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AACHENER VERFAHRENSTECHNIK

Acid-Base Reactions Enhancing Membrane Separation: Model Development and Implementation

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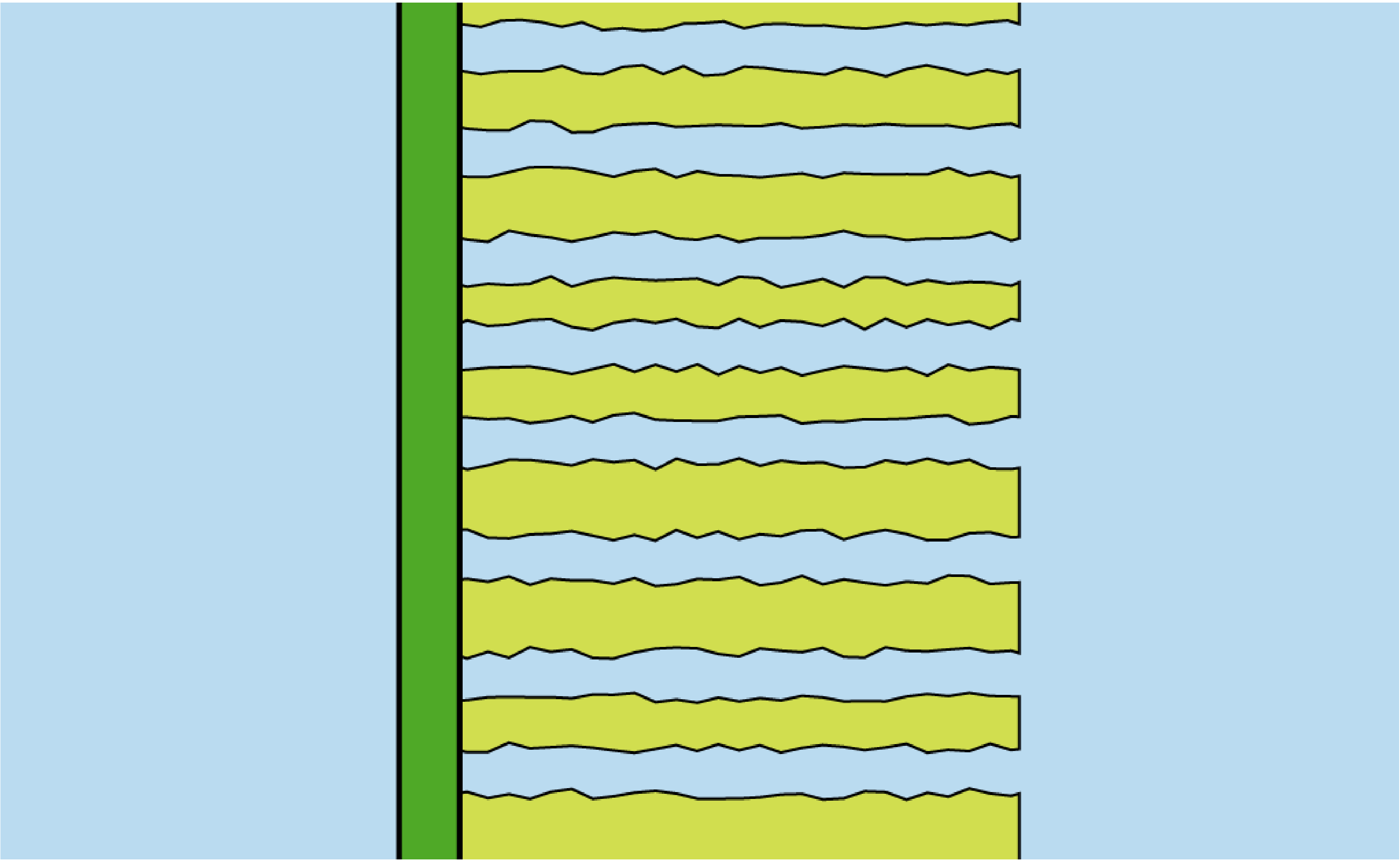
RWTH

