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Methodik zur schnellen Bewertung von Syntheserouten auf Basis von Exergiebilanzen

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outline

- why exergy?
- short-cut method
- example process
- results: comparison
- conclusions



calculation of exergy

exergy of a material stream

$$E_i = \sum_{i=1}^N (E_{i,\text{chem}} + E_{i,\text{phys}}) + \Delta E_{\text{mix}}$$

chemical exergy of a material stream

$$E_{i,\text{chem}} = \Delta^{\circ}G_i + \sum_{i=1}^j v_{i,j} E_{j,\text{chem}}^{\circ}$$

physical exergy of a material stream

$$E_{i,\text{phys}} = \int_{T_U}^{T_R} C_i(T) dT + V_i^{\text{IF}} (P_R - P_U) - T_U \int_{T_U}^{T_R} \frac{1}{T} C_i(T) dT$$

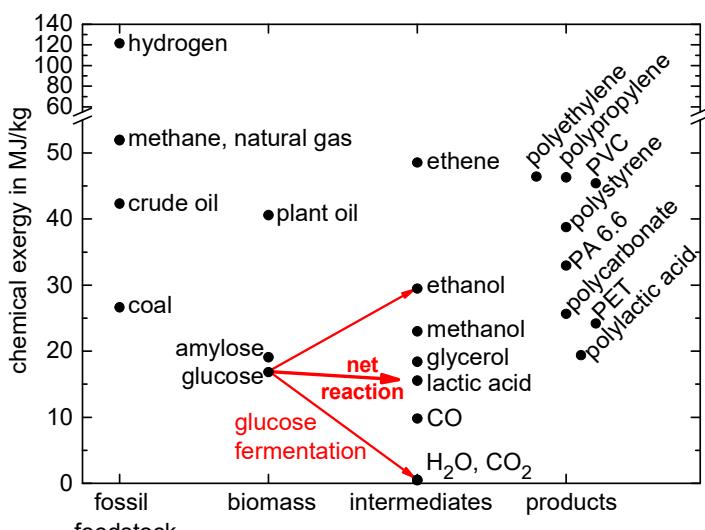
+ exergy losses in processes and equipment



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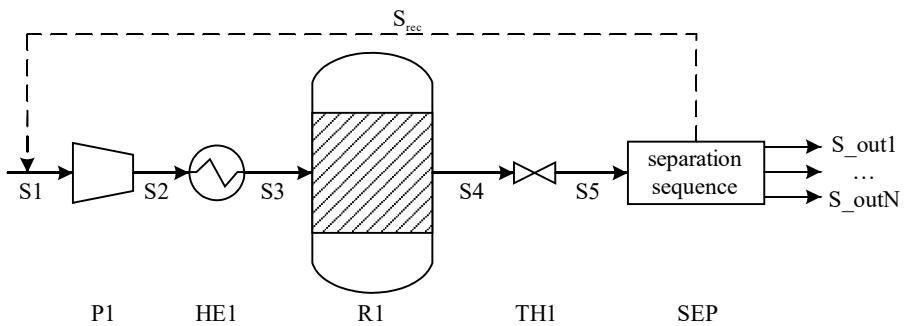
exergy as measure sorting the options



