



Simulation-based Optimization of Mass Transport Processes in Thermal Drying in the Recycling Process of Lithium-Ion Batteries

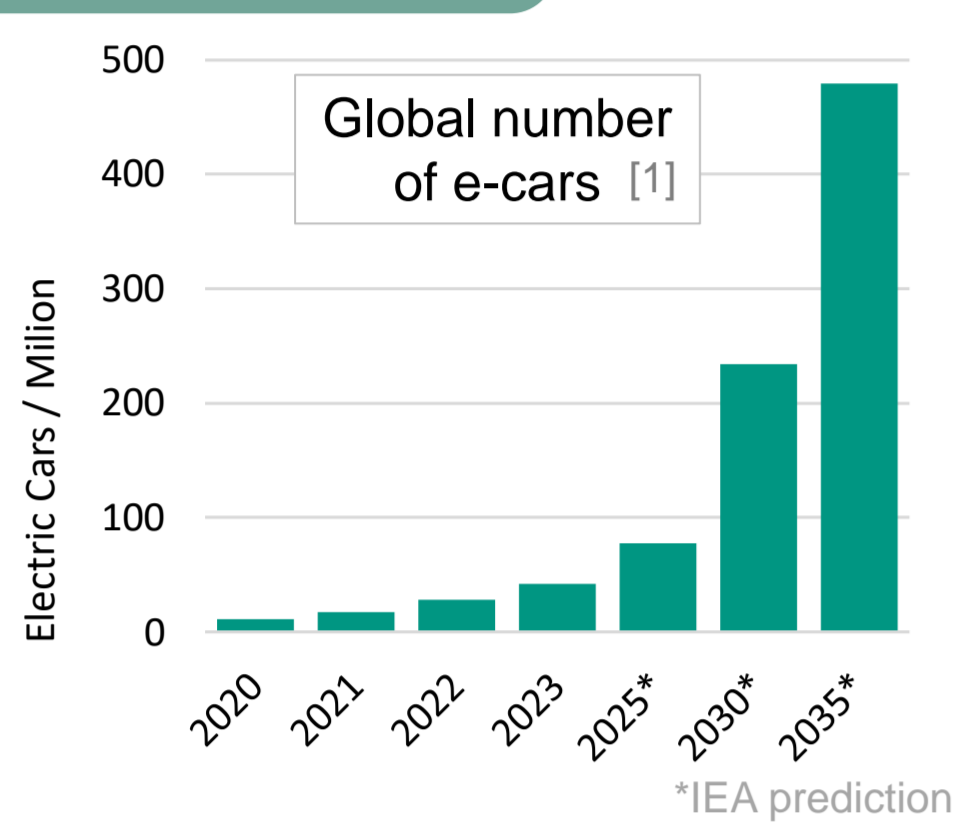
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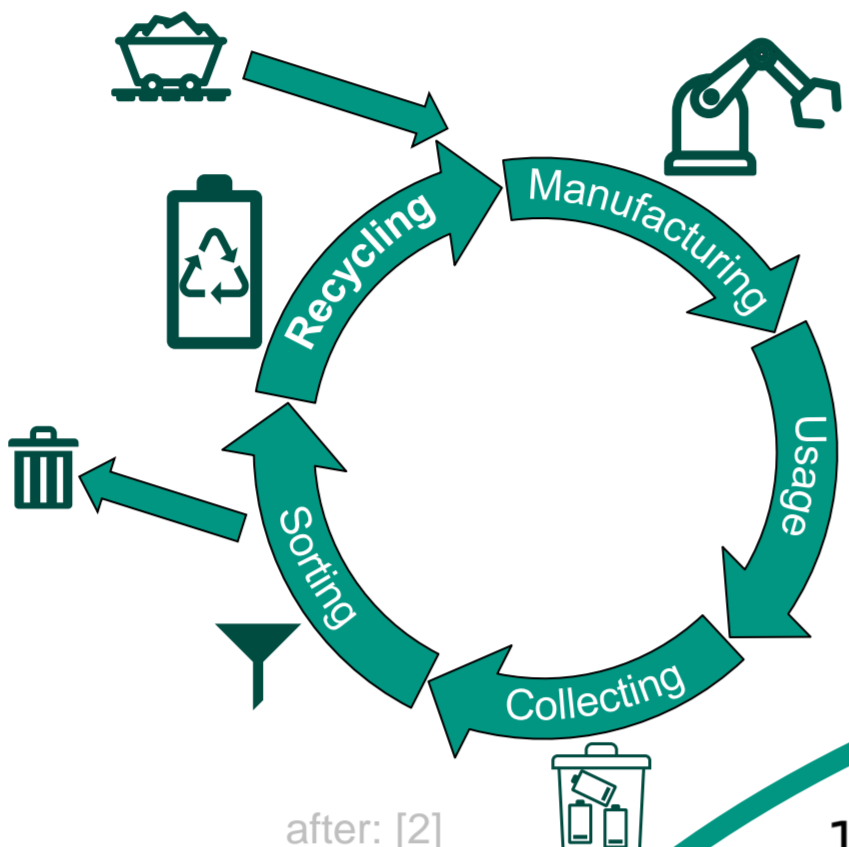
Lab-scale thermal drying model developed

Motivation

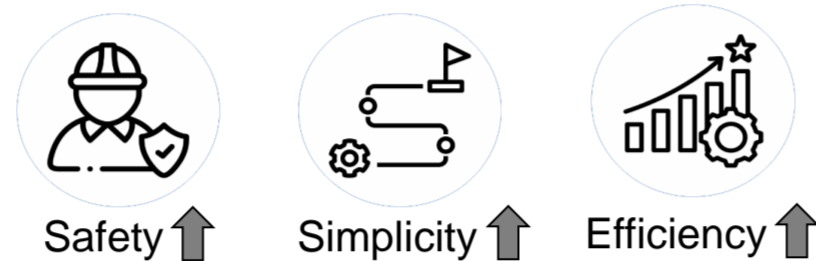


Key challenges

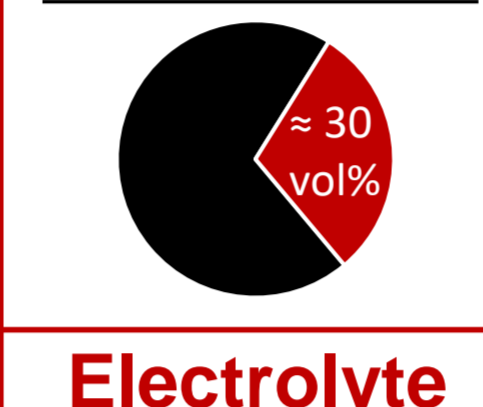
- Material cost and shortage
- Recovery rates by legislation



