MOST-H2

Novel metal organic framework
adsorbents for efficient storage of hydrogen

MODELLING CHEMICALS IN OPENLCA

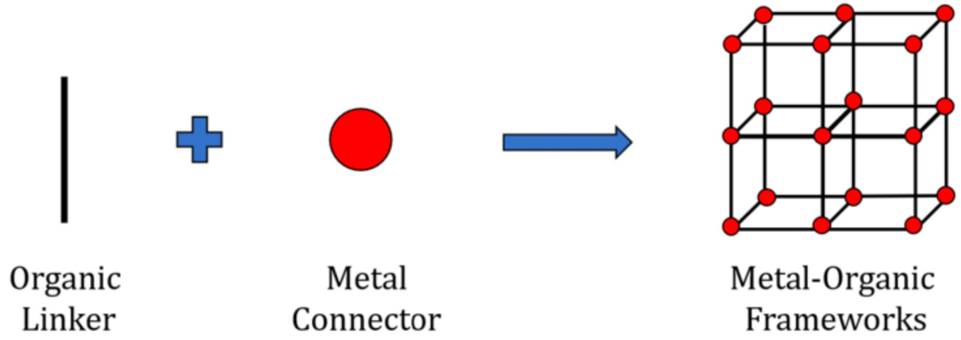
EXEMPLARY APPROACH BASED ON METAL-ORGANIC FRAMEWORKS

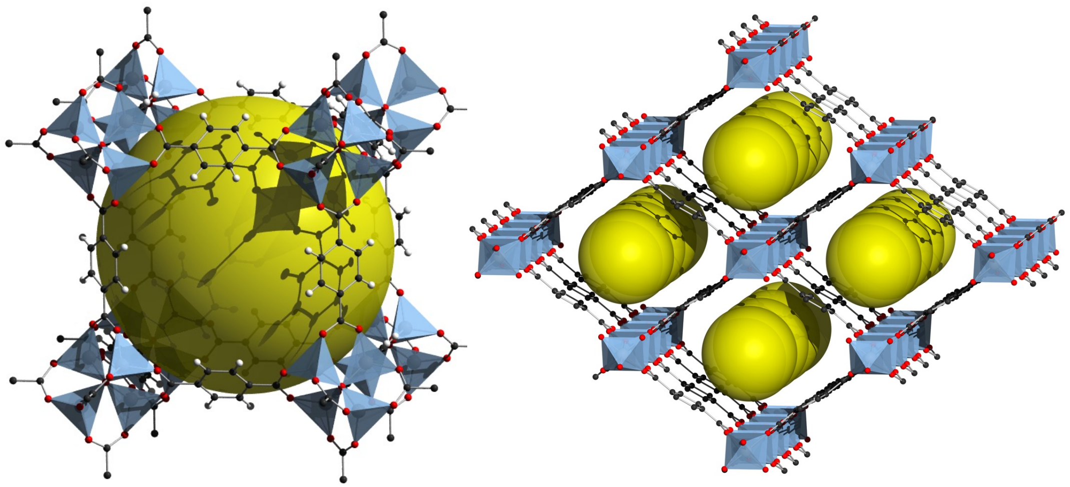
CONRAD SPINDLER

OPENLCA CONFERENCE

15.04.2024

METAL-ORGANIC-FRAMEWORK (MOF)





- “Lego”-structure with well-defined pores
- MOFs can store hydrogen with high capacities
- Only physical adsorption without chemical reaction

