“AI will never predict environmental impacts only from the molecular structure of a product…”

Tim Langhorst,
Senior Expert and Trainer, Carbon Minds GmbH;
formerly: EPSE group @ ETH

92nd LCA Discussion Forum - AI in LCA: Innovations, Applications, and Challenges
February 26th, 2026

carbonminds

From molecule to impacts

Molecule

Environmental impacts

Molecular structure-based models (MSM)

Molecular descriptors
(physical and chemical properties)

Training data
(Environmental impact metrics)

Most MSM estimate environmental impacts from the molecule structure or molecular properties

USE CASES: Molecule design, closing (minor) data gaps, screening (e.g., for cut-off decisions)

Examples for MSM: Zhang et al., 2024, Sun et al., 2023, Calvo-Serrano et al., 2019, Song et al., 2017, Wernet et al., 2009

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Molecule

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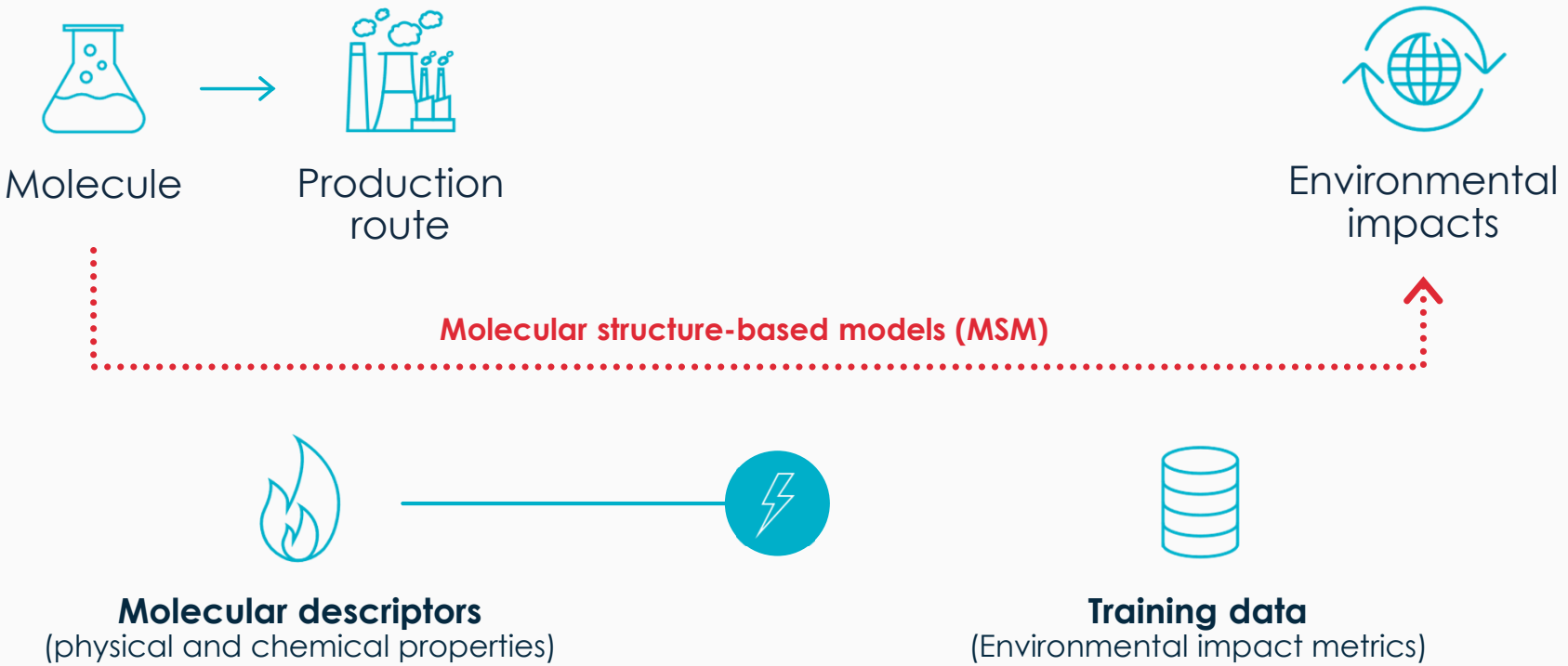
But this path is doomed.

Examples for MSM: Zhang et al., 2024, Sun et al., 2023, Calvo-Serrano et al., 2019, Song et al., 2017, Wernet et al., 2009