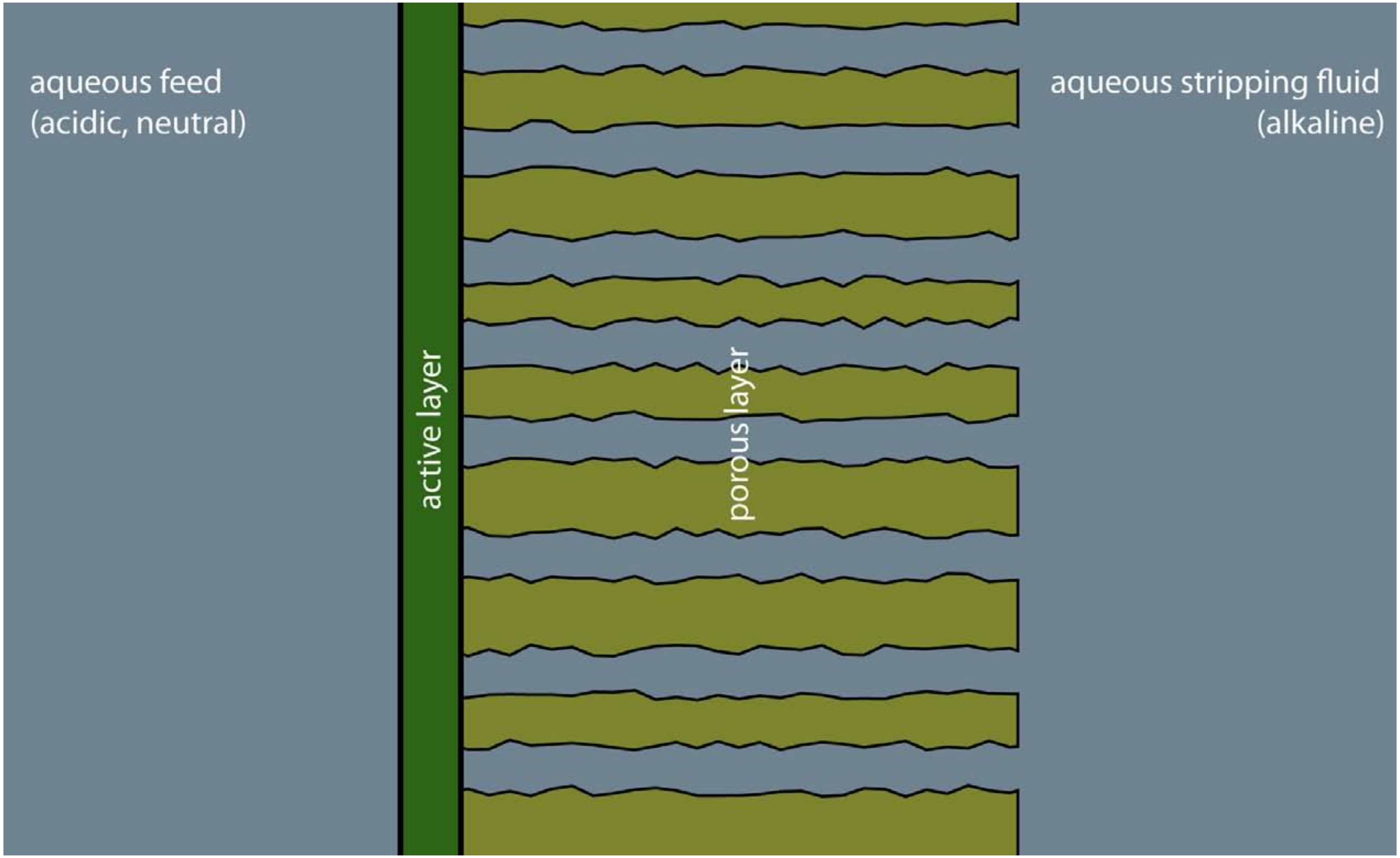
Overview

- Introduction
- Governing Equations
  - Differential-algebraic equations
  - Boundary conditions
  - Implementation
- Verification and Results
  - Alternative Model by Olander
  - Simulation results
- Summary and conclusion