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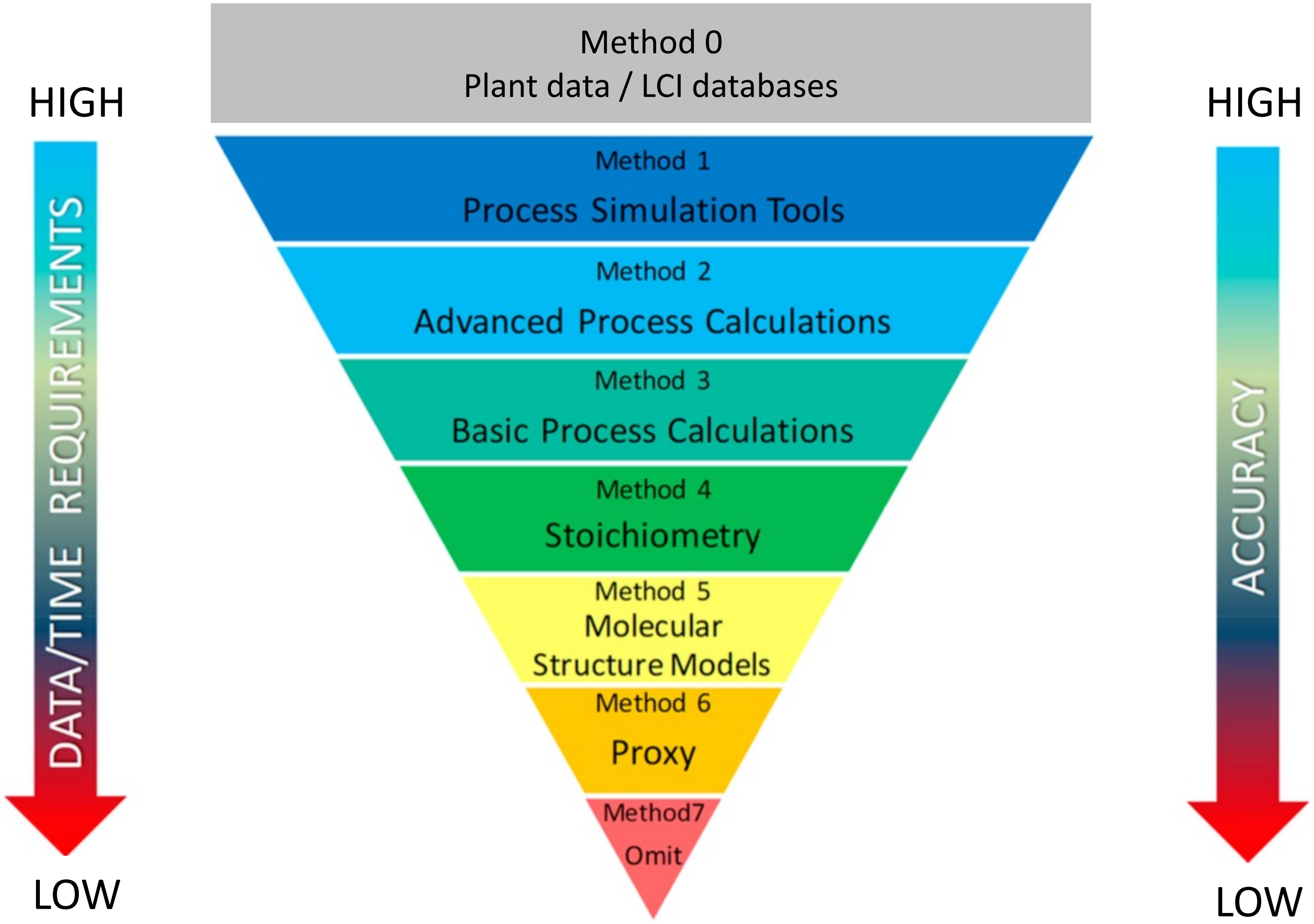
MODELLING MISSING CHEMICALS AND SYNTHESIS



[1] A. G. Parvatker and M. J. Eckelman, *ACS Sustainable Chemistry & Engineering* ***2019***, 7(1).
[2] R. Hischier et. al., *International Journal of Life Cycle Assessment* ***2005***, 10(1).