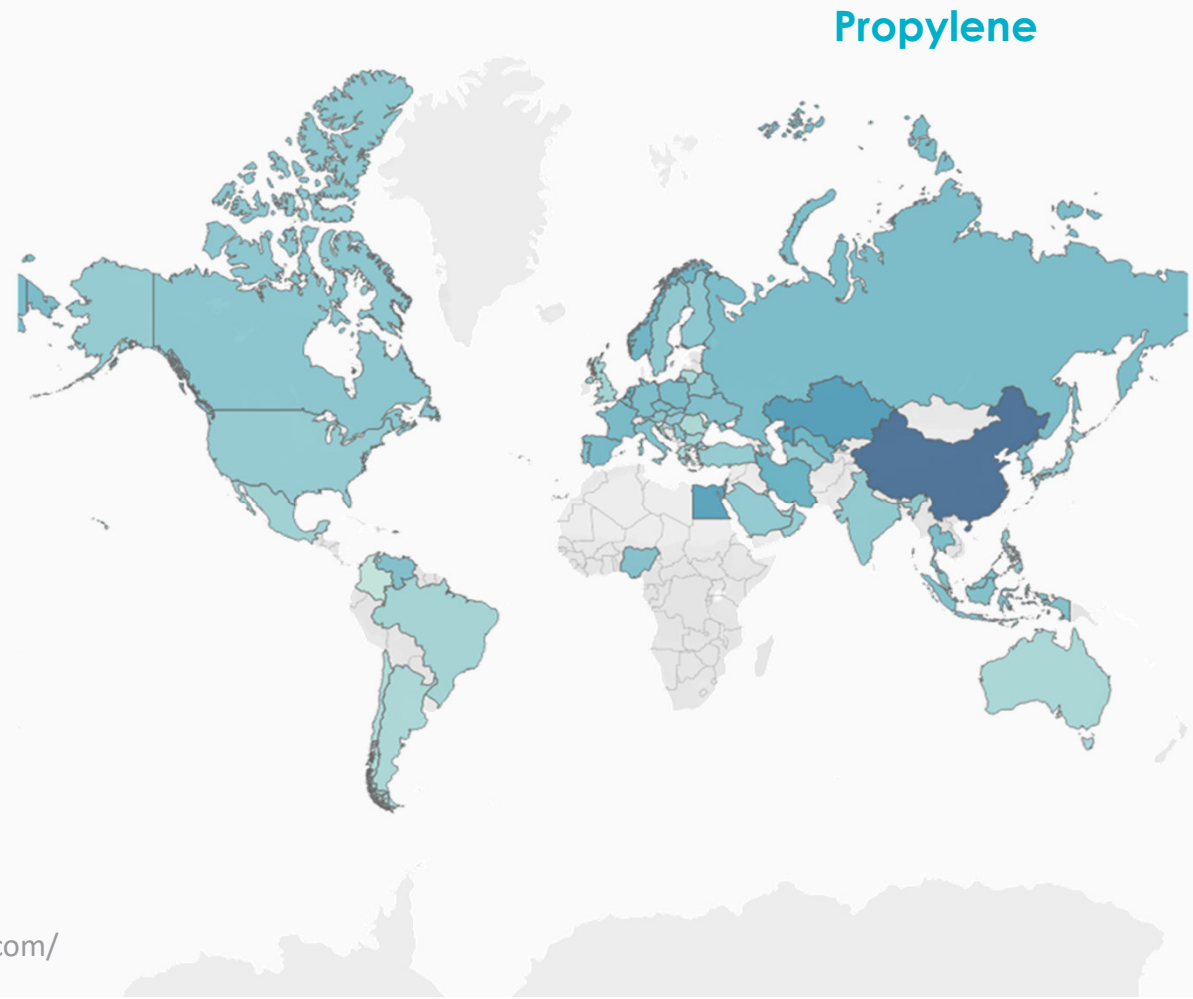
From molecule to impacts



Examples for MSM: Zhang et al., 2024, Sun et al., 2023, Calvo-Serrano et al., 2019, Song et al., 2017, Wernet et al., 2009

DATA BASED ON CM MODEL – NOT PRIMARY DATA

#1 Production mixes: domestic production
Climate impacts of propylene (in kg CO2-e/kg propylene)



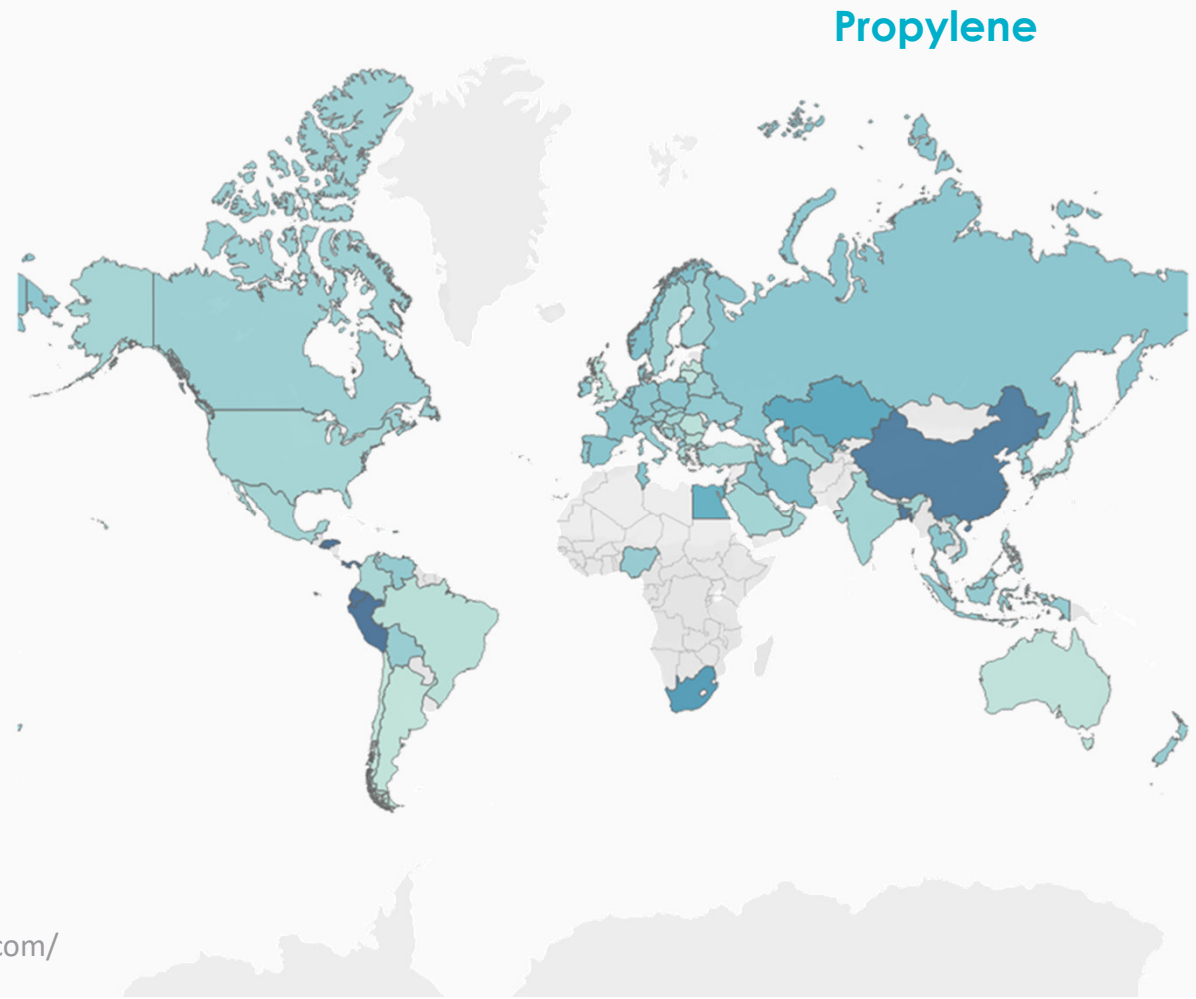
Large differences in climate impacts

- Feedstock use
- Technologies
- Energy

Source: https://dataplayground.carbon-minds.com/

DATA BASED ON CM MODEL – NOT PRIMARY DATA

#2 Consumption mixes: domestic production plus imports
Climate impacts of propylene (in kg CO2-e/kg propylene)



