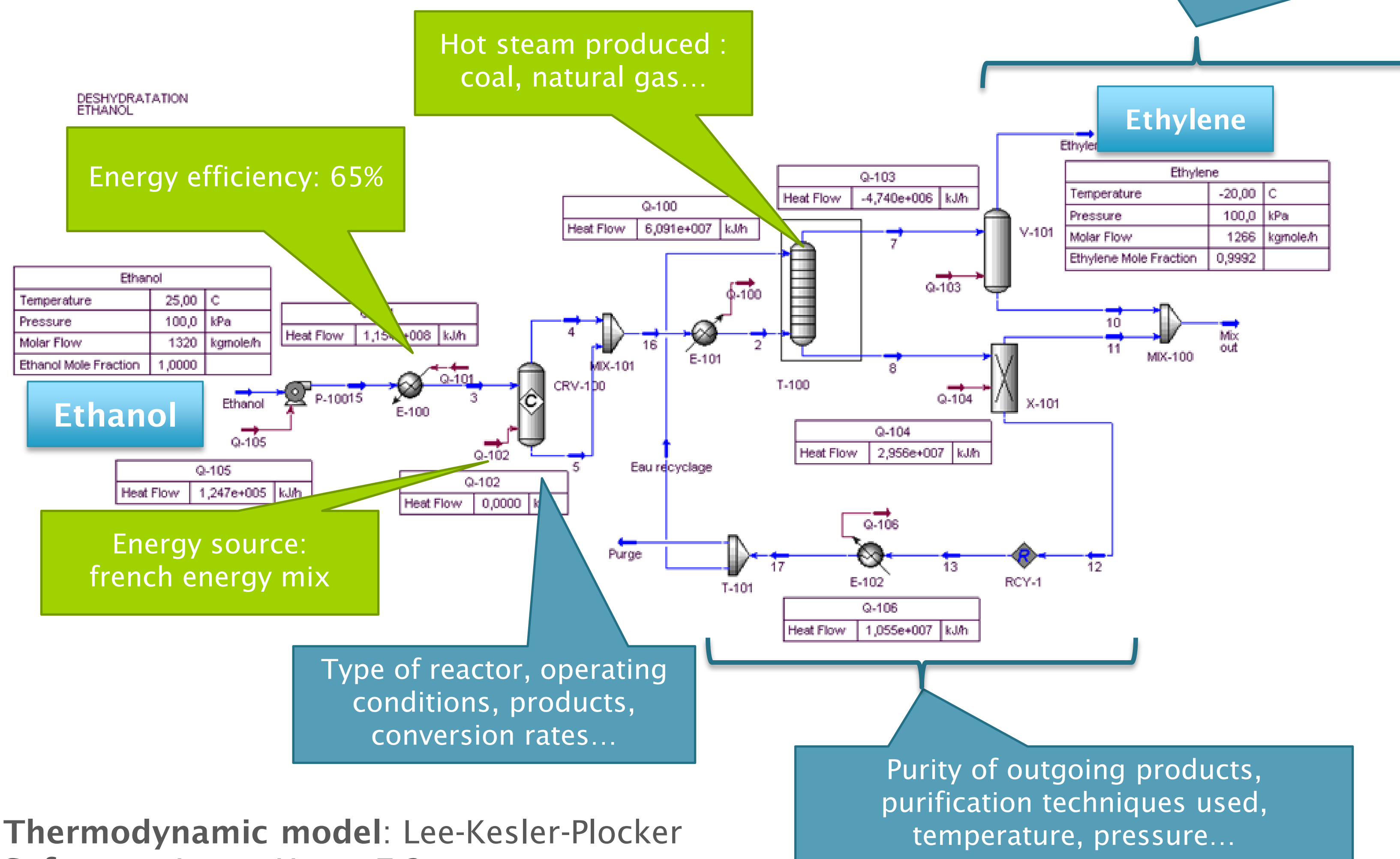
- **Ecoinvent database** considers that conversion rates and purity levels are 100%.
- **SIMULATED process**:
  - Oxidation step has a low conversion rate (42%)
  - For oxidation and hydration, two reactions compete with the expected reaction, which makes the purification step energy-consuming.