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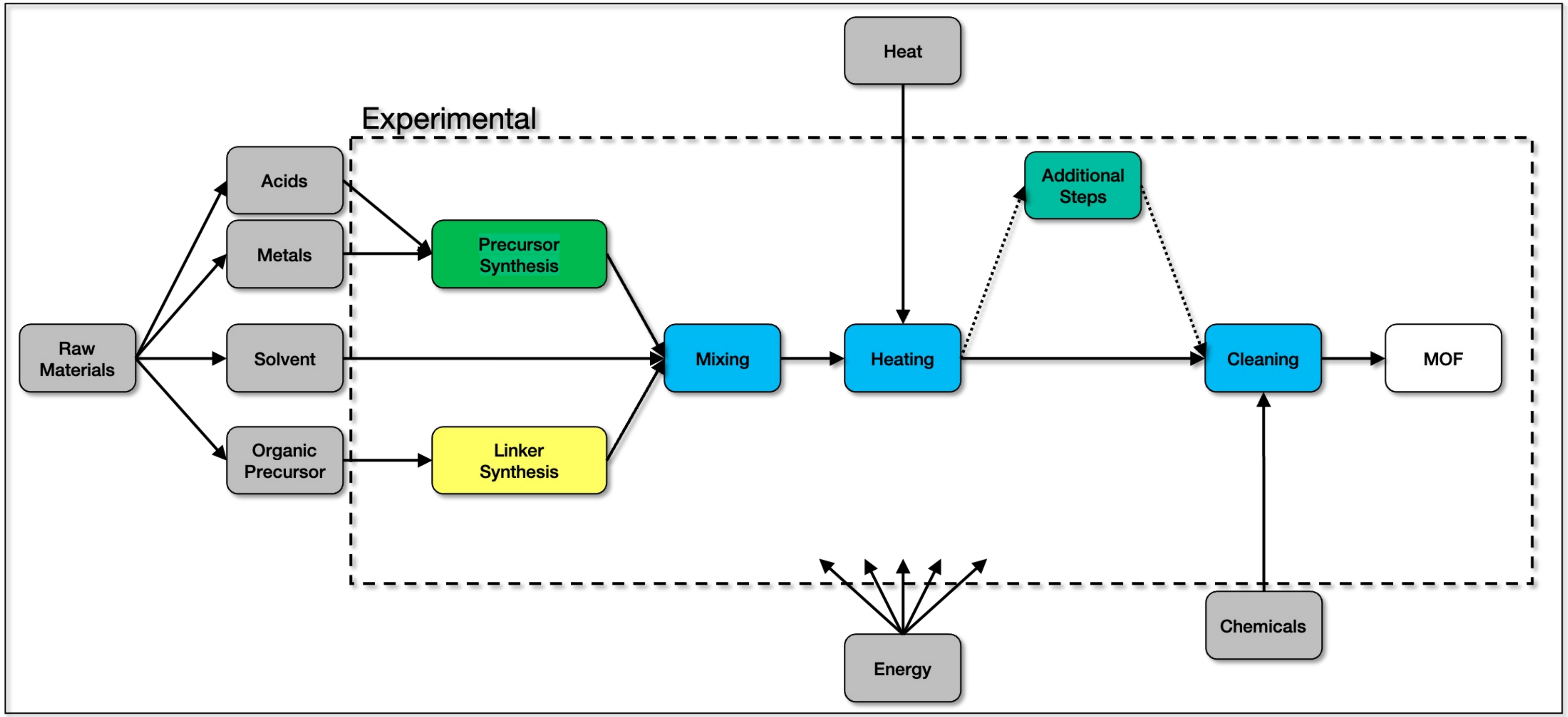
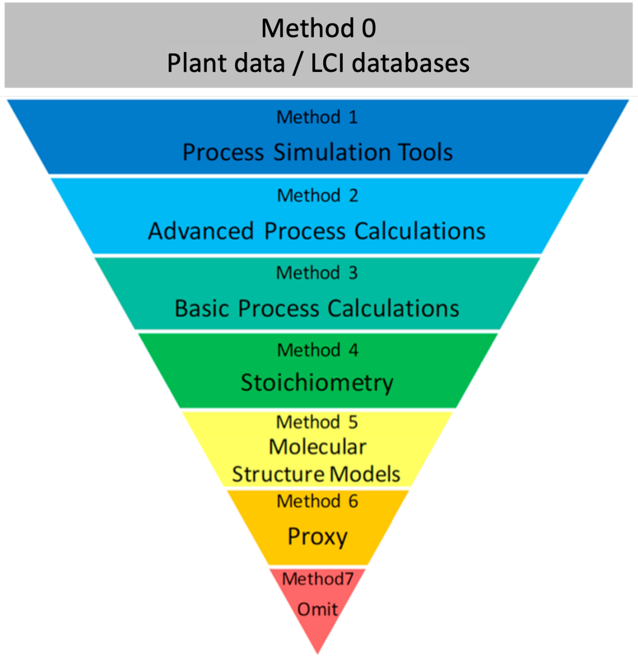
MODELLING MISSING CHEMICALS AND SYNTHESIS





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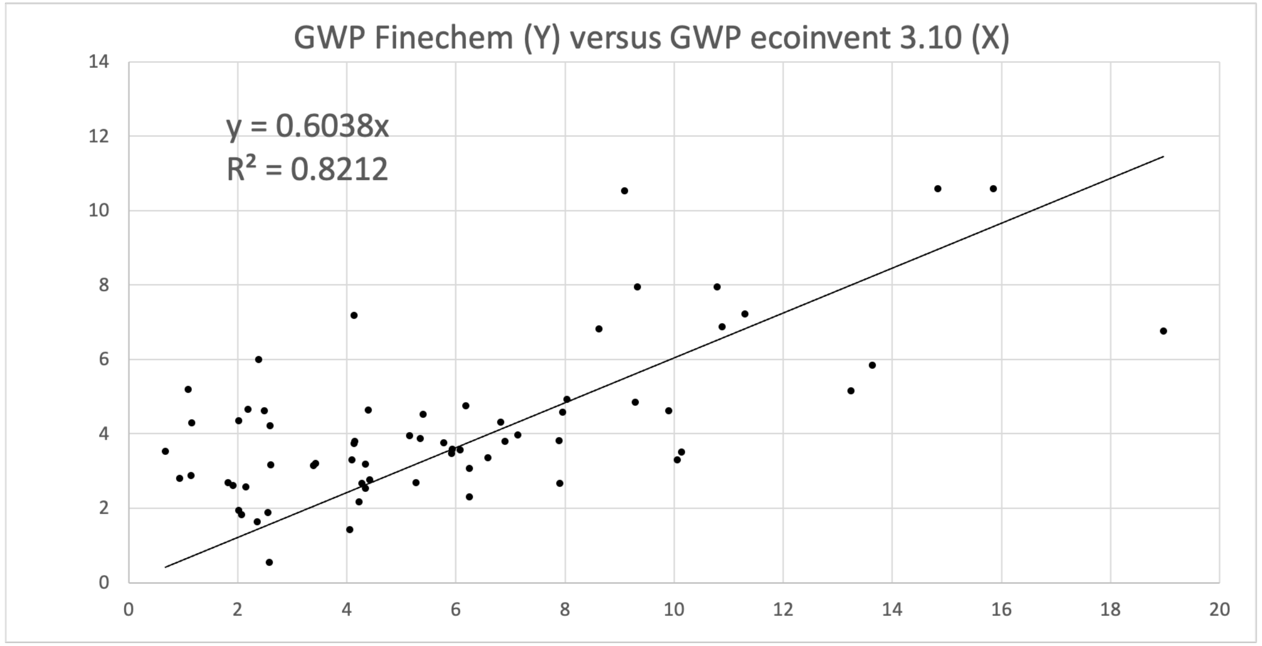
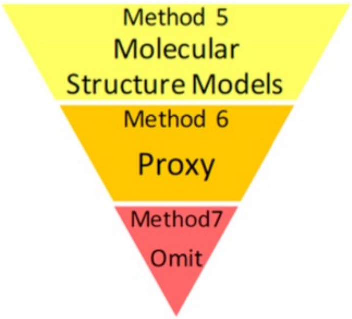
MOLECULAR STRUCTURE MODELS