Large differences in climate impacts

- Feedstock use
- Technologies
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- Trade

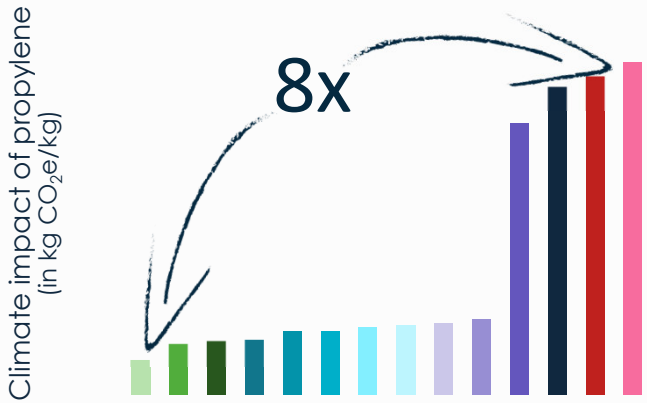
Source: https://dataplayground.carbon-minds.com/

DATA BASED ON CM MODEL – NOT PRIMARY DATA

#3 Technology specific data

Climate impacts of propylene (in kg CO2-e/kg propylene

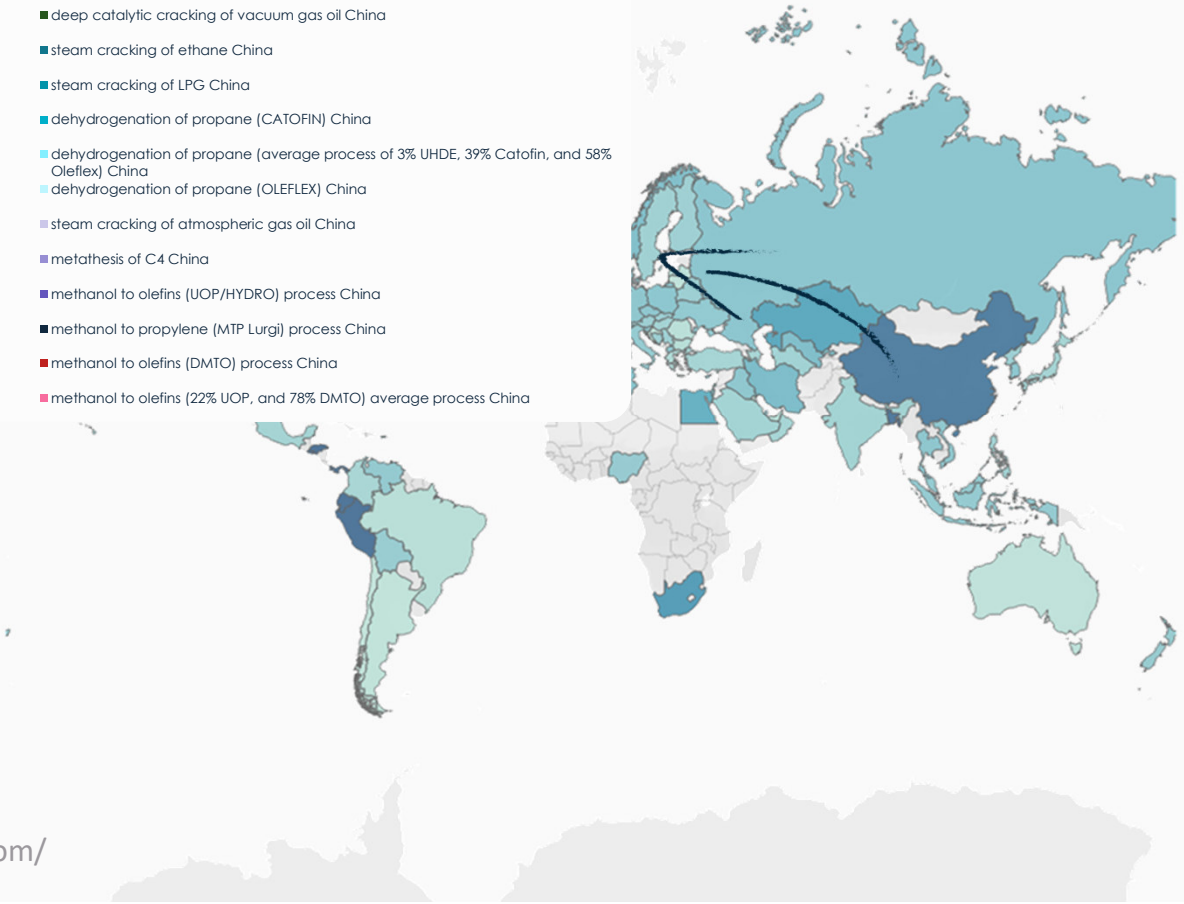
Technologies in China



- fluid catalytic cracking of vacuum gas oil China
- steam cracking of naphtha China
- deep catalytic cracking of vacuum gas oil China
- steam cracking of ethane China
- steam cracking of LPG China
- dehydrogenation of propane (CATOFIN) China
- dehydrogenation of propane (average process of 3% UHDE, 39% Catofin, and 58% Oleflex) China
- dehydrogenation of propane (OLEFLEX) China
- steam cracking of atmospheric gas oil China
- metathesis of C4 China
- methanol to olefins (UOP/HYDRO) process China
- methanol to propylene (MTP Lurgi) process China
- methanol to olefins (DMTO) process China
- methanol to olefins (22% UOP, and 78% DMTO) average process China