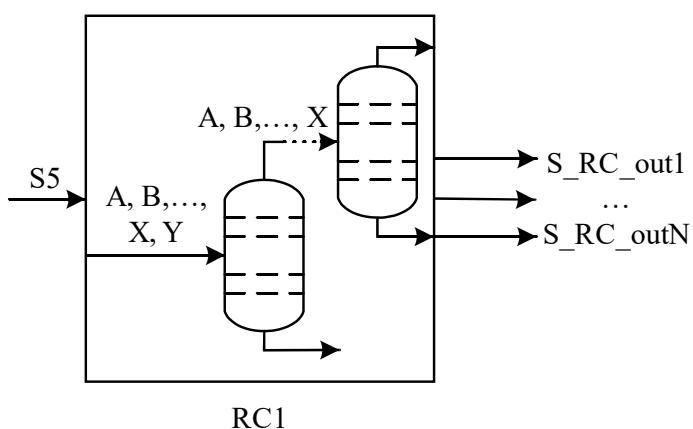
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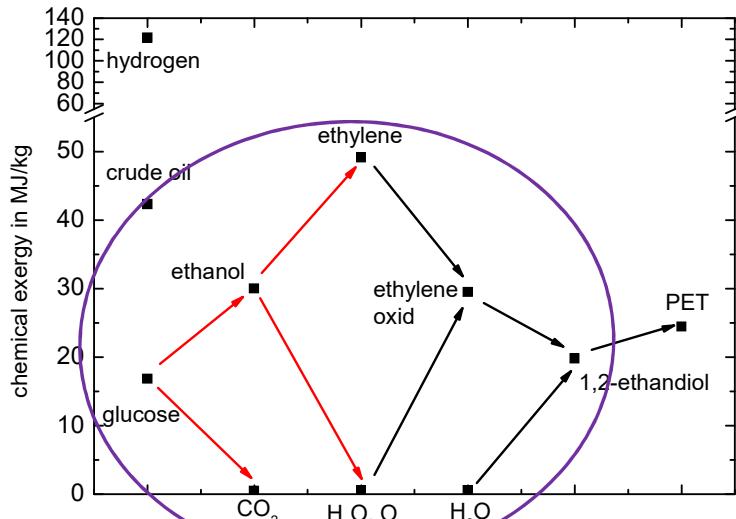
basic process scheme with recycle



separation by distillation cascade



synthesis pathways to PET



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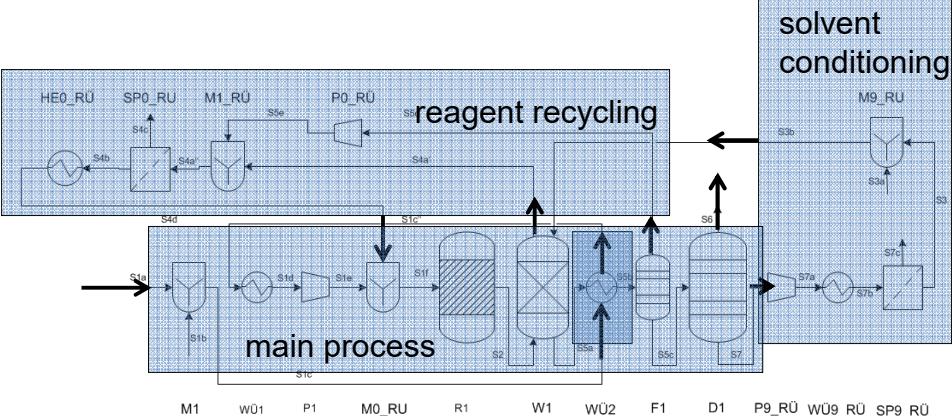
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process: ethylene → ethylene oxide