- FineChem Tool as the most prominent molecular structure model [1]

- Be careful with the limits and the uncertainty from the models





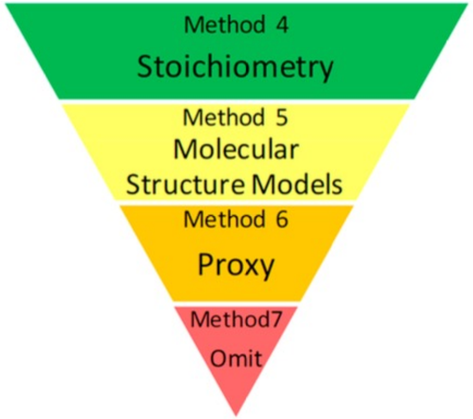
- FineChem2 from ETH Zurich is on the way to be published [2]

[1] G. Wernet et. al., *Green Chemistry* ***2009***, 11 (1826).
[2] D. Zhang et. al., *ACS Sustainable Chem. Eng.* ***2024***, 12 (2007).

MODELLING STOICHIOMETRY IN OPENLCA

- Example for MOFs is the production of metals salts = metal + acid
- Always good practice to parametrize models in openLCA

1. Add chemical equation with stoichiometric molecular masses
2. Add proxy for energy (often 2 MJ heat and 0.33 kWh electricity used)
3. Add proxy for yield (often 95 % is used)
4. Add proxy for factory (often 4E-10 items is used)



MODELLING STOICHIOMETRY IN OPENLCA

Inputs/Outputs: Sodium nitrate production

Inputs

Flow	Amount	Unit	Description
chemical factory, organics	4.00000E-10	Item(s)	General proxy
electricity, medium voltage	0.33000	kWh	General proxy
heat, district or industrial, natural gas	2.00000	MJ	General proxy
nitric acid, without water, in 50% solution state	2 * mol_HNO3	kg	Chemical synthesis standard reaction equation
soda ash, dense	1 * mol_Na2CO3	kg	Chemical synthesis standard reaction equation
water, deionised	2 * mol_HNO3	kg	Chemical synthesis standard reaction equation

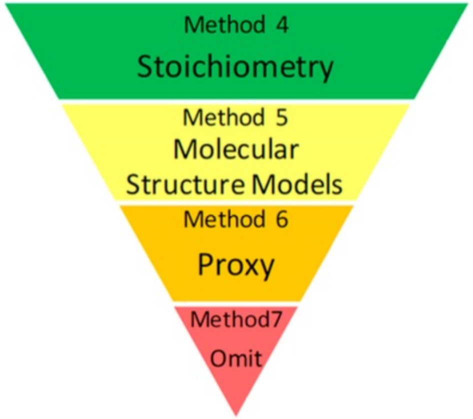
Outputs

Flow	Amount	Unit	Description
sodium nitrate	**2 * mol_NaNO3**	**kg**	**Chemical synthesis standard reaction equation**
wastewater, average	1 * mol_H2O	m3	Chemical synthesis standard reaction equation
Carbon dioxide, fossil	1 * mol_CO2	kg	Chemical synthesis standard reaction equation

Notes:
- "Water, deionised" added with same amount as the acid (50% solution)
- The amount could be added to the wastewater to keep mass balance
- Waste heat sometimes added to the output to keep energy balance
- Small proxy residues of 0.2% input material could be added to the output
- Yield in this example is 100%