	Chemical reactions	Conversion rate %	Required Purity % molar
Dehydration	$C_2H_5OH \rightarrow C_2H_4 + H_2O$	95.8	99.9
Oxidation	(1) $C_2H_4 + 1/2\ O_2 \rightarrow C_2H_4O$ (2) $C_2H_4 + 3O_2 \rightarrow 2CO_2 + 2H_2O$ (3) $C_2H_4O + 5/2\ O_2 \rightarrow 2CO_2 + 2H_2O$	42.0	99.7
Hydration	(1) $C_2H_4O + H_2O \rightarrow HOC_2H_4OH$ (2) $HOC_2H_4OH + C_2H_4O \rightarrow HOC_2H_4OC_2H_4OH$ (3) $HOC_2H_4OC_2H_4OH + C_2H_4O \rightarrow HOC_2H_4OC_2H_4OC_2H_4OH$	88.5	99.5

Example of process simulation

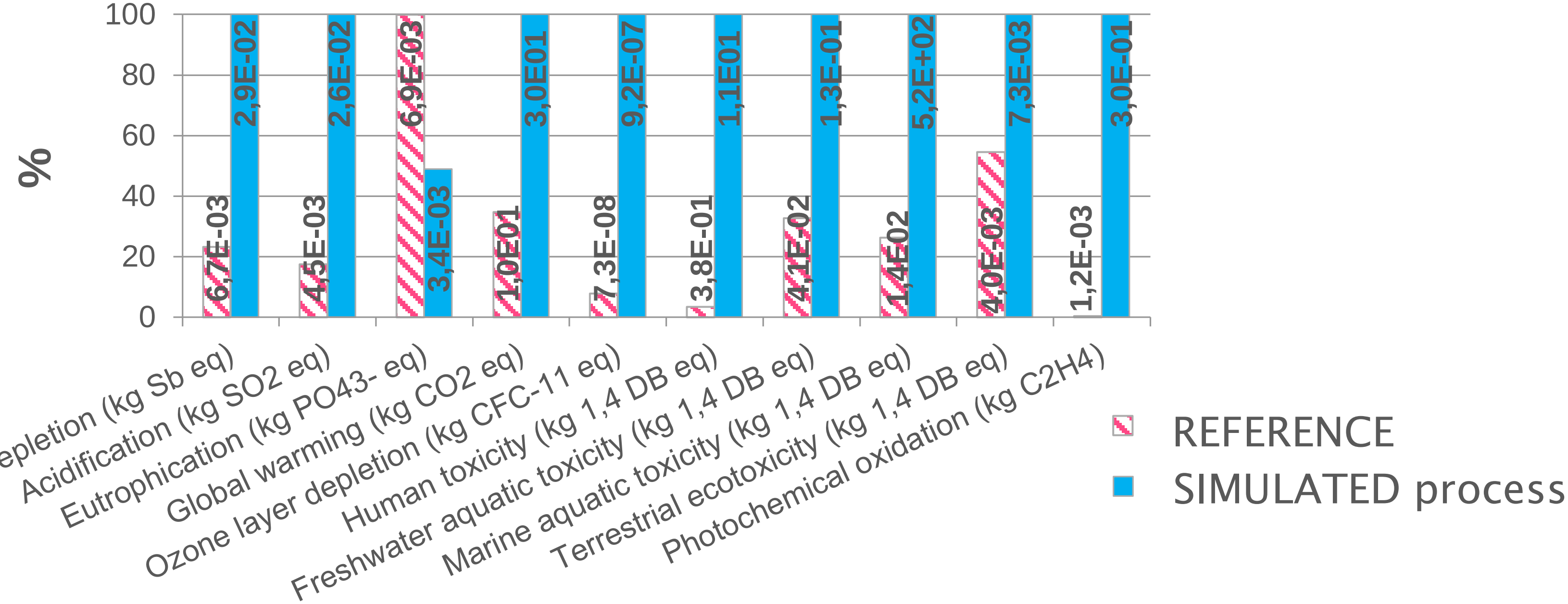
1 Dehydration

Purity of outgoing products, purification technique used, temperature, pressure …