Recycling in Circular economy



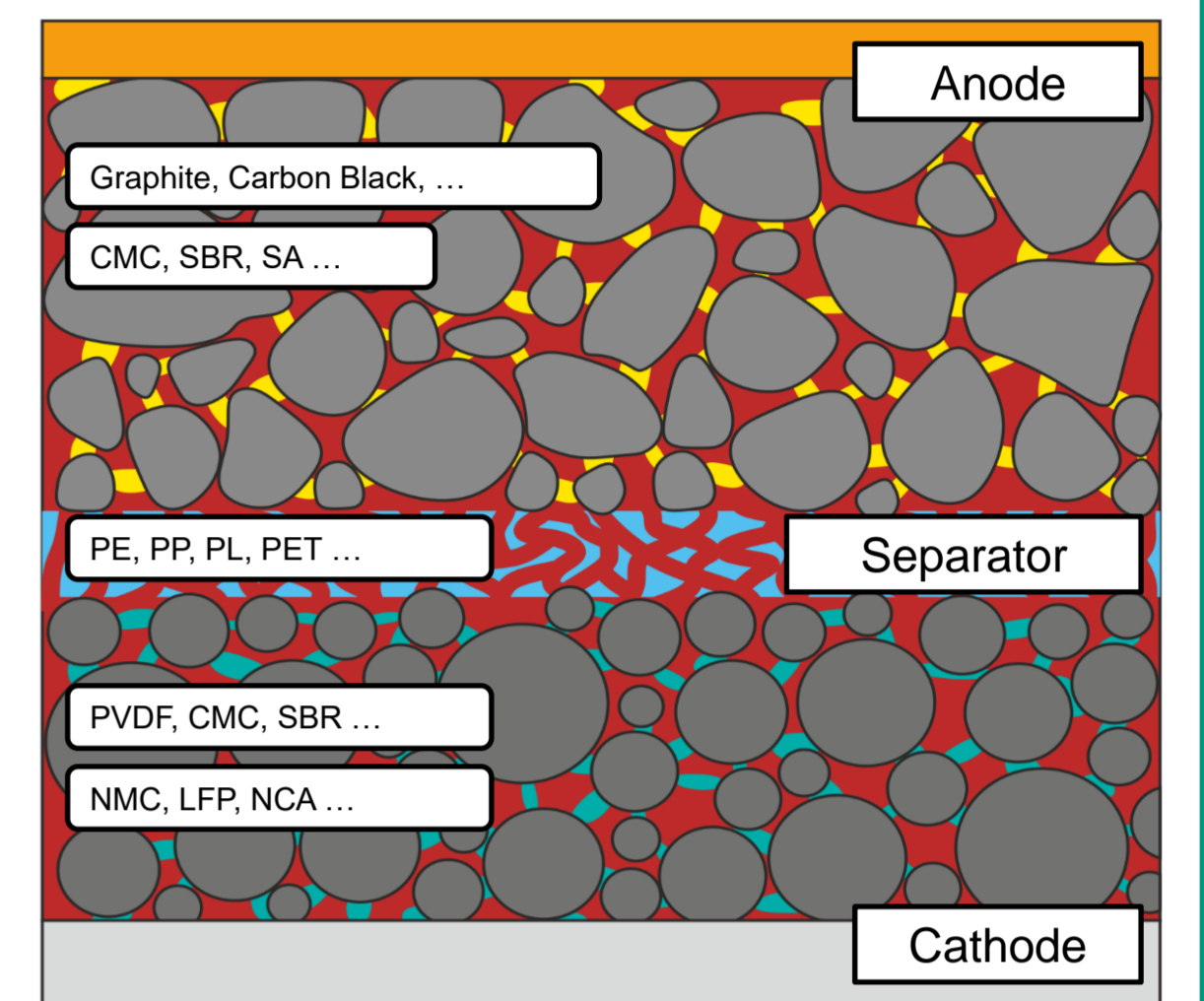
Share on cell level



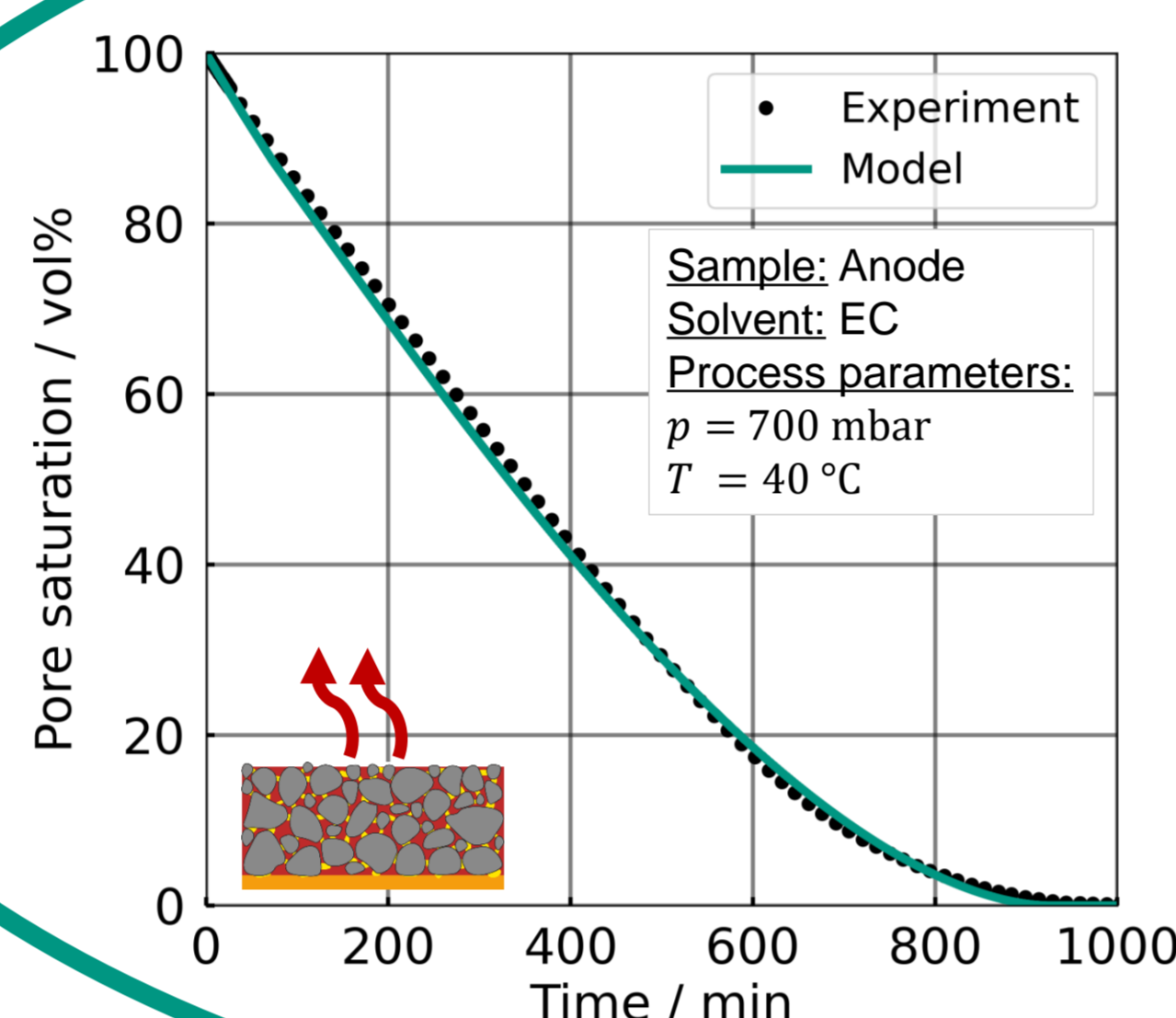
Key electrolyte solvents

Boiling temperature $T_B / ^\circ\text{C}$	Molar mass $\bar{M} / \text{g mol}^{-1}$
DMC	~72
EMC	~84
DEC	~108
EC	~74