- Feedstock use
- Technologies
- Energy
- Trade

Propylene



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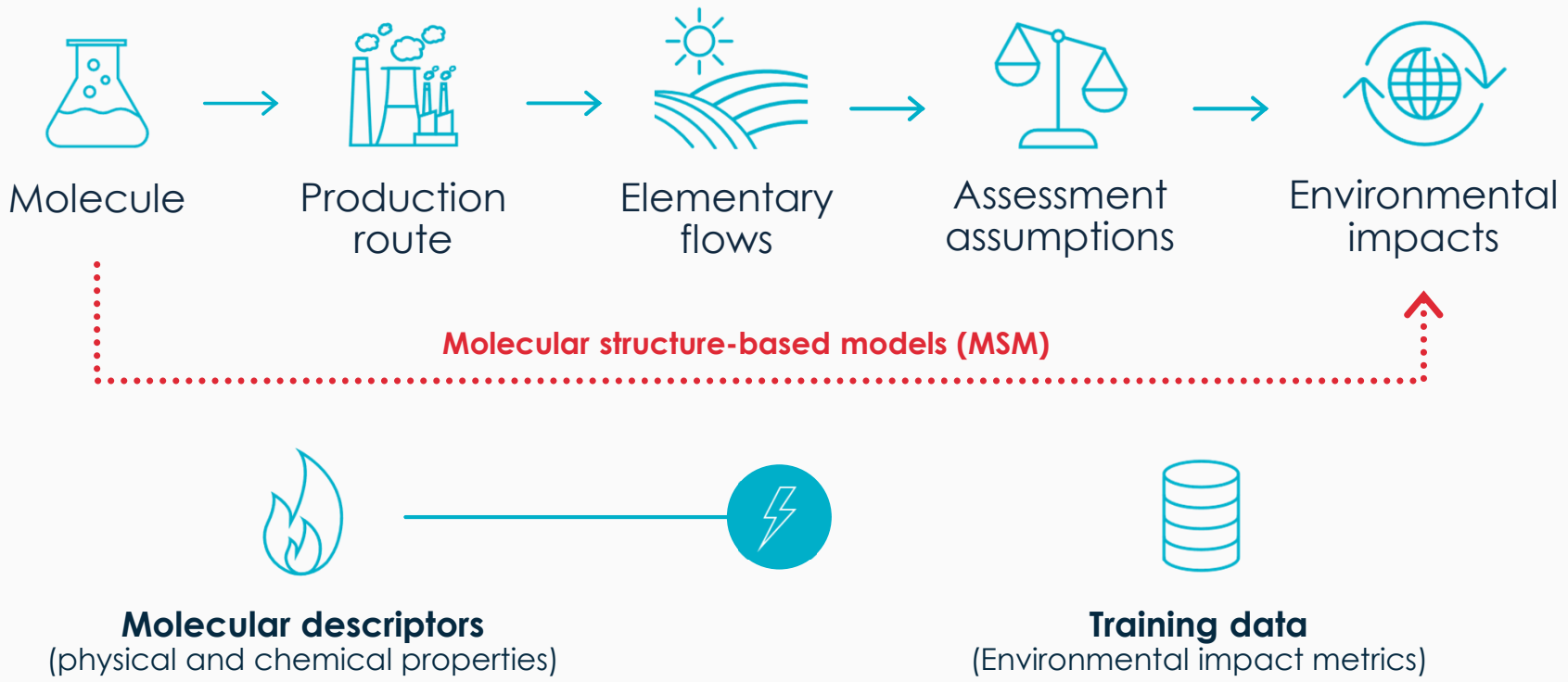
From molecule to impacts

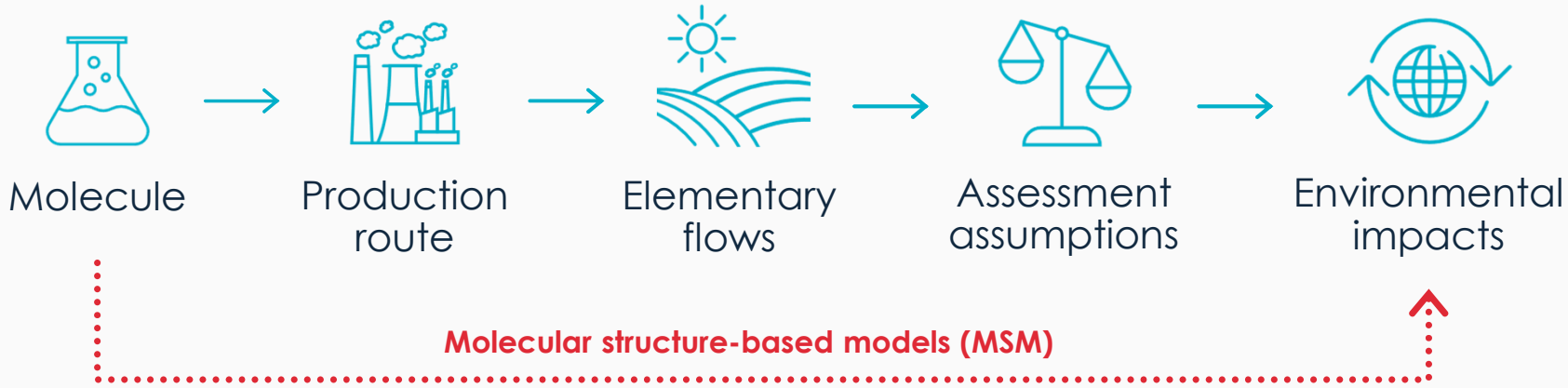


Examples for MSM **considering the production route**: Kleinekorte et al., 2023; Karka et al., 2019

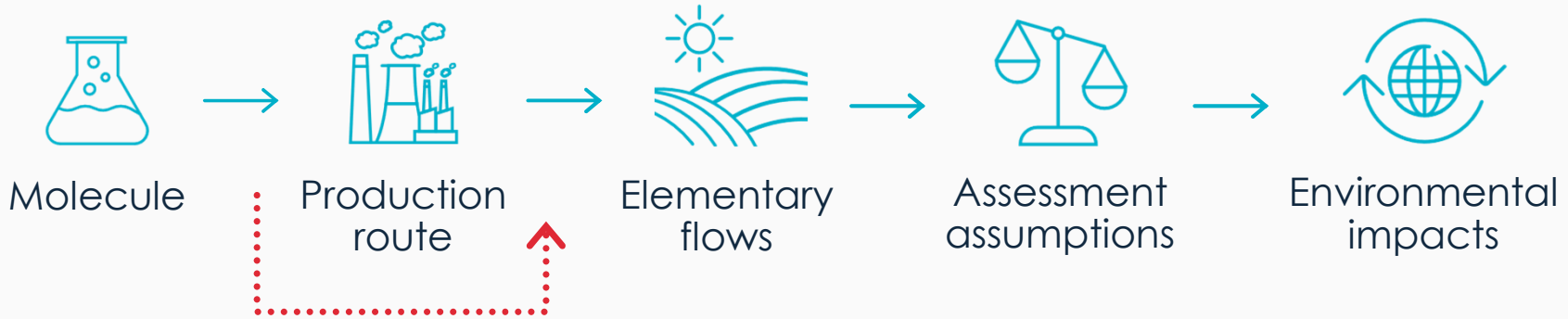
What can we do to fix this?

