An estimation method for the production of fine chemicals

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Overview

- Motivation

- Structure and methodology of the existing procedure

- Results of a case study

- Description of further plans

- Possible Applications

Motivation

Lack of LCI data for fine chemicals due to:

- Large amount of substances

- Production in batch plants

- Complex process tree

$\rightarrow$ Estimation procedure necessary

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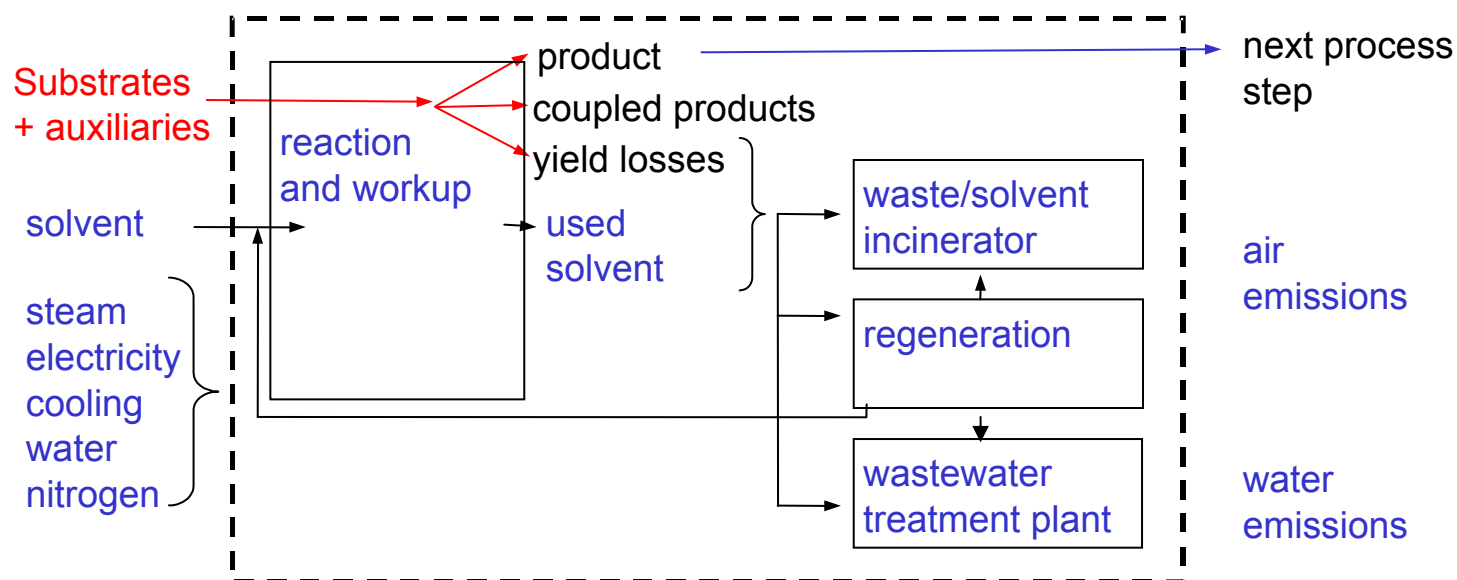Eidgenössische Technische Hochschule Zürich
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The existing estimation procedure

- Process tree is split into building blocks of individual process steps


Red: required   Blue: optional

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The existing estimation procedure

- Default values for all optional parameters based on expert advice

- Best-case and worst-case estimation ranges

→ Estimates LCI data from an incomplete or minimal set of input data

Case study

- Two crop protection substances

- 22 and 4 process steps calculated

- Verification of 11 process steps

- Sensitivity analysis

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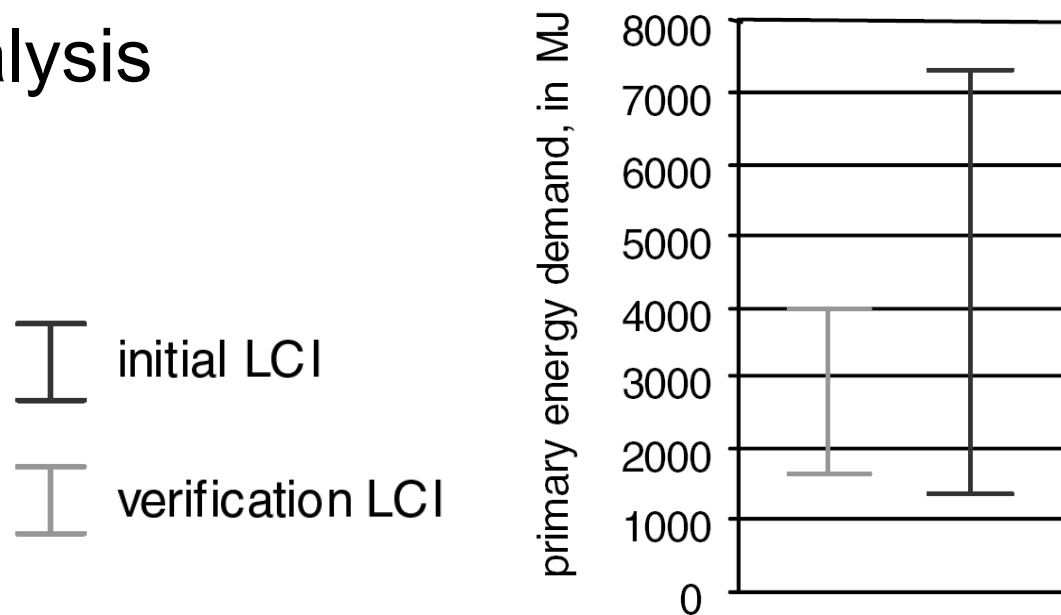
Further plans

- Calculation of a probable value and uncertainties

- Inclusion of several existing models to increase accuracy:
  - Waste treatment
  - Solvent recycling
  - Energy use in batch plants

- Inclusion machine learning algorithms:
  - Applicable even without a process tree
  - Based on substance structure and properties

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Applications

- Accurate estimation of LCI data with minimal input data

- Comparison of alternative substances

- Supply-chain analysis

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Thank you for your attention!

- ## Acknowledgements
  - Syngenta Crop Protection
  - Ciba Specialty Chemicals
  - SF-Chem

- ## Further information
  - gregor.wernet@chem.ethz.ch

- ## Reference
  - Geisler G, Hofstetter TB, Hungerbühler K; **Production of fine and specialty chemicals: Procedure for the estimation of LCIs**; *Int J Life Cycle Ass 9 (2): 101-113;* ***2004***