Components

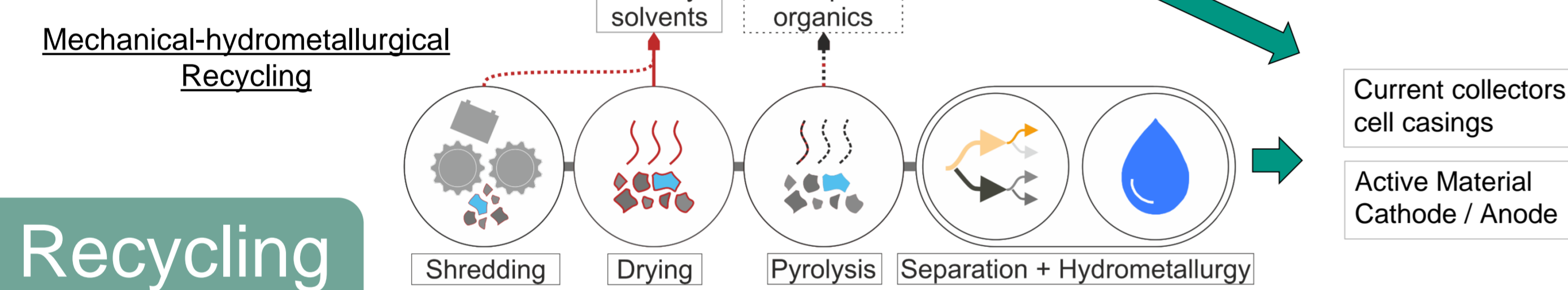
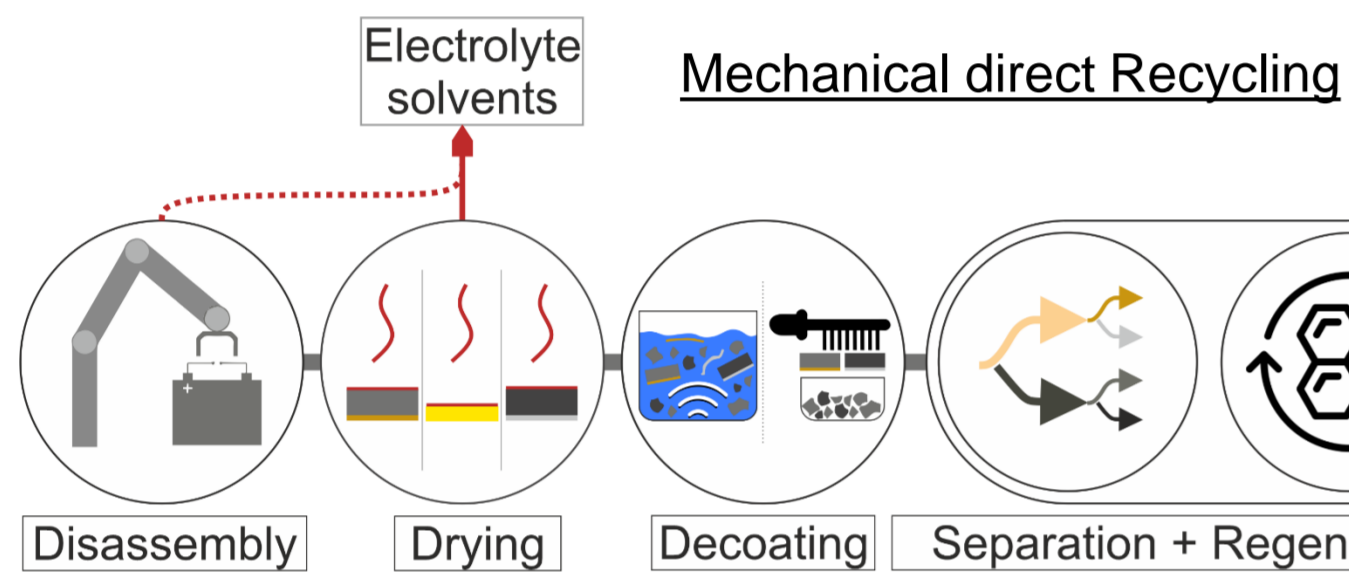


Achievements

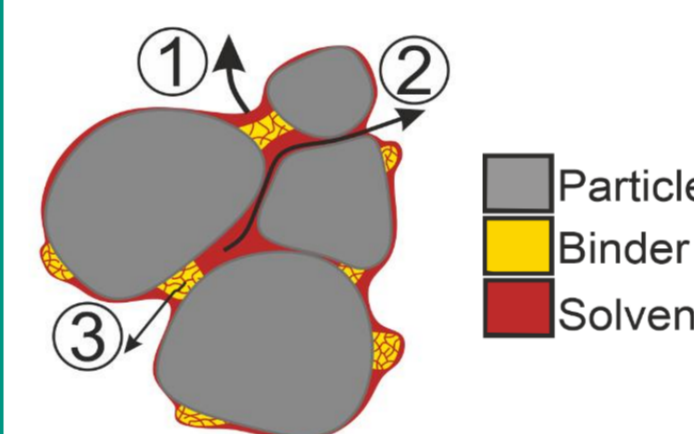
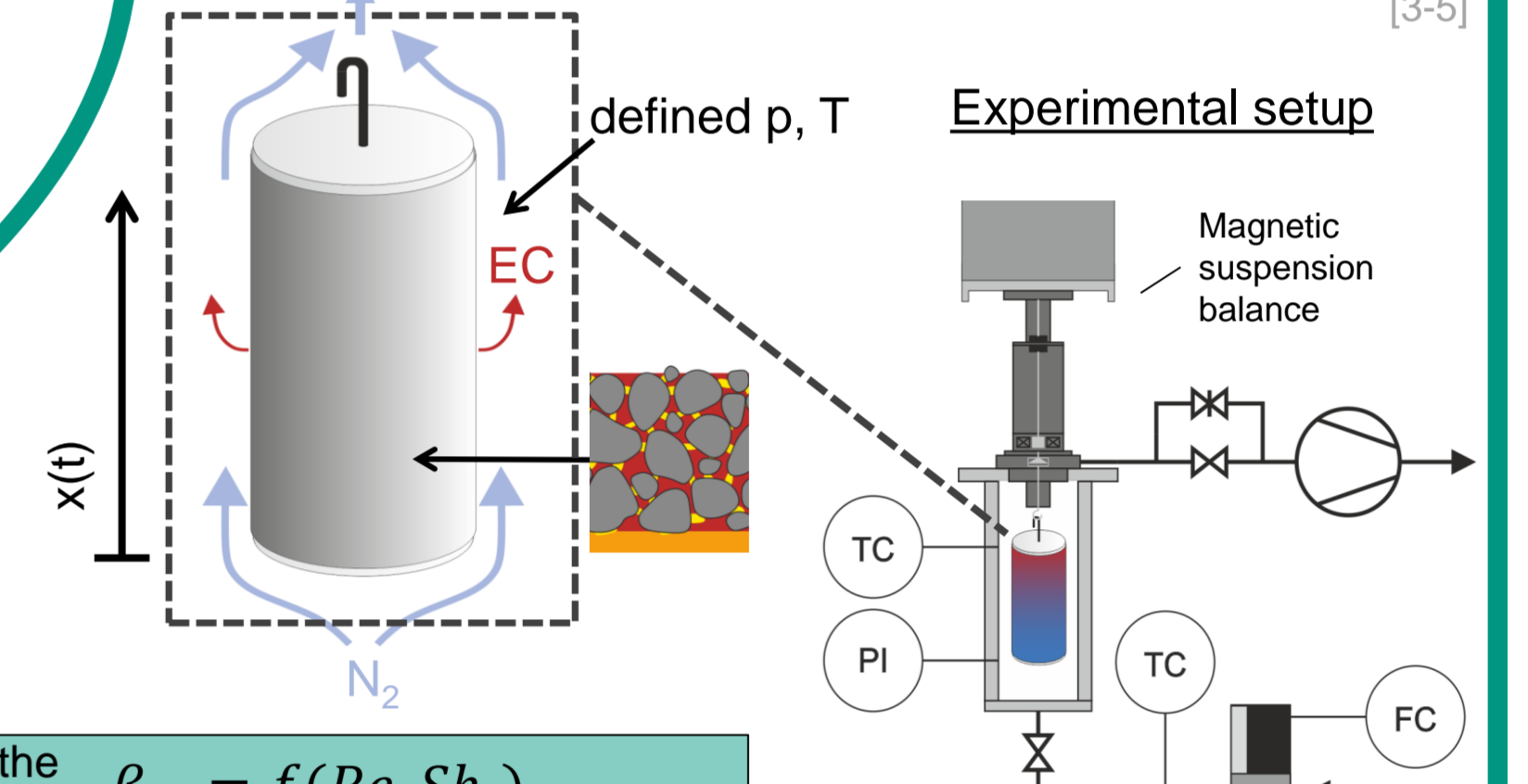