- Look at production routes, rather than molecular properties
- Predict Life Cycle Inventories, rather than Impacts
- Predict mass & energy balances, rather than elementary flows

From **reactions** to **mass & energy balances**



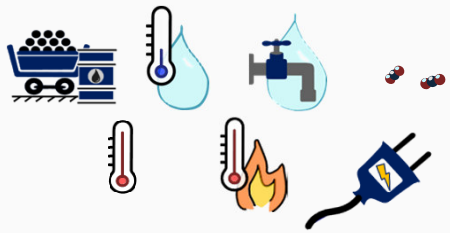
From **reactions** to **mass & energy balances**



Reaction-based models to estimate LCI:

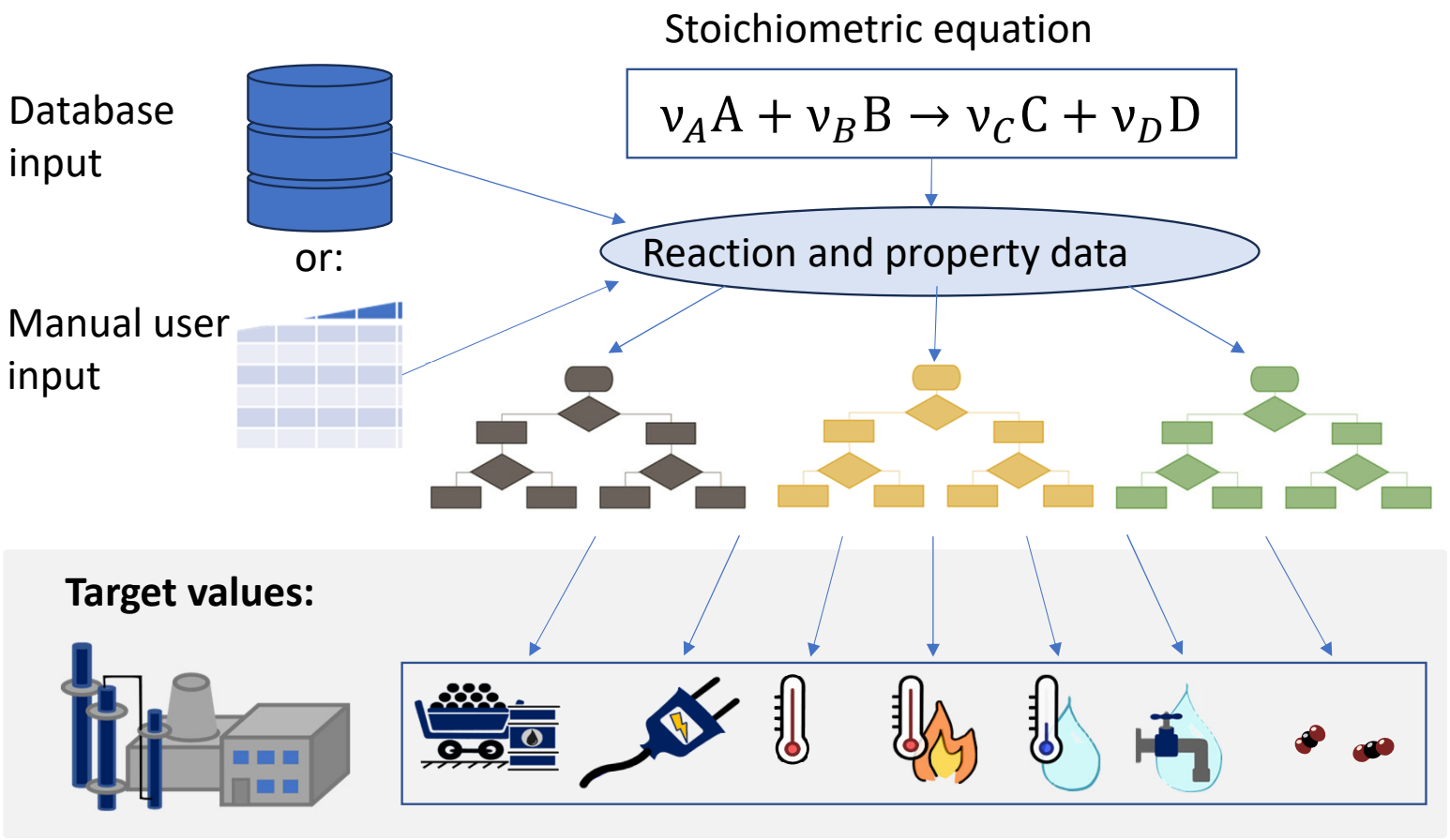
$$\nu_A \mathrm{A} + \nu_B \mathrm{B} \rightarrow \nu_C \mathrm{C} + \nu_D \mathrm{D}$$

Reaction equation
(properties derived for the whole reaction, not only the target molecule)

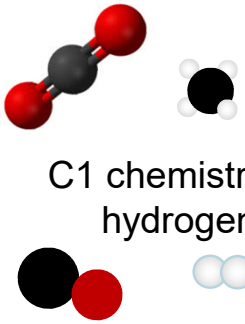


Training data
(Mass and energy balances needed to build the Life Cycle Inventory)