Reactive Extraction of Organic Acids



Reactive Extraction of Organic Acids



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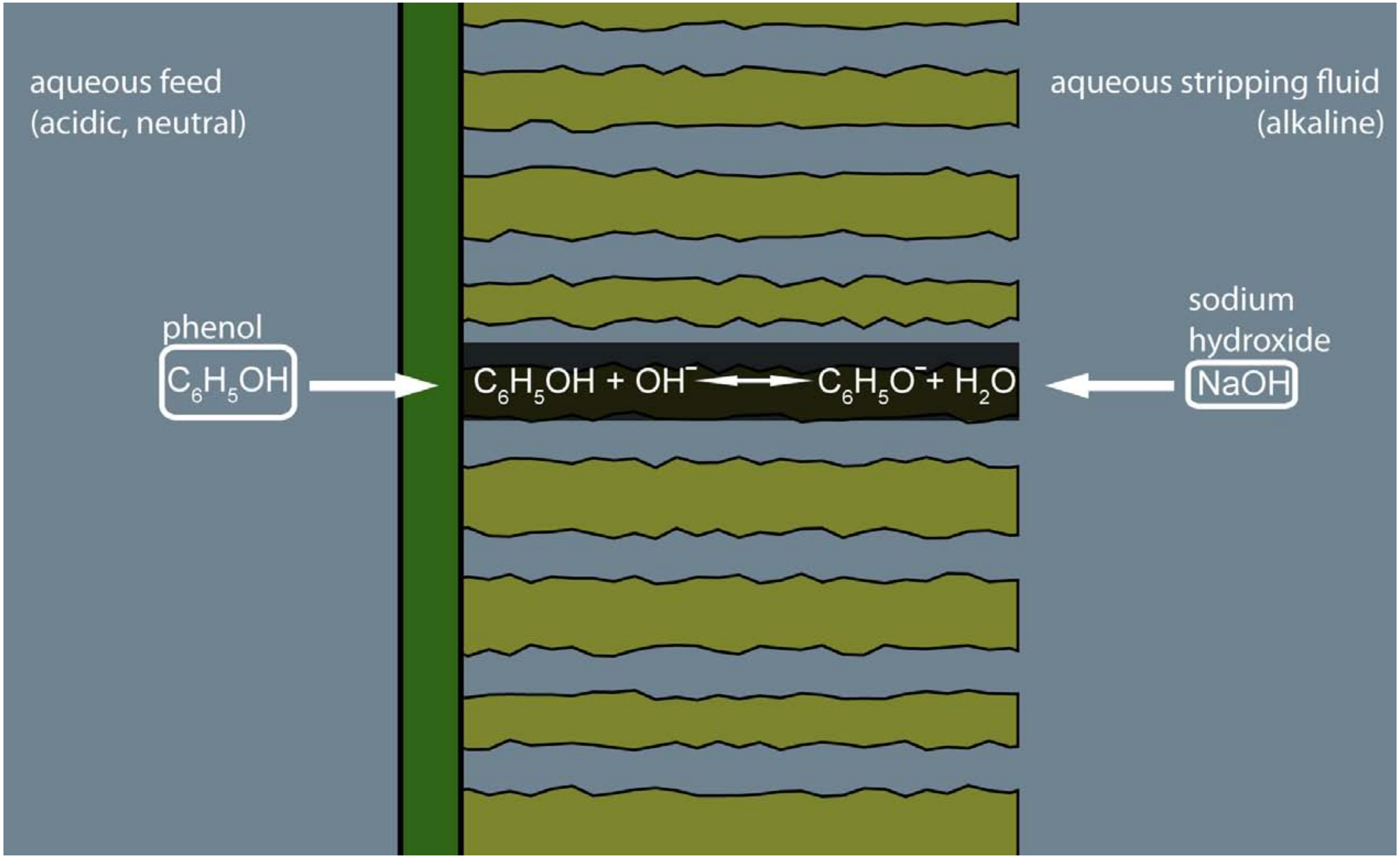