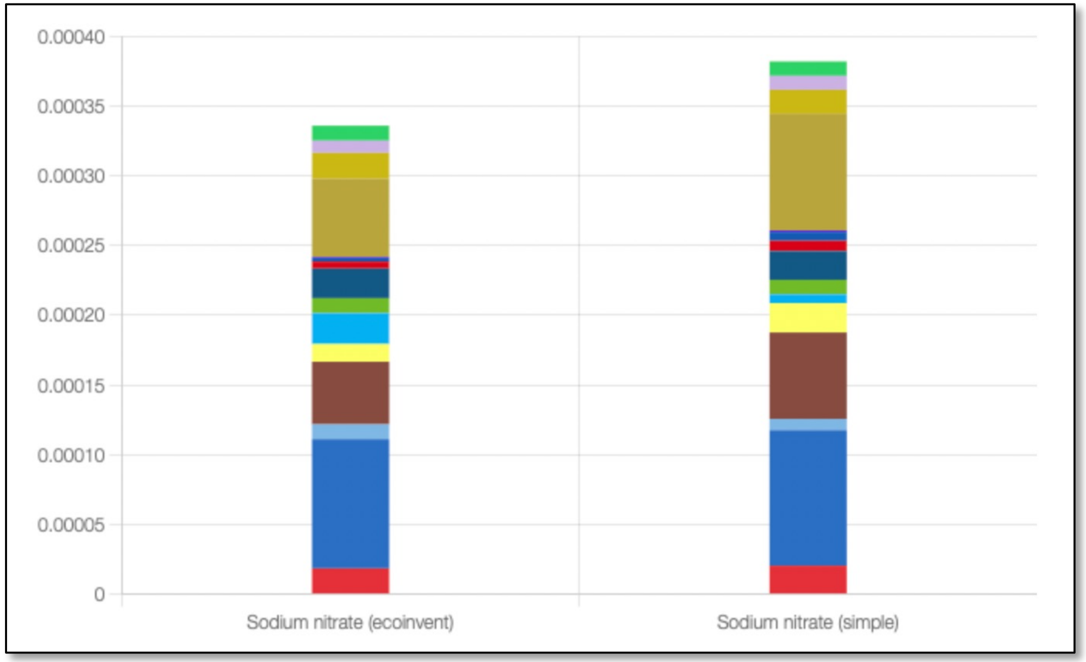
Input parameters

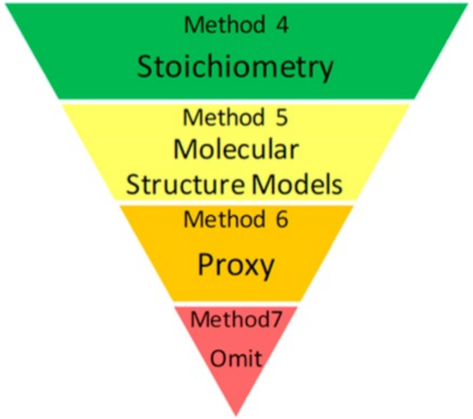
Name	Value	Description
Mol_CO2	0.044	kg / mol
Mol_H2O	1.8E-5	m3 / mol
Mol_HNO3	0.063	kg / mol
Mol_Na2CO3	0.106	kg / mol
Mol_NaNO3	0.085	kg / mol