- Mass transport model
- Validation through experiments in a magnetic suspension balance

- Hazard of health damage, fire, explosion, ...
- Adverse effects on various downstream processes



Recycling

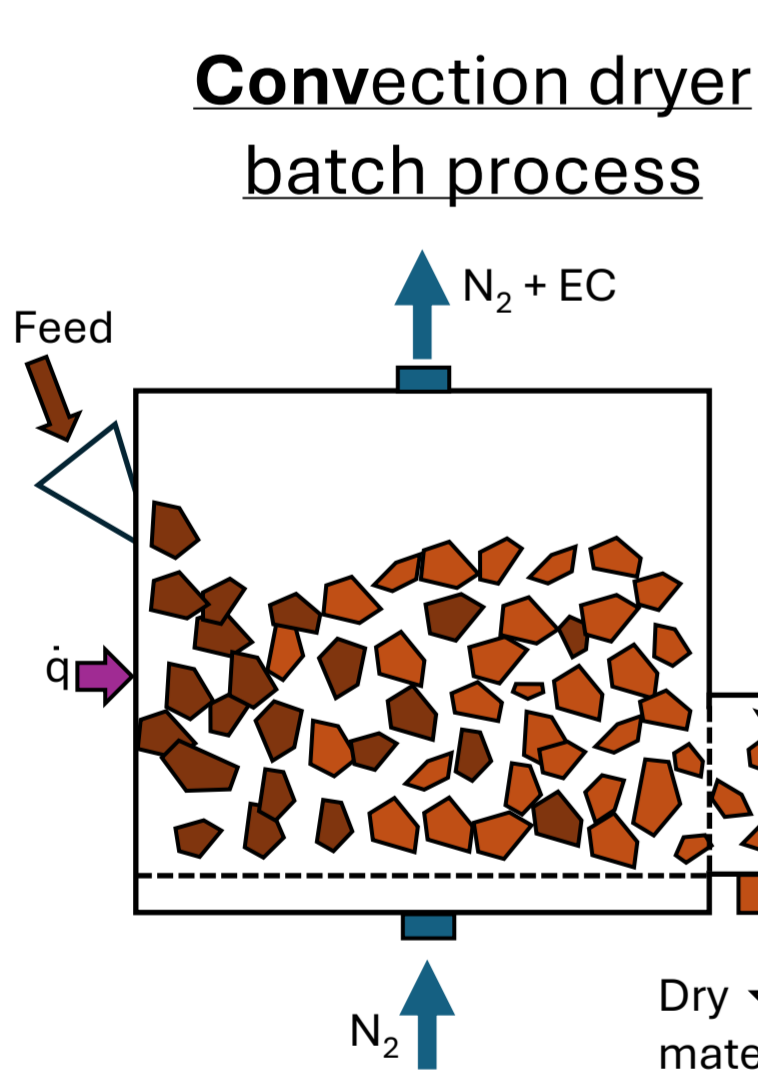


- 1 Mass transport in the external gas phase $\beta_{i,g} = f(Re, Sh_i)$
- 2 Mass transport in the porous network $\delta_{i,eff} = f(T, p, \epsilon, \tau, d_{pore})$
- 3 Mass transport in absorbing materials $D_{i,j} = f(T, X_{solvent})$

Mass transport

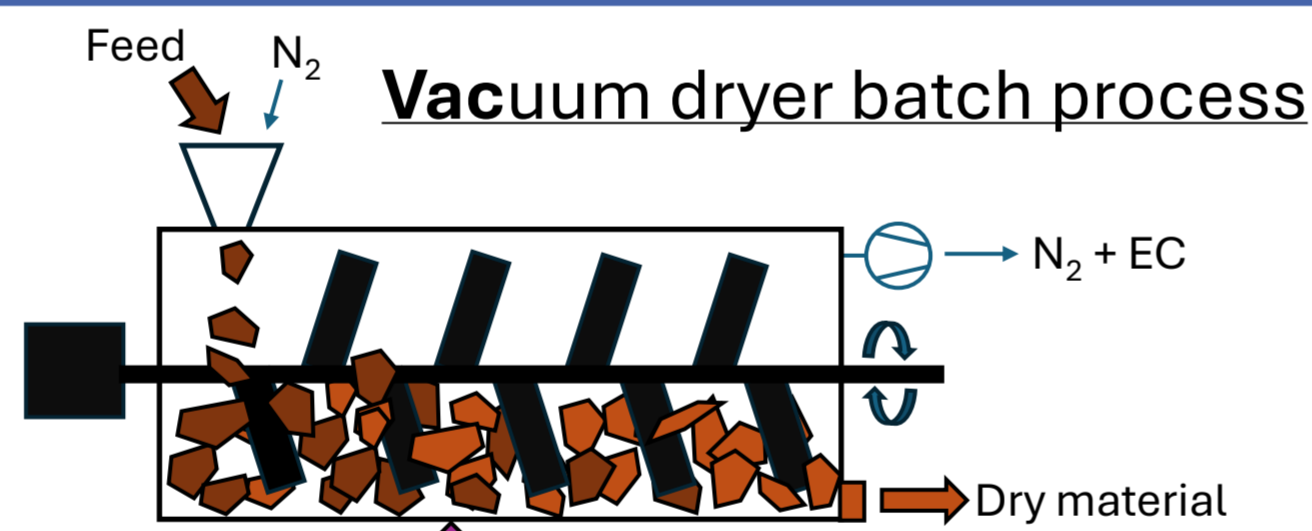
Transition to a real-application thermal drying model – a parameter study