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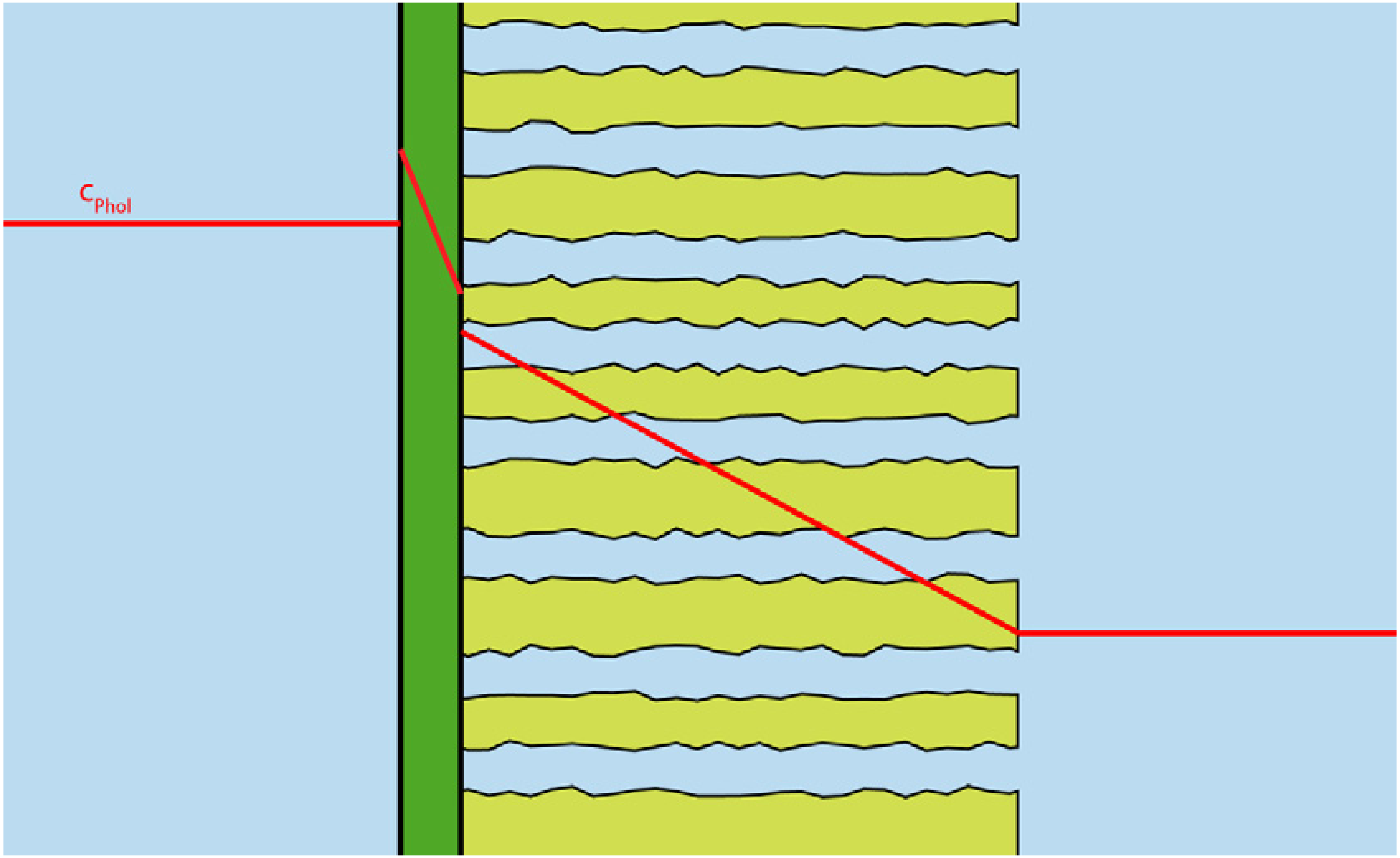

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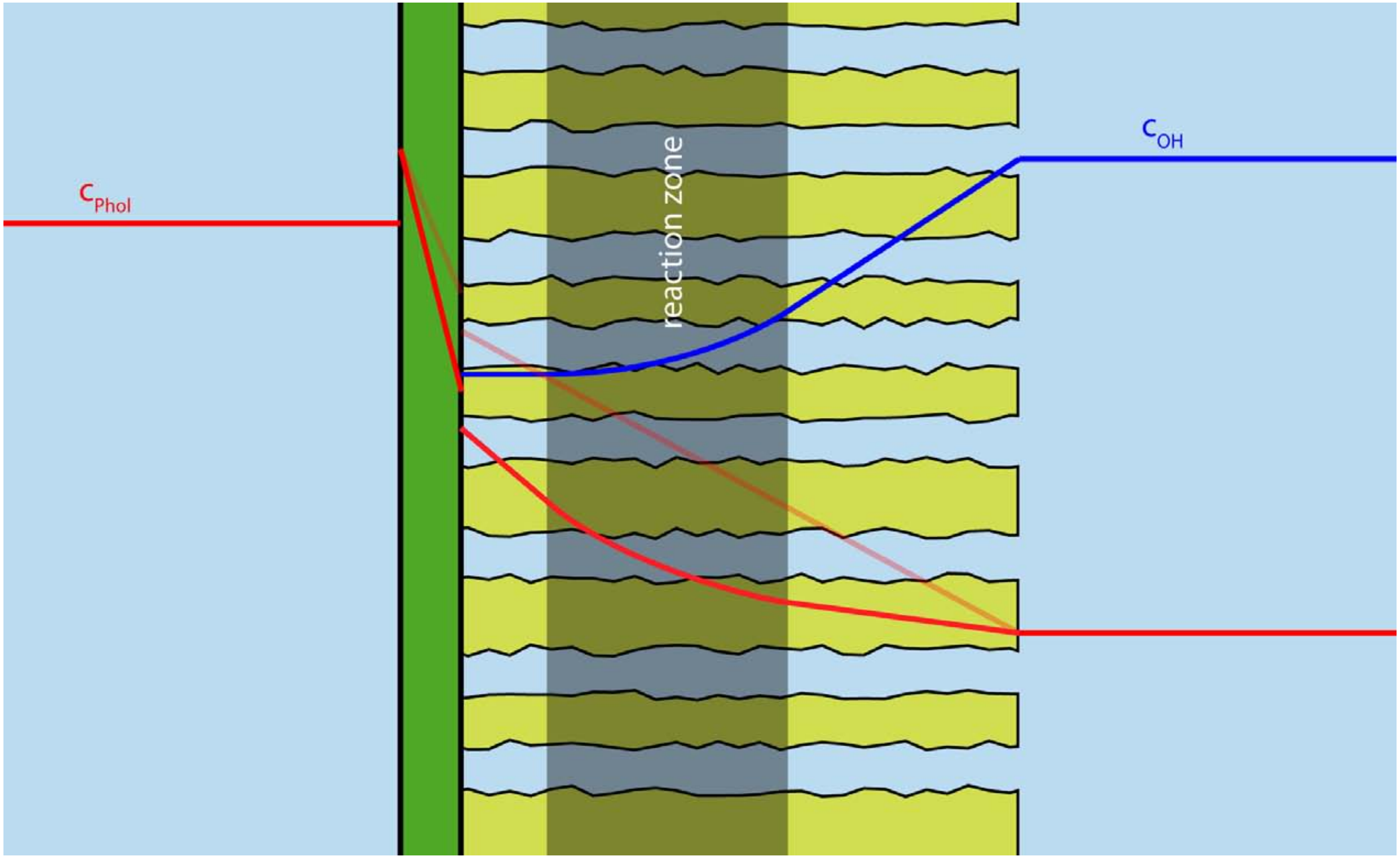