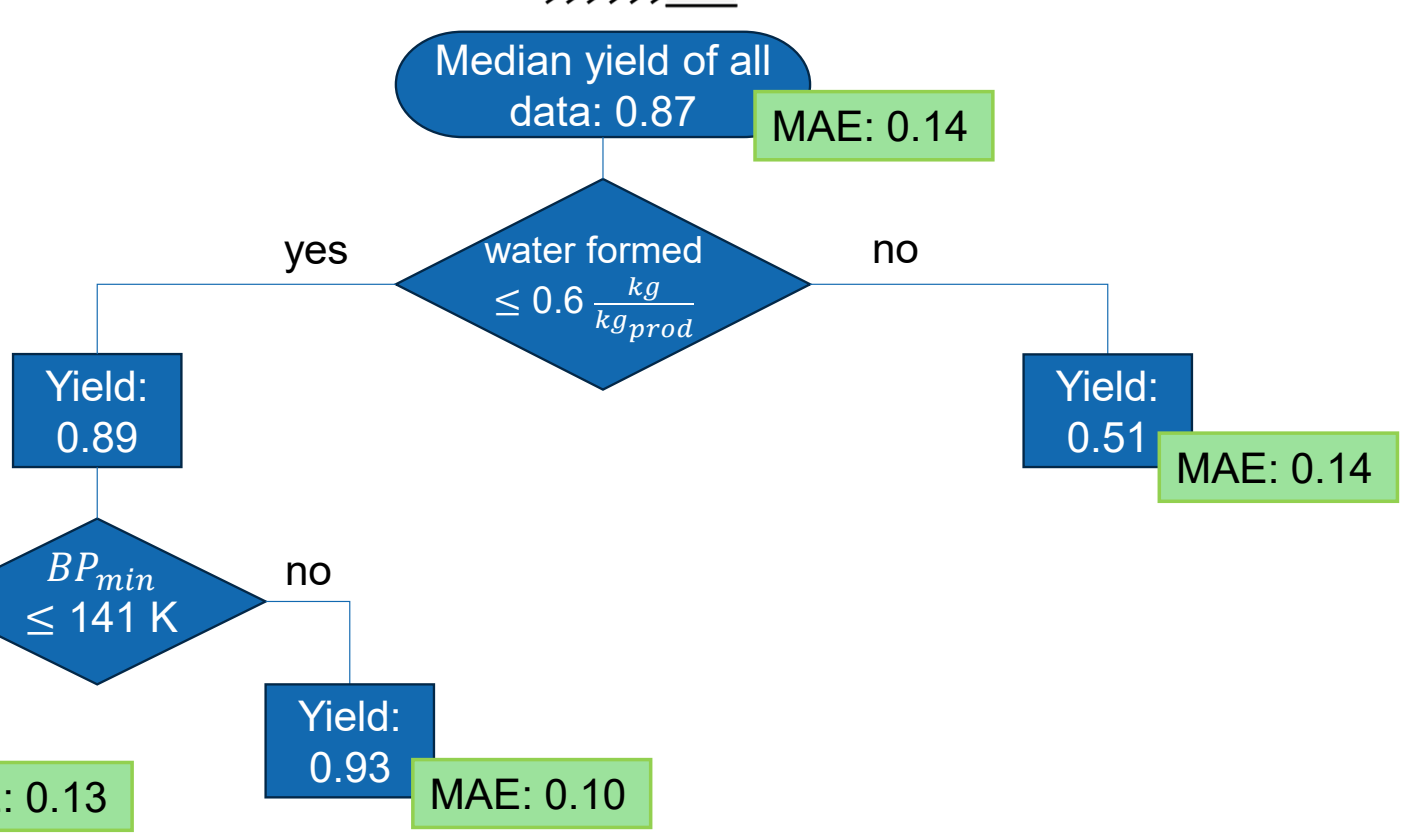
Example for reaction-based LCI prediction:



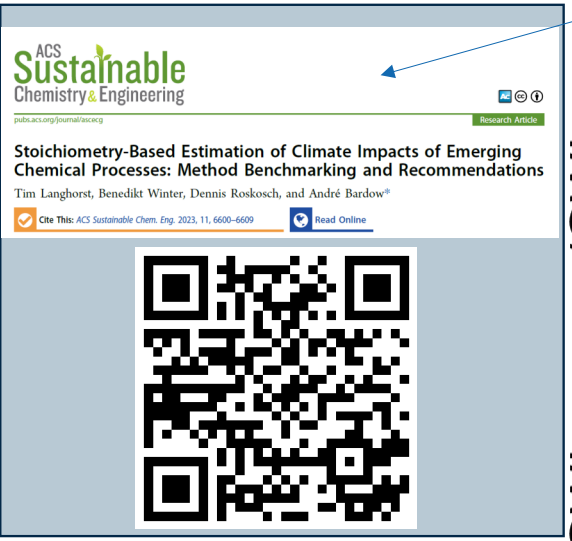
Regression trees = white boxes

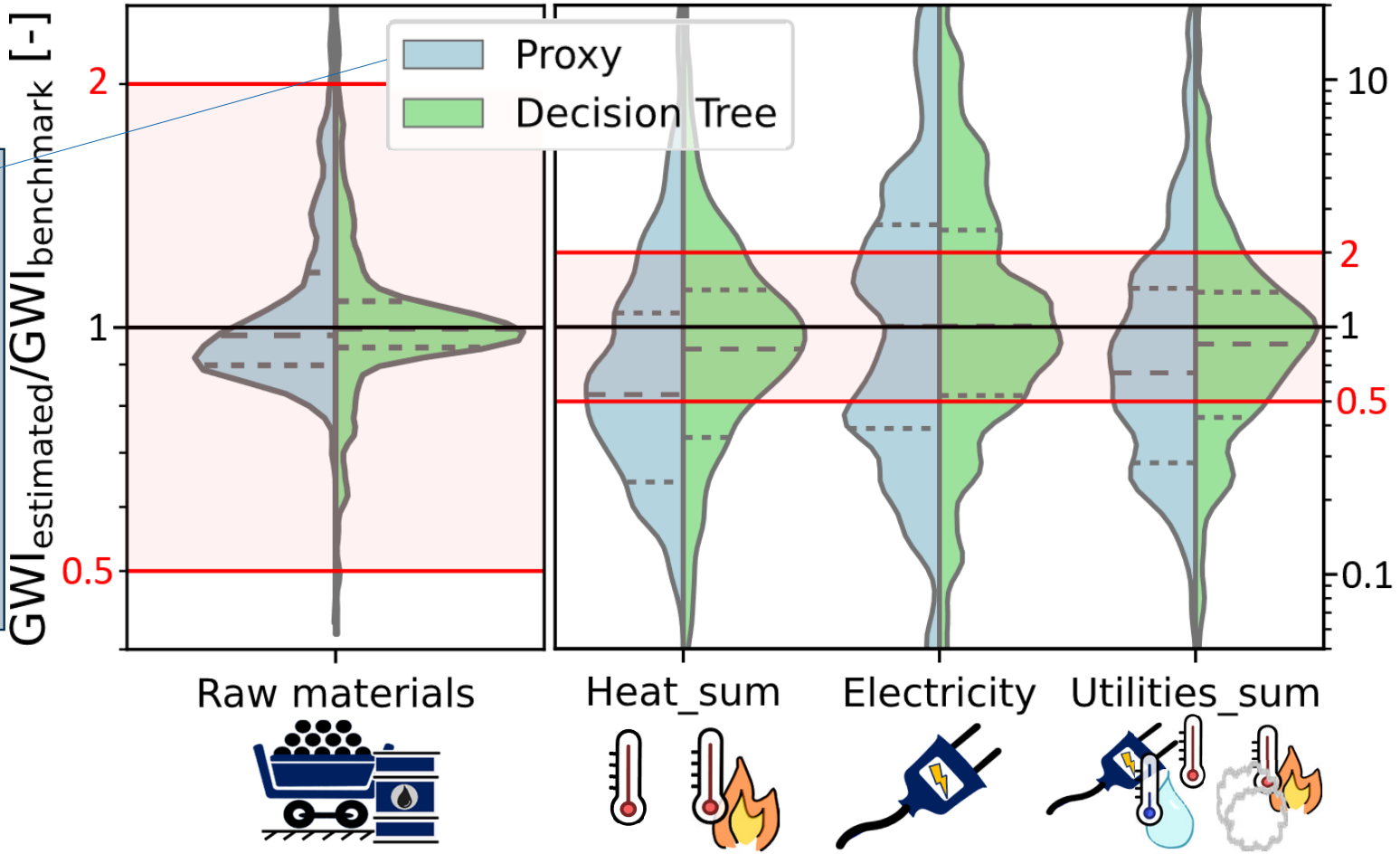


C1 chemistry or hydrogen



Results based on leave-one-out predictions





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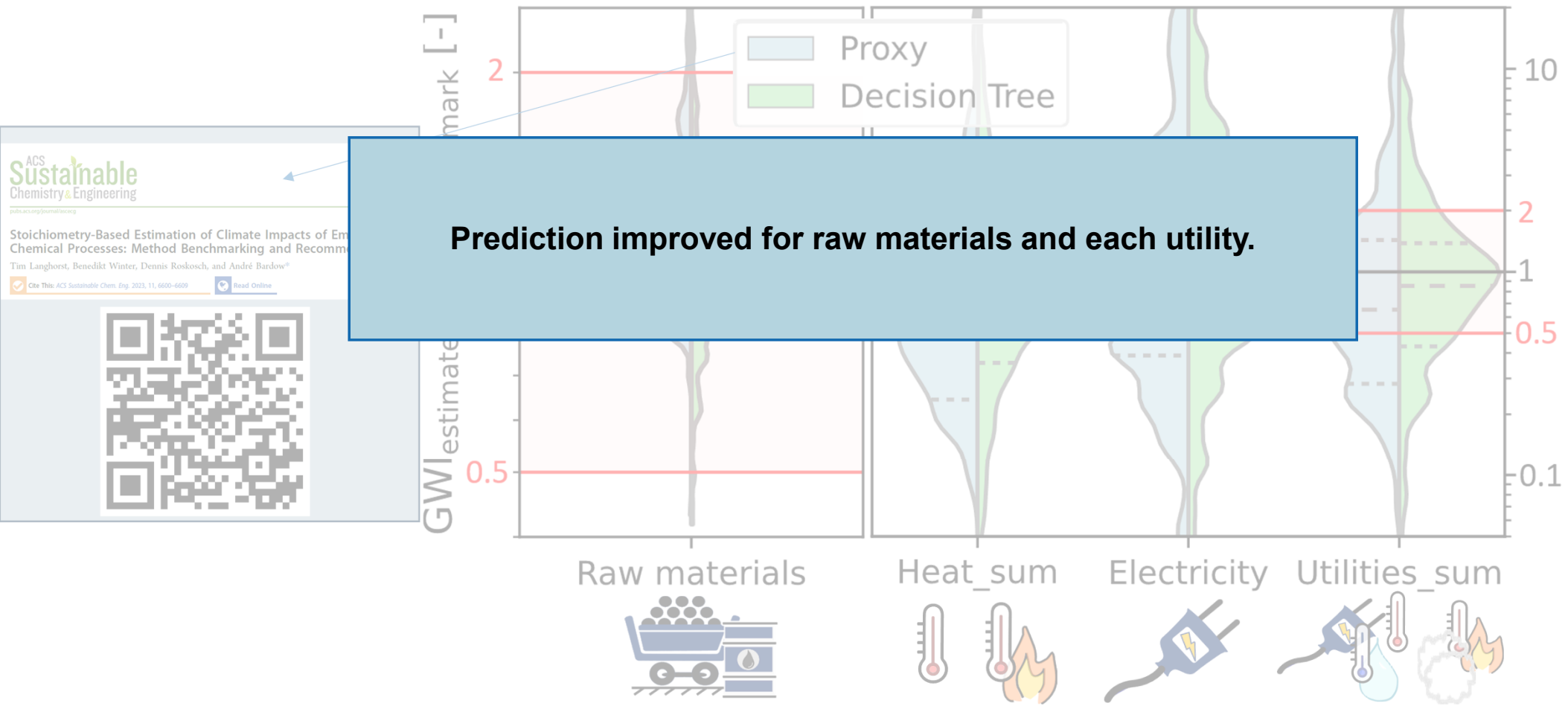
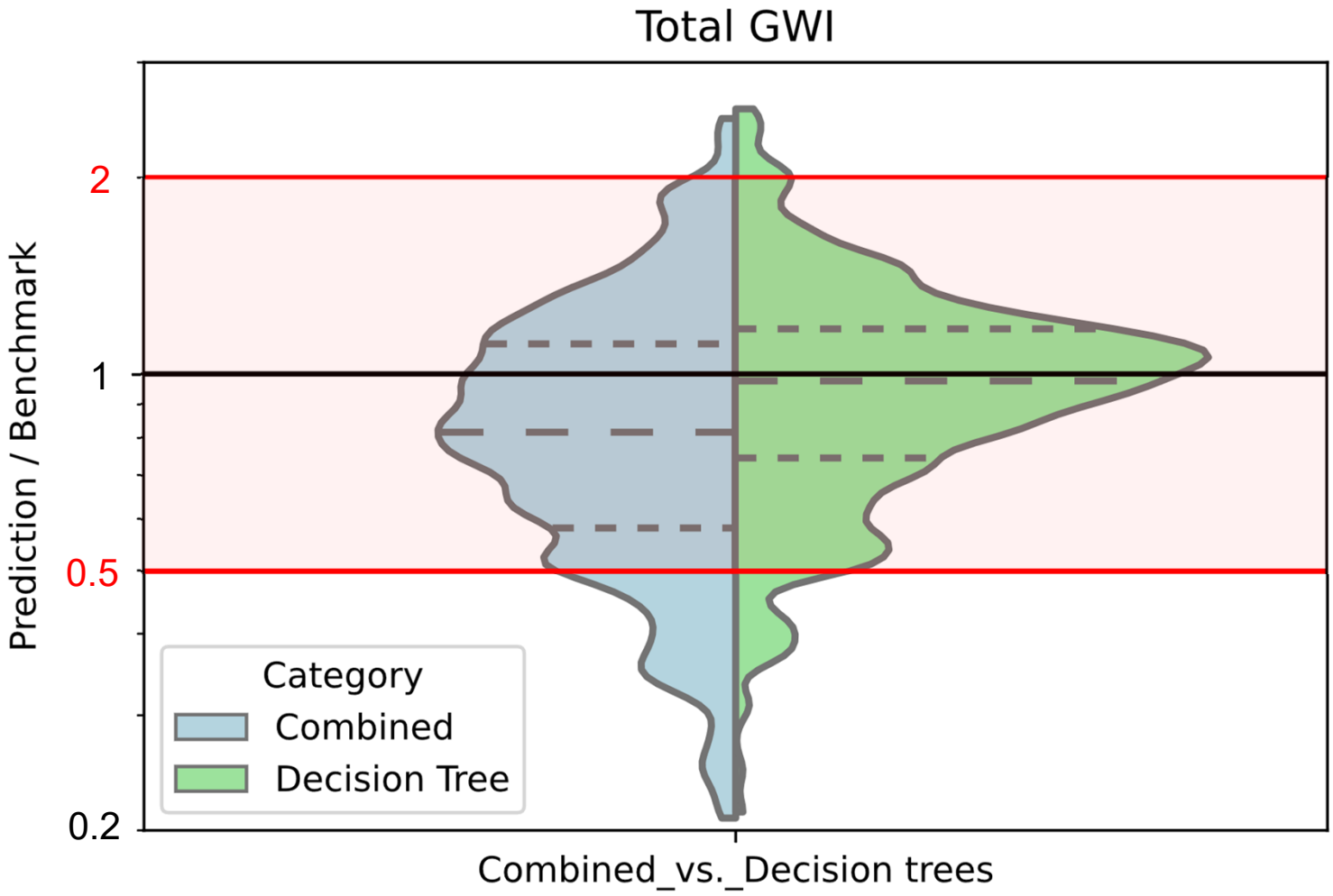