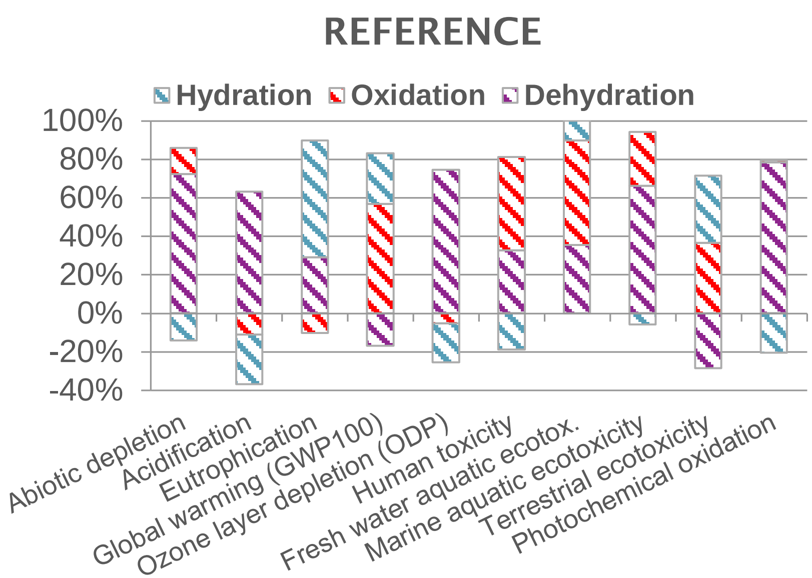
- **Thermodynamic model**: Lee-Kesler-Plocker
- **Software**: Aspen Hysys 7.2

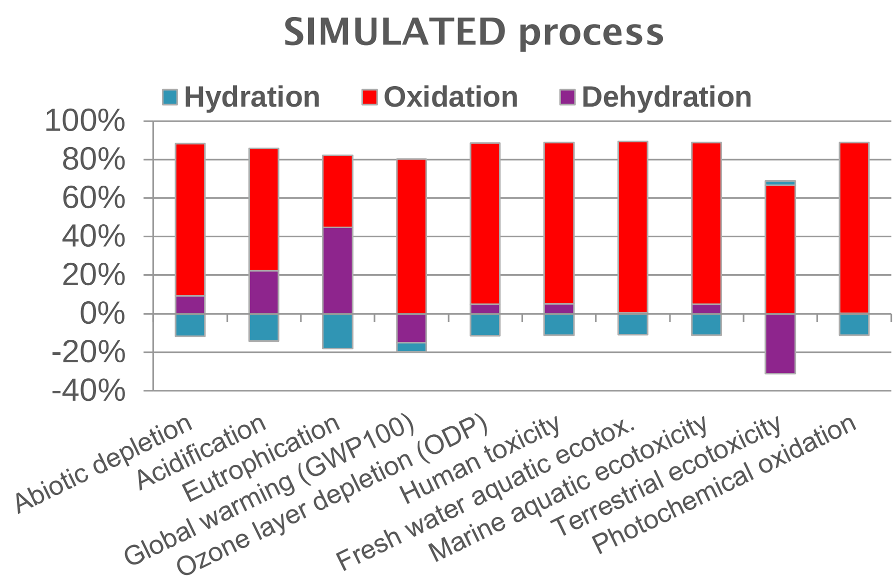
The classical approach (based on the Ecoinvent data) underestimates the environmental impacts.



- Environmental impacts of the SIMULATED process are higher than REFERENCE results except for **Eutrophication**.
- Taking into account real conversion rates and the need for separation steps to get the expected purity drastically increases the fossil energy consumption, thus the environmental impacts.
- Surprisingly, eutrophication is much higher in the classical method. This might be due to an error in the COD (chemical oxygen demand) for the hydration step (factor 1000 in comparison with oxidation and dehydration steps).

Contribution of each unit process to the total impacts





- Oxidation has a predominant effect, as the real conversion rate is 42% and the purity is 99.7%.
- Hydration step promotes other products (propylene glycol and butylene glycol) so the environmental impacts decrease.

Conclusion

- Coupling process simulation and life cycle assessment is an efficient tool for environmental assessment.
- Process simulation is a relatively simple method. This work has been realized with six parameters: the type of chemical reaction, the conversion rate, the temperature, the pressure, the purification technique, the purity level of the products.
- Process simulation is of particular interest when data are not available : incomplete or imprecise, as in our case (bioresources transformation processes).
- Most of all, process simulation makes it possible to take into account real conversion rates and the need for separation steps to get required purity. These purification steps drastically increase the environmental impacts.

Perspective

For further studies, we want to:

- Simulation with 100%
- Sensibility
- Identify the relevant indicators instead of using the preconceived list of indicators
- Assess other aspects related to agricultural production such as land use

INNOVATION MAKERS

Thank for your attention!