Dryer



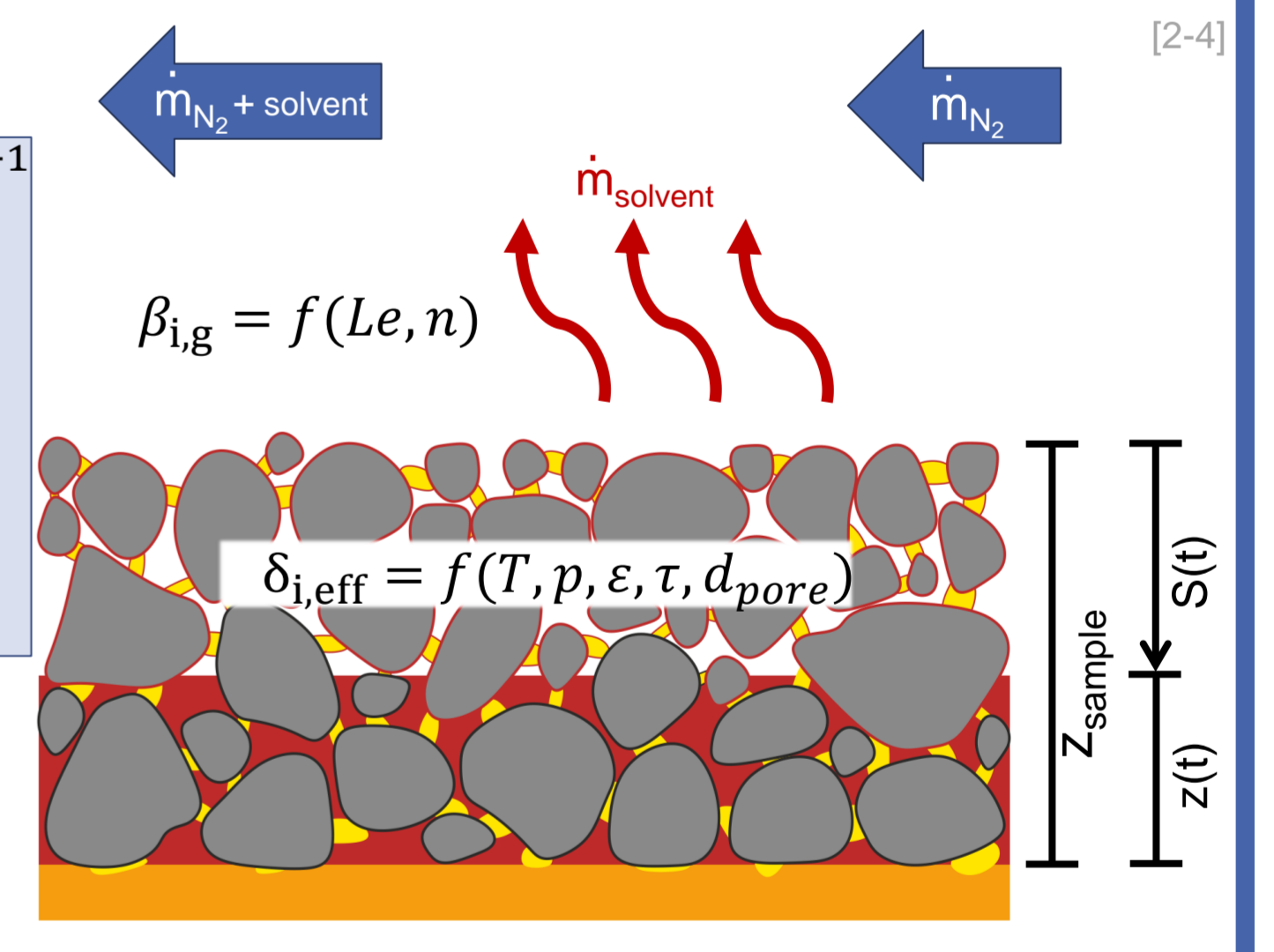
Default parameters	Conv.	Vac.
p / mbar	1000	50
$T / ^\circ\text{C}$	40	40
$Y_{EC,w} / -$	0	0
sgt^* / s^{-1}	0.1	0.002
$\alpha_g / \text{W m}^{-2} \text{K}^{-1}$	150	20
$\alpha_w / \text{W m}^{-2} \text{K}^{-1}$	20	200
$wbr^* / -$	0.1	0.5

*sgt: specific gas throughput $[sgt] = \frac{\dot{m}_{N_2}}{\dot{m}_{solids}}$
*wbr: wall-bulk-ratio $[wbr] = \frac{\tau_{wall}}{\tau_{bulk}}$



- Virgin battery material
- Steady-state process
- $\alpha_{gas}, \alpha_{wall}$ pre-defined (depending on dryer)
- $\beta_{i,g}$ through Lewis-analogy with $n = 1/3$
- Single component solvent
- No capillary transport
- 1st, 2nd drying stage