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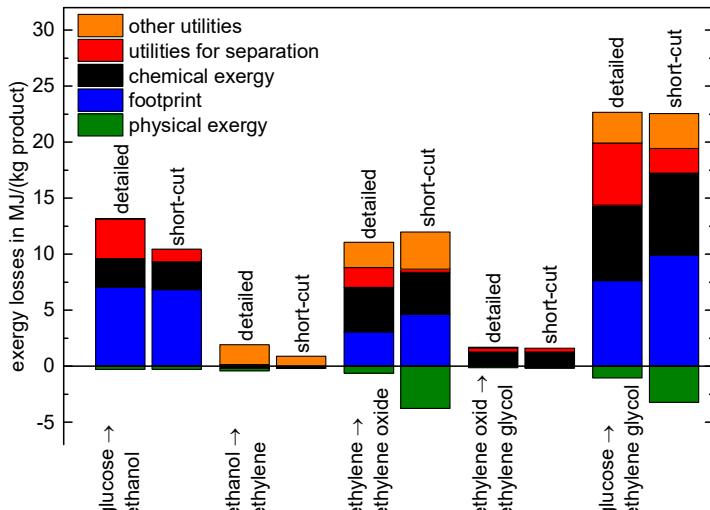
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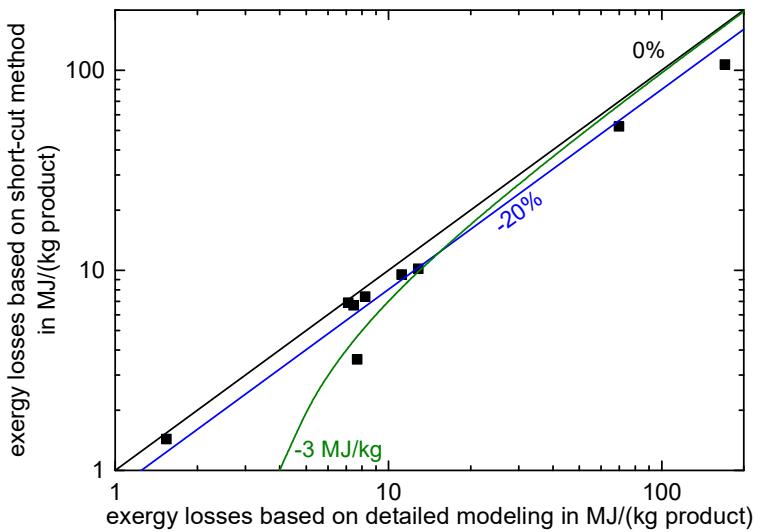
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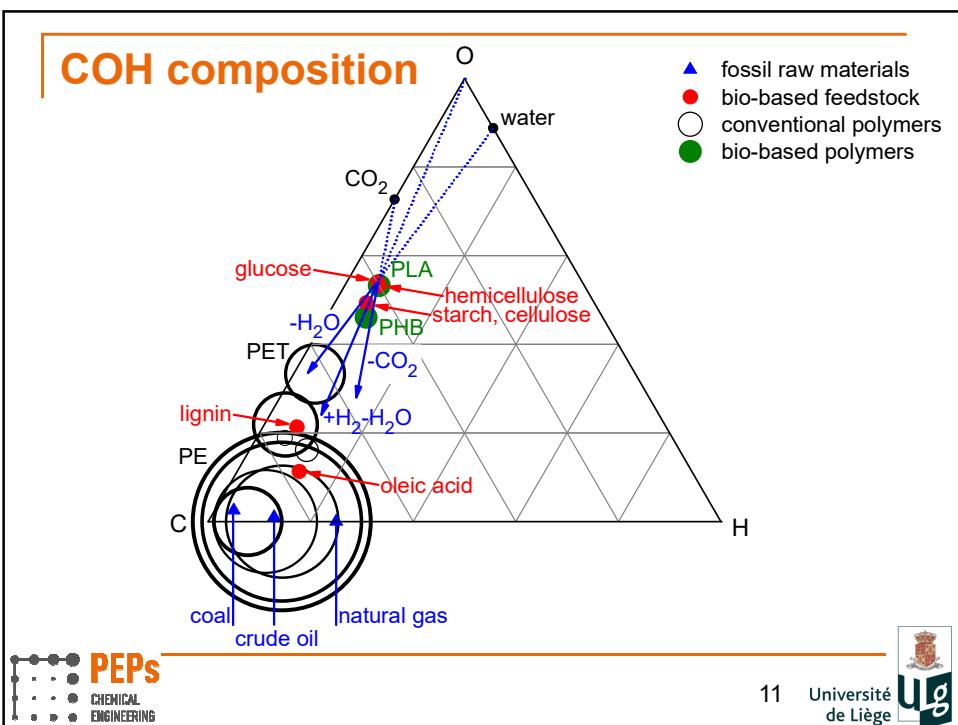