MODELLING STOICHIOMETRY IN OPENLCA

EF 3.1 Single score comparison for sodium nitrate





MODELLING PROCESS CALCULATIONS IN OPENLCA

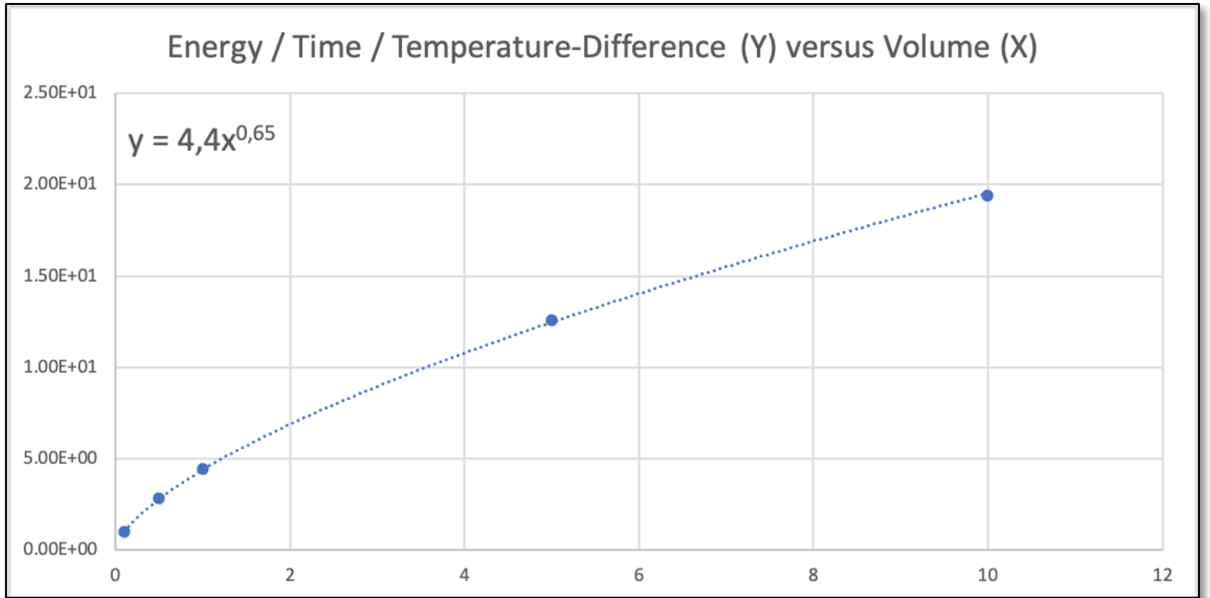
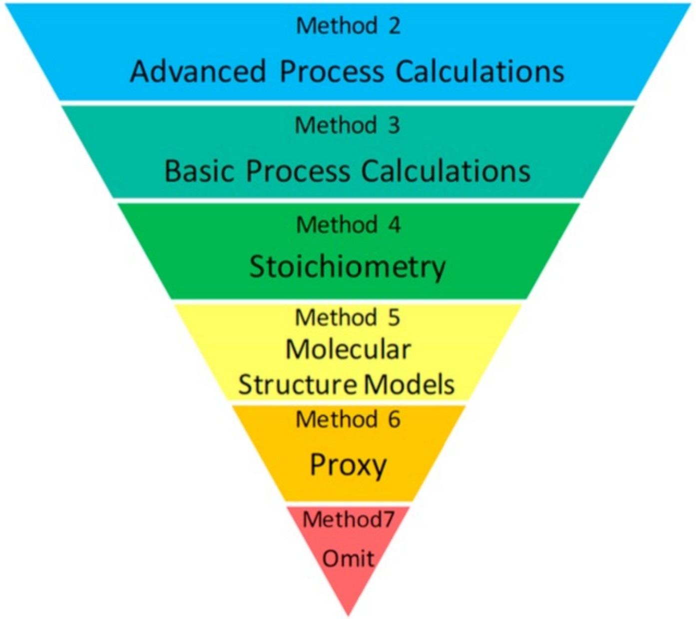


Table 2
Suggested scale-dependent data for the calculation of heating energy.

Physical entity	Symbol	Unit	100 l	500 l	1′000 l	5′000 l	10′000 l
Reaction mixture volume	$V_{(mix)}$	m^3	0.1	0.5	1	5	10
Height of reactor	L	m	0.519	0.888	1.119	1.913	2.410
Diameter of reactor	D	m	0.519	0.888	1.119	1.913	2.410
Surface area	A	m^2	1.271	3.716	5.899	17.249	27.381
Reactor volume	$V_{(reactor)}$	m^3	0.11	0.55	1.1	5.5	11
Insulation material	–	–	Glass fiber	Glass fiber	Glass fiber	Glass fiber	Glass fiber
Thermal conductivity of insulation	k_a	$\frac{W}{m*K}$	0.042	0.042	0.042	0.042	0.042
Insulation thickness	s	m	0.075	0.075	0.075	0.075	0.075
Heat transfer coefficient of insulation	k_a/s	$\frac{W}{m^2*K}$	0.56	0.56	0.56	0.56	0.56
Efficiency of heating element	η_{heat}	%	72%	74%	75%	77%	79%
Impeller diameter	d	m	0.173	0.296	0.373	0.638	0.803
Rate of heat loss per Kelvin	$\frac{A*k_a}{s}$	$\frac{W}{K}$	0.712	2.081	3.303	9.659	15.333
Starting and outside temperature	$T_0 = T_{out}$	K	298.15	298.15	298.15	298.15	298.15



[1] F. Piccinno et. al., *Journal of Cleaner Production* ***2016***, 135(1085).

MODELLING PROCESS CALCULATIONS IN OPENLCA

Parameters: Service | Heating

Global parameters

Input parameters

Name	Value	Description
A	4.4	power law amplitude (constant)
k	0.65	power law coefficient (constant)
t	3600.0	heating time [s]
T0	20.0	room temperature outside reactor [°C]
Tr	130.0	reactor temperature [°C]
V	0.2	heating volume [m3]

Dependent parameters

Name	Formula	Value	Description
energy	A * V^k * t * dT	612092.9249235917	heating energy [J]
dT	Tr - T0	110.0	temperature difference (K)