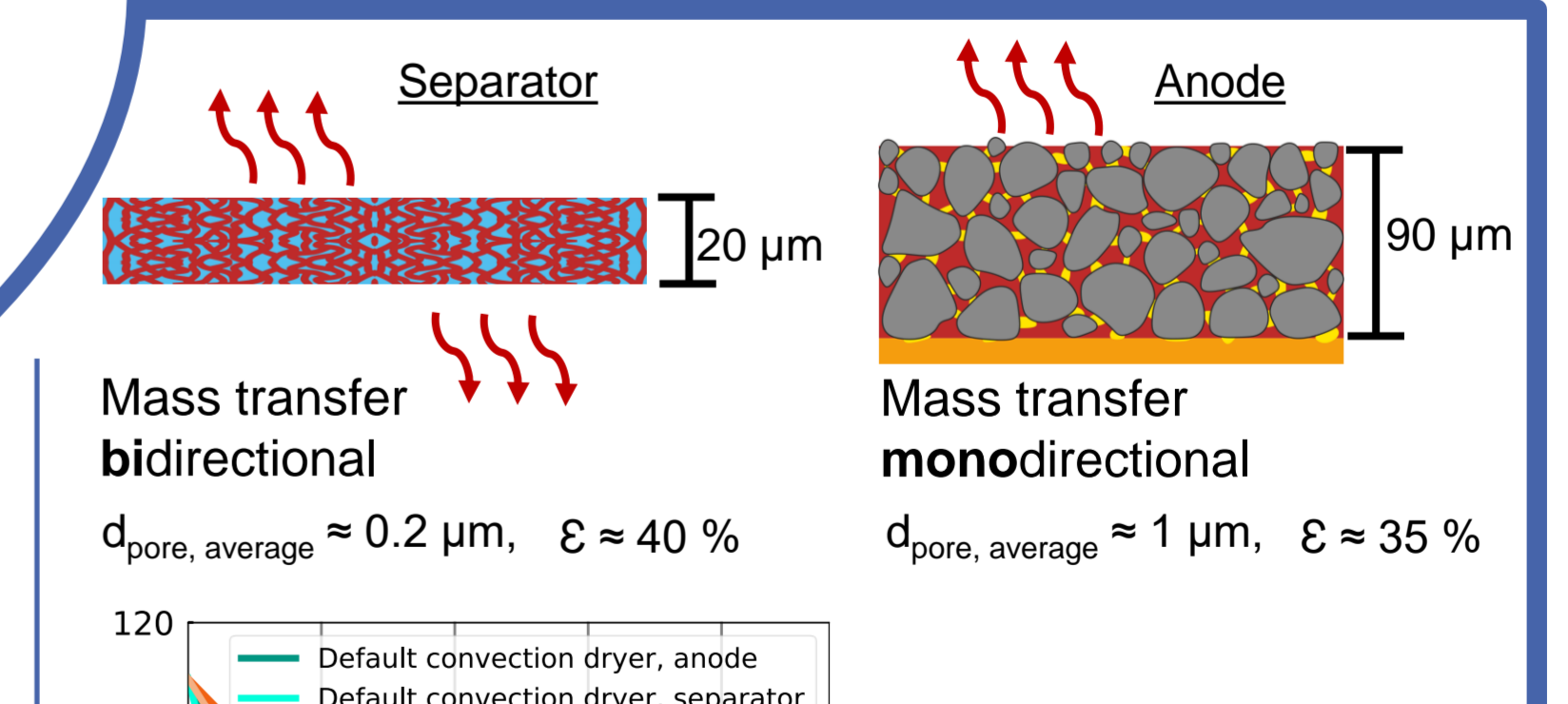
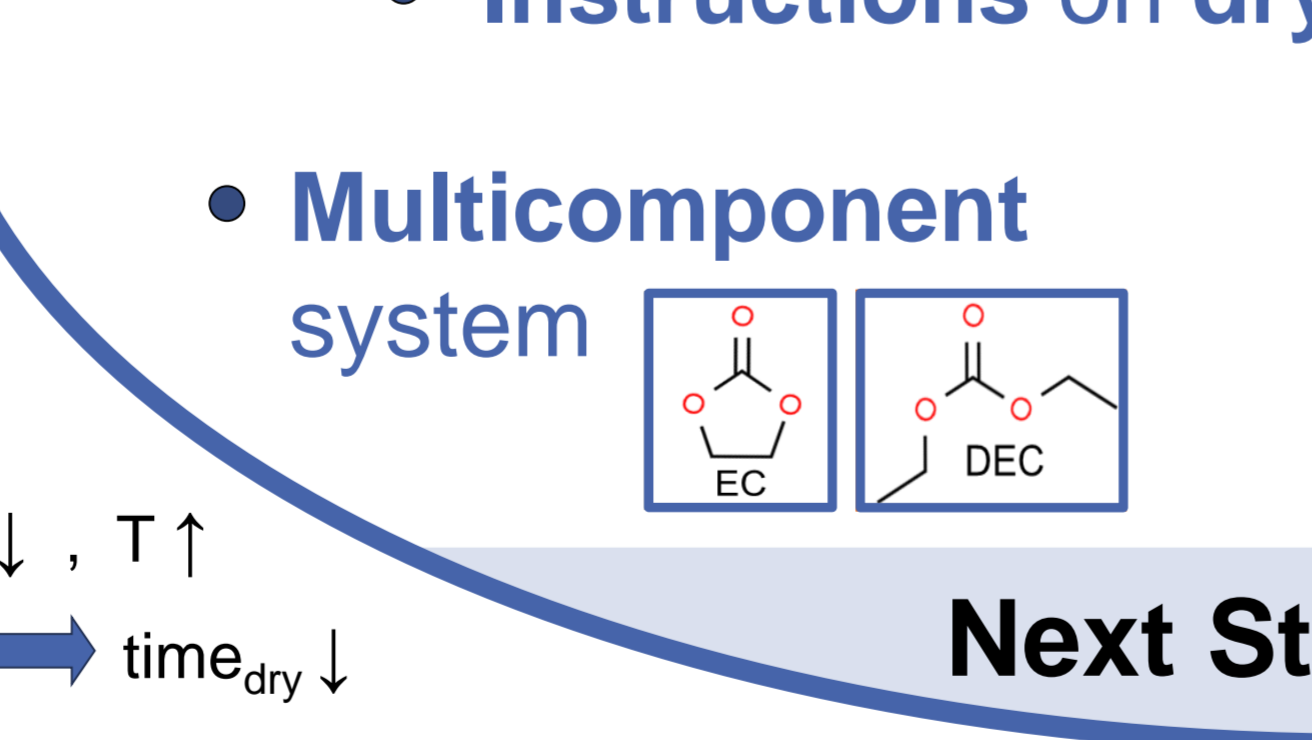
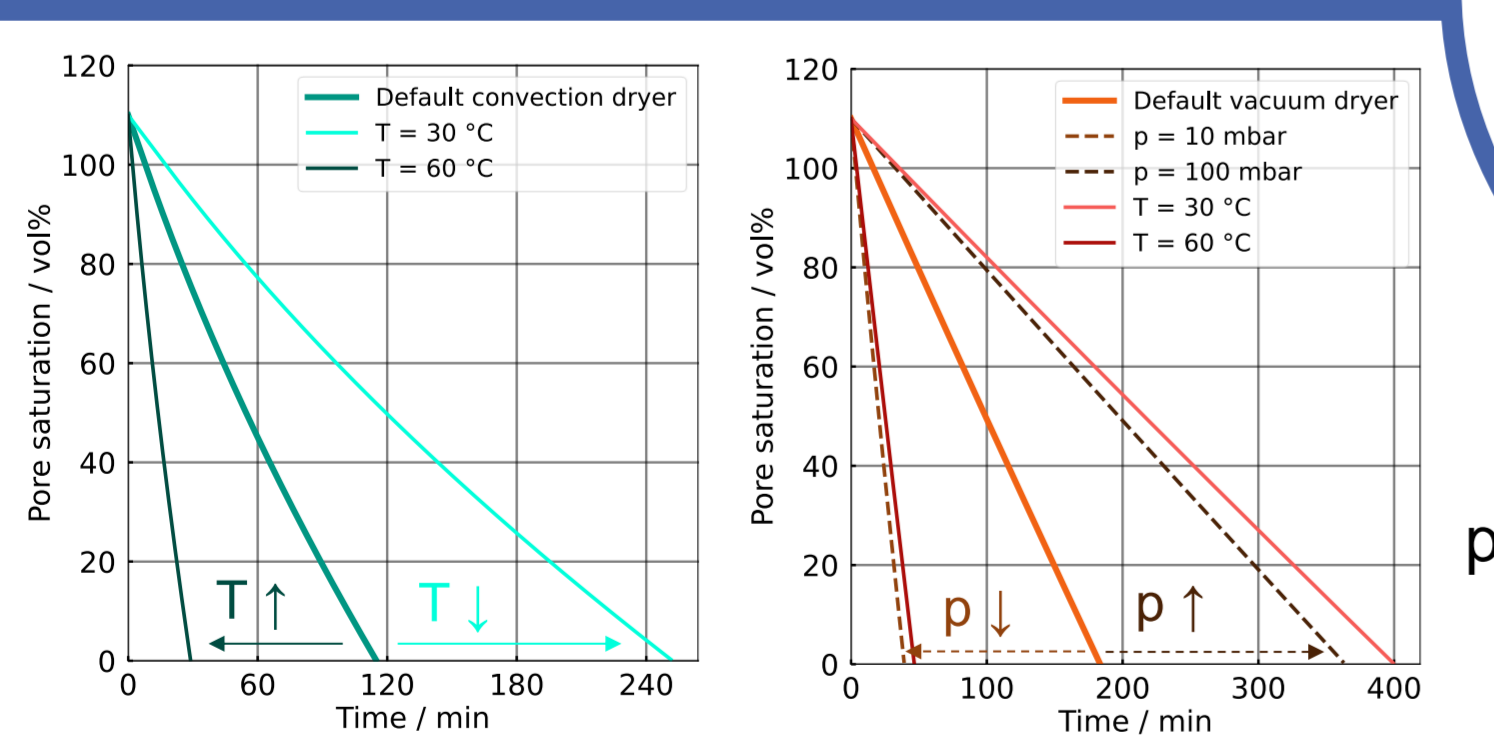
Model & Assumptions