comparison of routes and methods



order almost unchanged by short-cut





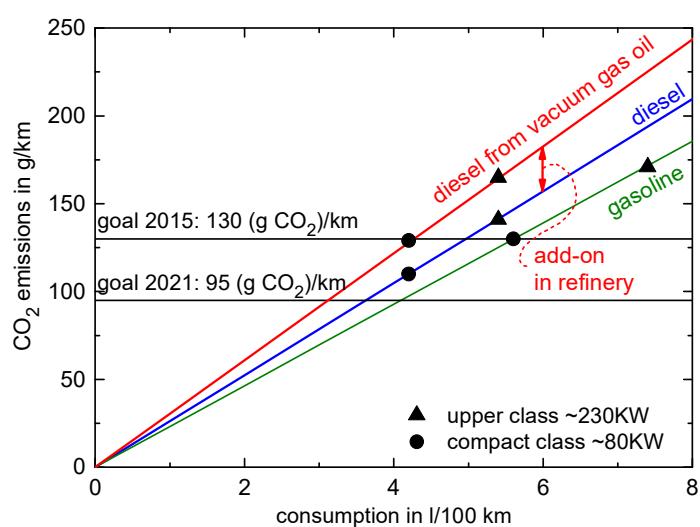
- ### evaluation of options
- exergy as universal measure:
 - short-cut gives proper order
 - can be used on variable level of refinement
 - glucose → products with more oxygen
 - plant oil → products with less oxygen
 - energy demand for processes will increase
 - land area required for biobased feedstock:
200 to 800 m²/capita (food ≈ 7000 m²/capita)
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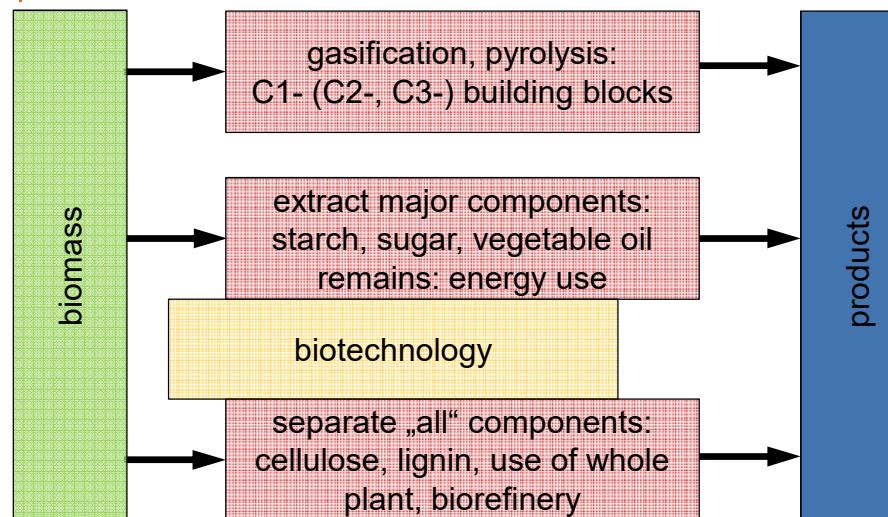
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CO₂ of diesel may not be as good as it seems



possible biobased synthesis pathways



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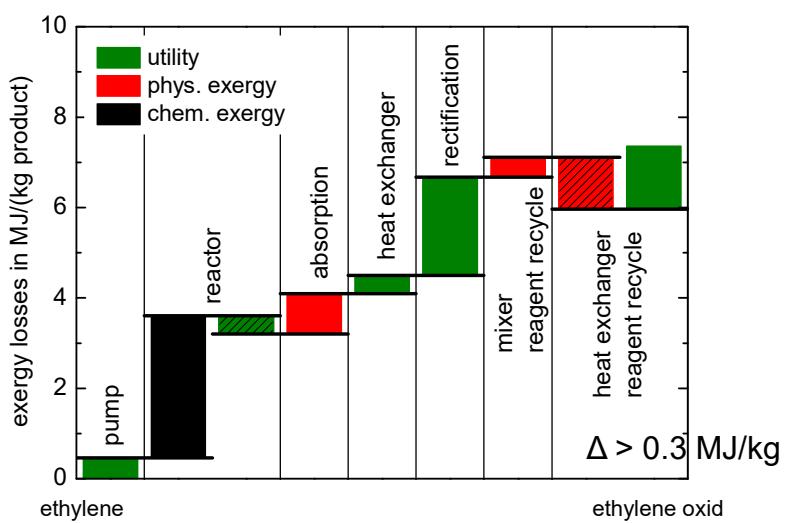
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results of exergy analysis



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comparision of the processes

