

Current models and approaches for data matching and modeling of chemical production

Gregor Wernet, Tereza Levova, Guillaume Bourgault

What is ecoinvent?



- A Swiss **not-for-profit** association
- Publishes the ecoinvent database, which contains **Life Cycle Inventory** data on many thousands of products and services
- Tens of thousands of users from over 80 countries
 - Primary users are industry, researchers, consultants and policy makers

What does the database contain?

- **Background database**, which contains average data on different materials and services at a product level, originally for process LCA
 - e.g. energy, basic materials, agriculture, transport, machinery, ...
- More than **12'500** datasets for over **2'700** products
- Data for up to **157** distinct geographies and over **80** countries
- Core features of **consistency**, **reliability** and **transparency**



ecoinvent as a PEF data provider



- ecoinvent is a data provider for the PEF pilot phase
 - Many of the data tenders are based on ecoinvent data in the background
 - ecoinvent was a direct data supplier for **270 products**, and over 800 datasets, on the **production of chemicals**
- Roughly 3 months for delivery
- How to deal with significant data needs on chemical products on short notice, while delivering quality and integrating primary data?

The PEF chemicals tender

- Prepare the background database
 - Integrate PEF energy and transport data, export and format questions
- Screen our existing data against the quality criteria
 - Existing data received updates or replacements if needed
- Around 80 chemicals needed completely new datasets
 - Upstream supply chains also needed
 - Around 200 new chemicals unit process datasets created
- Industry stakeholder group discussion
 - Timeframe made collaboration difficult, but several sources provided data

The PEF chemicals tender

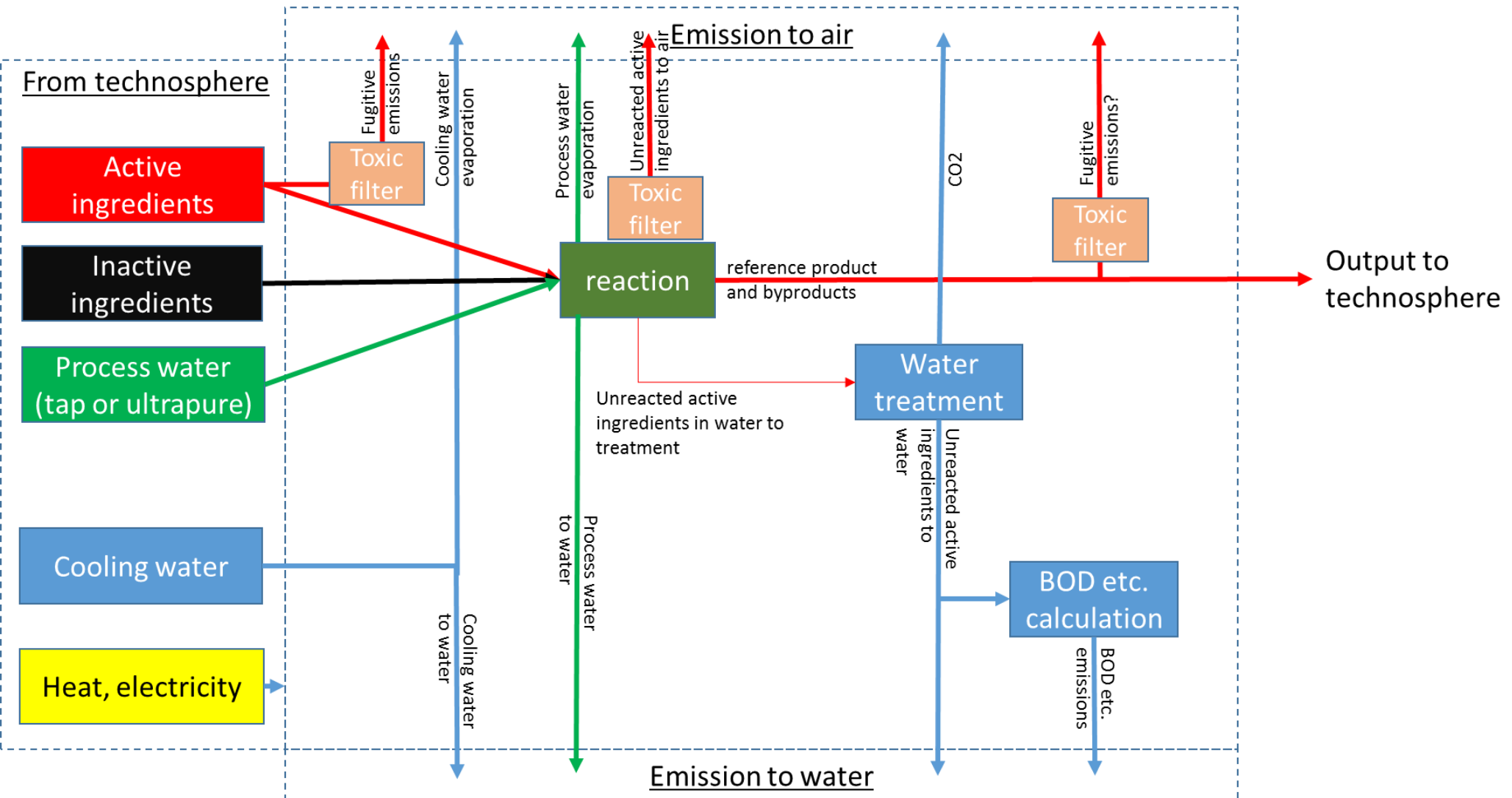


- Created a framework model that provides a unit process result, with each part of the process adaptable
 - Integrate primary data and more specific models in the project, often at the **data point** level
- “Modular model” approach
 - Datasets can be upgraded on specific topics when data becomes available, but fallback options are available if there are issues in data supply

The PEF chemicals tender

- Create **stoichiometric model** of the reactions required, with reactants and other reagents
- Average values for **yield, heat, electricity, water and supporting processes** are available from industry reports
- Air emission model based on vapor pressure, filtering systems and toxicity
- Waste water treatment model determines water emissions
- Previous models existed but all aspects of the model have been updated and extended for this project

Process flow diagram



The unit process model

- Start with a simple model and add what can be added
 - Yield factors
 - By-product fates
 - Energy demand
 - Solvents, disposal pathways
- Additional supporting activities were also updated (e.g. thermal energy)
- Discuss results with experts
- Review, compare, validate, repeat
- Documentation, metadata, quality indicators

The unit process model

- Project was an interesting combination of data format and data requirement issues and high-efficiency data generation
- The flexible model of chemical unit processes allows users to work with various data availabilities
 - Model is accessible, with all values and sources
 - Datasets list source types and acknowledge industry sources in coordination with the data providers
- Data are now used in the PEF pilot projects, and many will also be published in the upcoming ecoinvent 3.4

The world's most
consistent and
transparent Life Cycle
Inventory database



Thank you for your attention!