Prediction improved for raw materials and each utility.

Let’s combine the trees for a full inventory:



Summary

MSM are great for screening

- → Impacts are no molecular properties
- → MSM are limited

Workaround:

- → Look for process related properties
- → Predict mass and energy balances rather than impacts

Thank you for your attention!

Tim Langhorst
tim.langhorst@carbon-minds.com

Stay in touch:
www.carbon-minds.com
linkedin.com/in/tim-langhorst-b56817170

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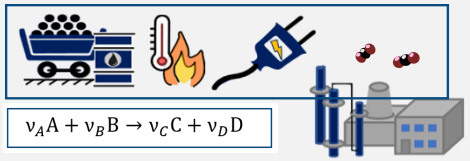
Prediction of LCIs: State-of-the-Art

Input

Stoichiometric equation

$$\nu_A A + \nu_B B \rightarrow \nu_C C + \nu_D D$$

Benchmark data [2, 3]



- 409 chemical processes
- Detailed inventories from the PEP yearbook
- Expanded to LCA needs

Prediction method

Best practice today:

- Default values, e.g., from averaged data

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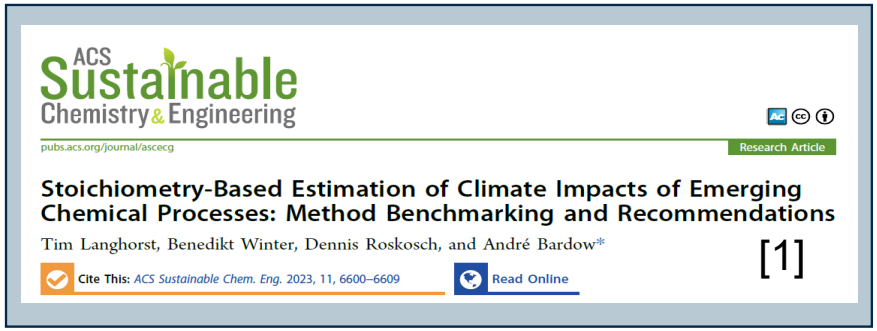
ACS Sustainable Chemistry & Engineering

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Research Article

Stoichiometry-Based Estimation of Climate Impacts of Emerging Chemical Processes: Method Benchmarking and Recommendations

Tim Langhorst, Benedikt Winter, Dennis Roskosch, and André Bardow*

Cite This: *ACS Sustainable Chem. Eng.* 2023, 11, 6600−6609 Read Online

[1]

Targets


yield


direct emissions


heat, steam


heat, natural gas


electricity


cooling & process water

[1] Langhorst T, Winter B, Roskosch D, Bardow A. Stoichiometry-Based Estimation of Climate Impacts of Emerging Chemical Processes: Method Benchmarking and Recommendations. ACS Sus Chem Eng. 2023. doi: 10.1021/acssuschemeng.2c07624

[2] Process Economics Programm Yearbook, S&P Global

[3] Kätelhön A, Meys R, Deutz S, Suh S, Bardow A. Climate change mitigation potential of carbon capture and utilization in the chemical industry. PNAS. 2019. doi: 10.1073/pnas.1821029116

From best practices to even better practices

Learnings from benchmarking

1. Distinguish between processes rather than using averaged proxies
2. Estimate LCIs rather than impacts
3. Provide target values and a measure for uncertainty

New prediction method

- Decision trees
- Regression with mean absolute error
- Only stoichiometry-based information
- **Reproducible and transparent**
- **Easy to use**