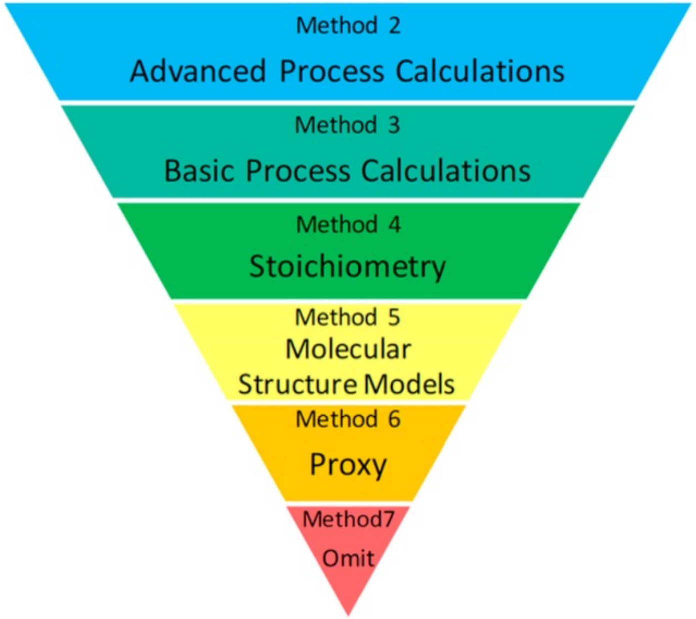
Inputs/Outputs: Service | Heating

Inputs

Flow	Amount	Unit
heat, district or industrial, natural gas	energy	J

Outputs

Flow	Amount	Unit
Service | Heating	**V**	**m3**



KEY TAKE AWAYS

System process

Sodium nitrate production

Inputs

Name	Amount	Unit
Aluminium	0.00075	kg
Anhydrite	4.20137E-10	kg
Antimony	8.94323E-10	kg
Argon	4.54888E-5	kg
Arsenic	3.82372E-8	kg
Barium	0.00062	kg
Basalt	0.00019	kg
Beryllium	0.00000	kg
Borax	6.07889E-11	kg
Boron	5.83011E-7	kg
Bromine	1.12587E-8	kg

Outputs

Name	Amount	Unit
1,1,1,2-Tetrafluoroethane	6.38007E-10	kg
1,1,1,2-Tetrafluoroethane	1.35178E-11	kg
1,1,1,2-Tetrafluoroethane	6.71778E-10	kg
1,1,1-Trichloroethane	9.27457E-21	kg
1,1,1-Trichloroethane	9.52946E-11	kg
1,1,1-Trichloroethane	1.65353E-12	kg
1,1,1-Trichloroethane	1.44289E-13	kg
1,1,1-Trifluoroethane	0.00000	kg
1,1,1-Trifluoroethane	1.20407E-35	kg
1,1,2-Trichloro-1,2,2-trifluoroethane	5.63429E-11	kg
1,1,2-Trichloro-1,2,2-trifluoroethane	1.05391E-10	kg

Unit process

Inputs/Outputs: Sodium nitrate production

Inputs

Flow	Amount	Unit
chemical factory, organics	4.00000E-10	Item(s)
electricity, medium voltage	0.33000	kWh
heat, district or industrial, natural gas	2.00000	MJ
nitric acid, without water, in 50% solution state	0.12602	kg
soda ash, dense	0.10599	kg
water, deionised	0.12602	kg

Outputs

Flow	Amount	Unit
sodium nitrate	**0.16999**	**kg**
wastewater, average	1.80153E-5	m3
Carbon dioxide, fossil	0.04401	kg

Unit process + model method

Inputs/Outputs: Sodium nitrate production

Inputs

Flow	Amount	Unit
chemical factory, organics	4.00000E-10	Item(s)
electricity, medium voltage	0.33000	kWh
heat, district or industrial, natural gas	2.00000	MJ
nitric acid, without water, in 50% solution state	2 * mol_HNO3	kg
soda ash, dense	1 * mol_Na2CO3	kg
water, deionised	2 * mol_HNO3	kg

Outputs

Flow	Amount	Unit
sodium nitrate	**2 * mol_NaNO3**	**kg**
wastewater, average	1 * mol_H2O	m3
Carbon dioxide, fossil	1 * mol_CO2	kg

Dependent parameters

Name	Formula	Value	Description
energy	A * V^k * t * dT	612092.9249235917	heating energy [J]
dT	Tr - T0	110.0	temperature difference (K)