Achievements

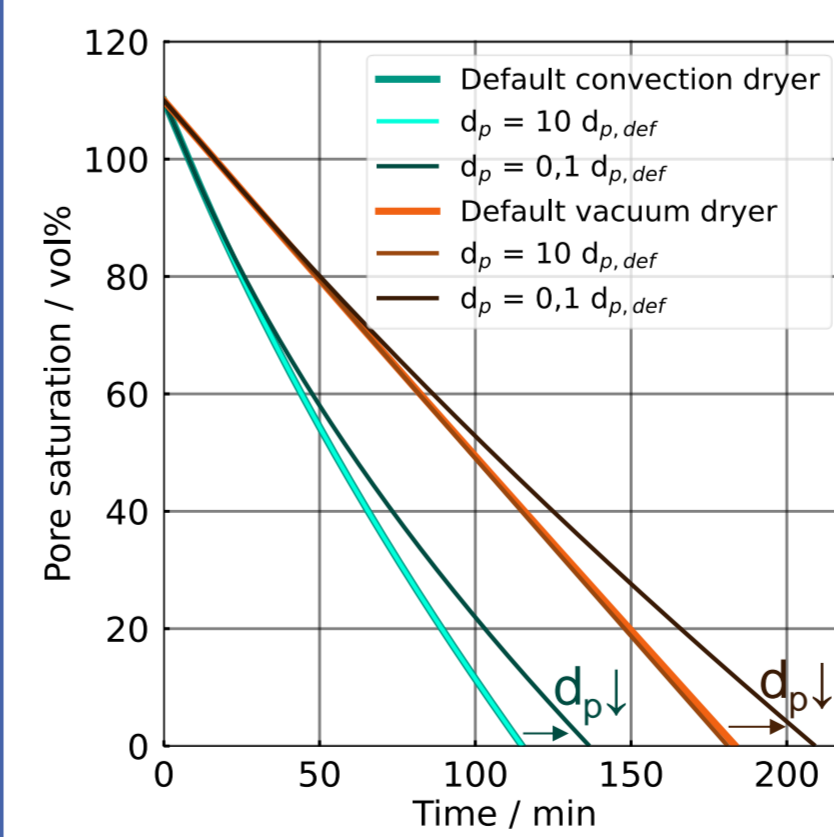
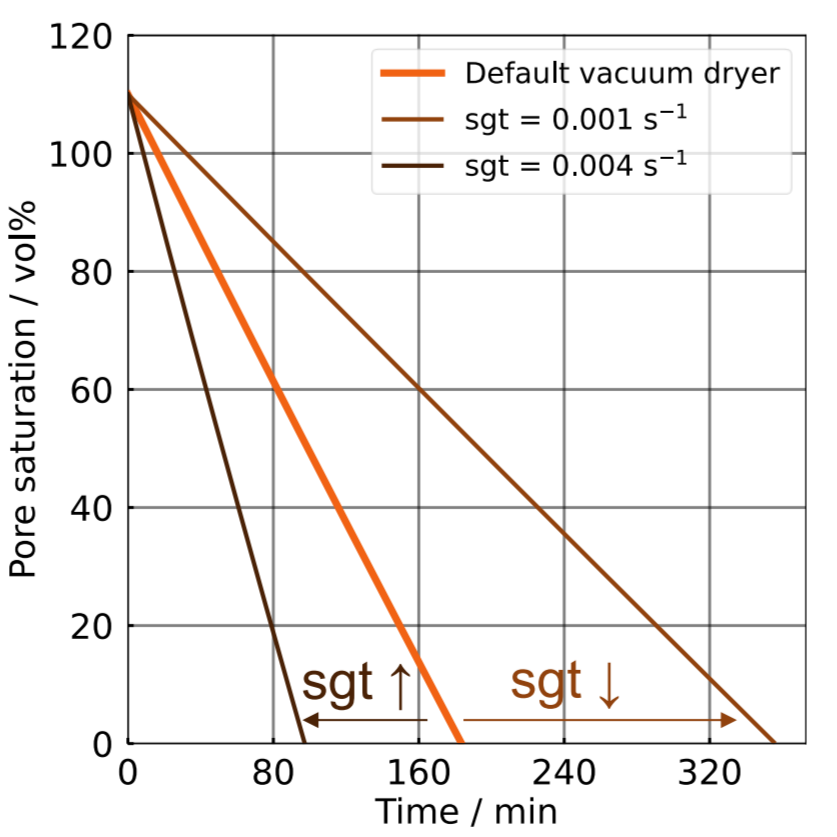
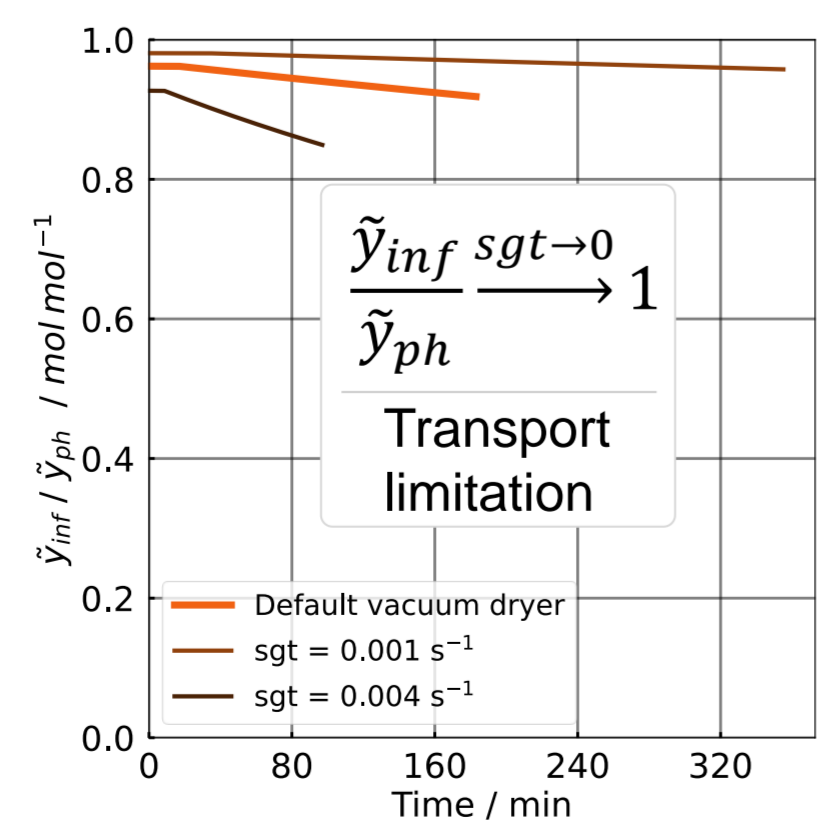
- Highly flexible model for different dryer setups
- Identified critical process and material properties
- Instructions on drying procedure
- Multicomponent system
- Validation through existing industrial dryers