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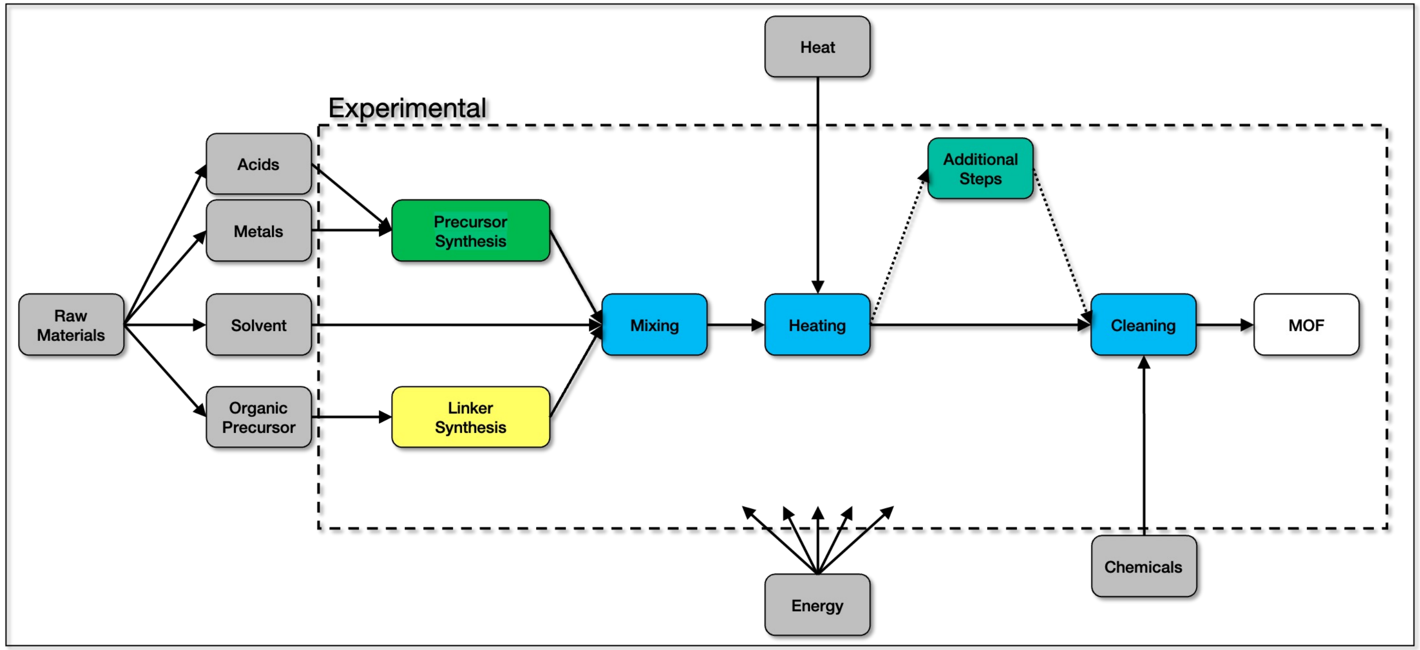
THANK YOU FOR YOUR ATTENTION



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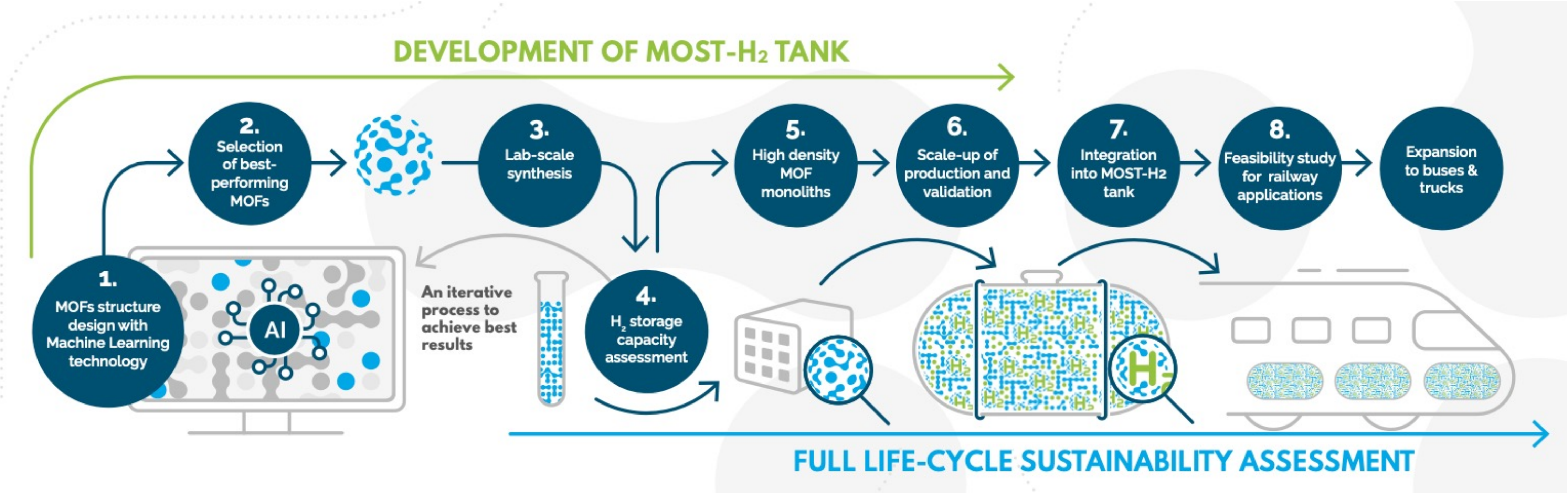
PROJECT OBJECTIVES



PROJECT PARTNERS

Project Partners

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