Next Steps

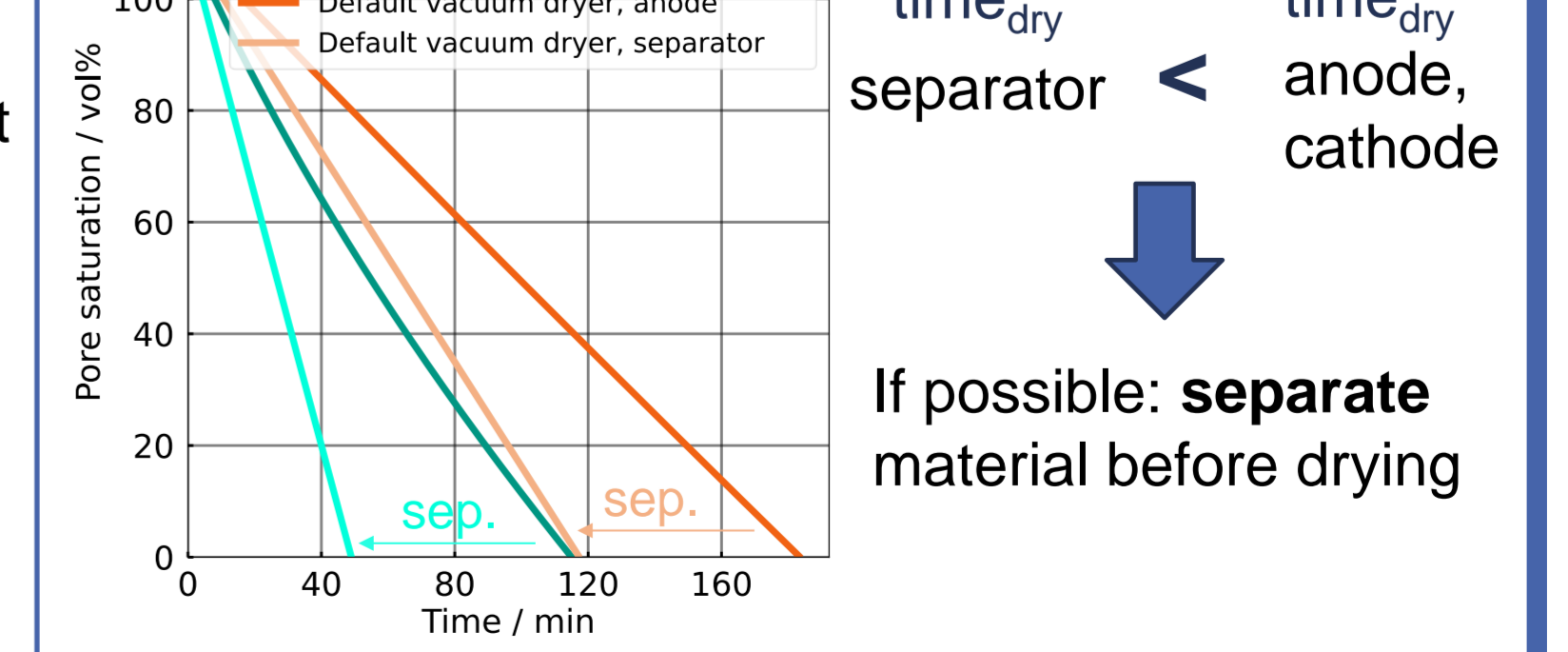
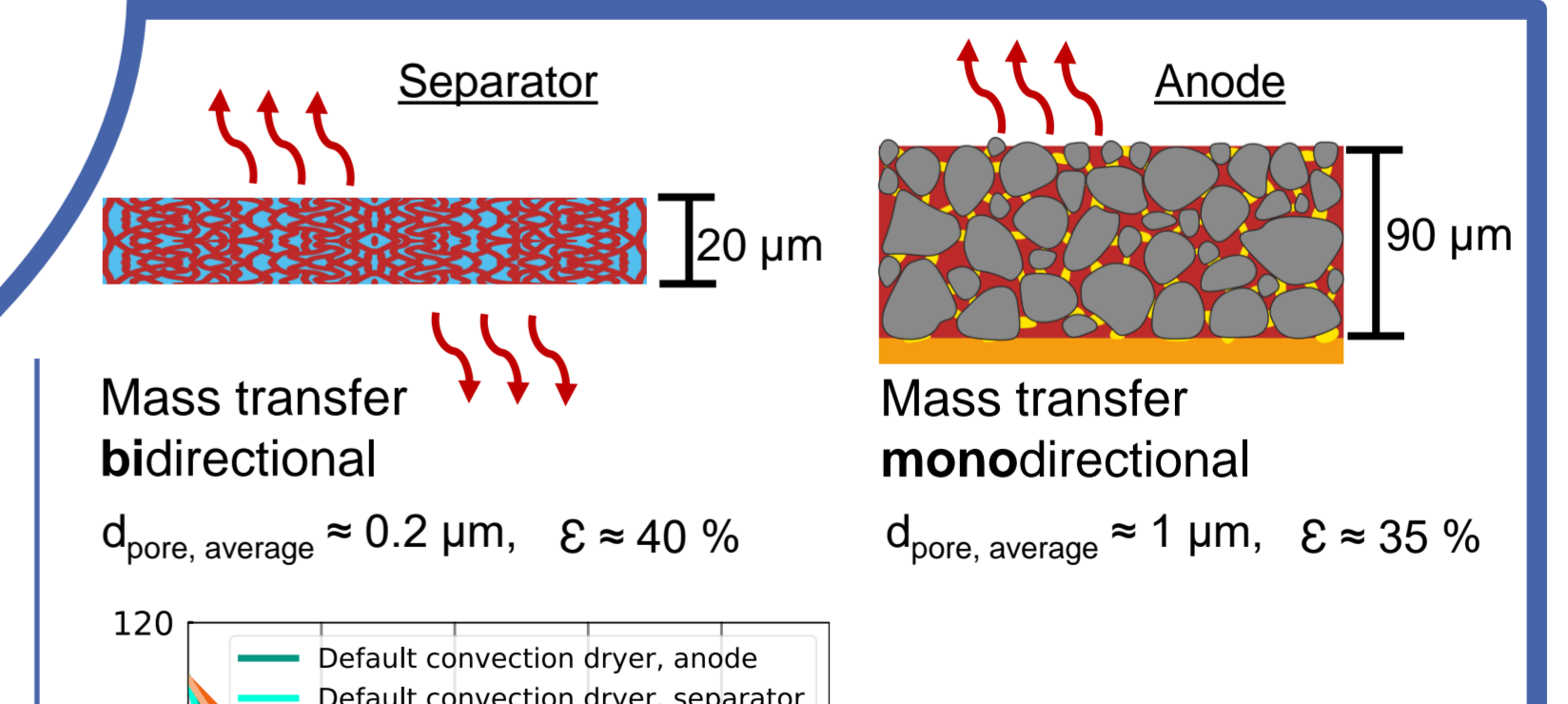


- Temperature limitation: $T < 60 \text{ }^\circ\text{C}$
- ➔ Unwanted decomposition reactions
- Feasibility of different process conditions?
- ➔ Cooperation with industry, get economical data

Process properties



- Pore size: only minor effects on drying time at small pore diameters
- Effect of Knudsen-diffusion in small pores!



Material properties

[1] ZSW, IEA. (2024). Anzahl von Elektroautos weltweit von 2013 bis 2023 und eine Prognose bis 2035. Statista. Statista GmbH. Zugriff: 26. Februar 2025. <https://de.statista.com/statistik/daten/studie/168350/umfrage/bestandentwicklung-von-elektrofahrzeugen/>
[2] Prgowska et al. (2022): The Application of Artificial Intelligence in the Effective Battery Life Cycle in the Closed Circular Economy Model - A Perspective, <https://doi.org/10.3390/recycling7060081>
[3] J. Eser, J. et al. P. Scharfer, W. Schabel (2020): Moisture Adsorption Behavior in Anodes for Li-Ion Batteries. *Energy Technology*, 8, 1801162
[4] T. Heckmann et al. P. Scharfer, W. Schabel (2023): Mass Transport in the Stefan-Knudsen Transition Region during Vacuum Drying at Different Pressures in a Porous Structure [...]. *Langmuir*, 39, 7, 2859-2869
[5] T. Heckmann et al. P. Scharfer, W. Schabel (2022): Experimental Investigation of the Temperature, Pressure, and Binder System Influence on Vacuum Postdrying Processes [...]. *Energy Technology*, 2200859