Governing Equations

- Transport equations for phenol, phenolate and OH-Ions

$$(1)\ 0 = \varepsilon D_{Phol} \frac{\delta^2 c_{Phol}}{\delta z^2} - R$$

$$(2)\ 0 = \varepsilon D_{OH} \frac{\delta^2 c_{OH}}{\delta z^2} - R$$

$$(3)\ 0 = \varepsilon D_{Phat} \frac{\delta^2 c_{Phat}}{\delta z^2} + R$$

$$\xrightarrow[(2)+(3)]{(1)+(3)}$$

$$0 = \varepsilon D_{Phol} \frac{\delta^2 c_{Phol}}{\delta z^2} + \varepsilon D_{Phat} \frac{\delta^2 c_{Phat}}{\delta z^2}$$

$$0 = \varepsilon D_{OH} \frac{\delta^2 c_{OH}}{\delta z^2} + \varepsilon D_{Phat} \frac{\delta^2 c_{Phat}}{\delta z^2}$$

$$R = k_1 c_{Phol} c_{OH} - k_2 c_{Phat}$$

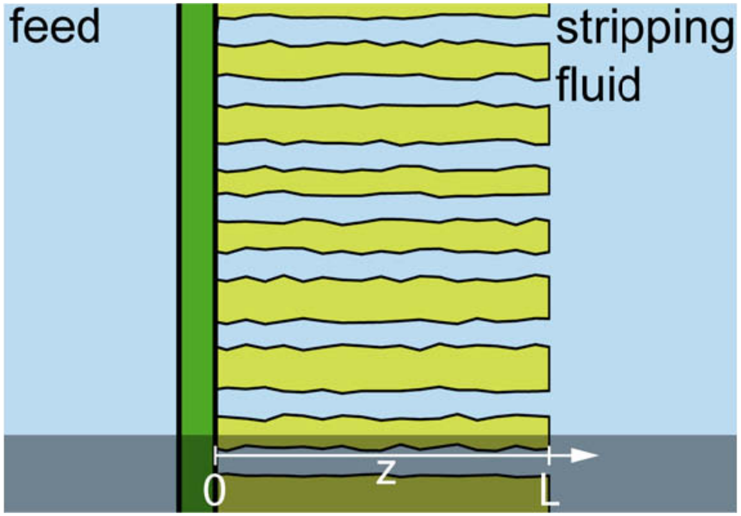
$$K = \frac{k_1}{k_2} = \frac{c_{Phat}}{c_{Phol} \cdot c_{OH}}$$

- Problem: Magnitude of Reaction Rate constants k1, k2 undefined
  - Too high: model instabilities
  - Too low: incomplete chemical equilibrium

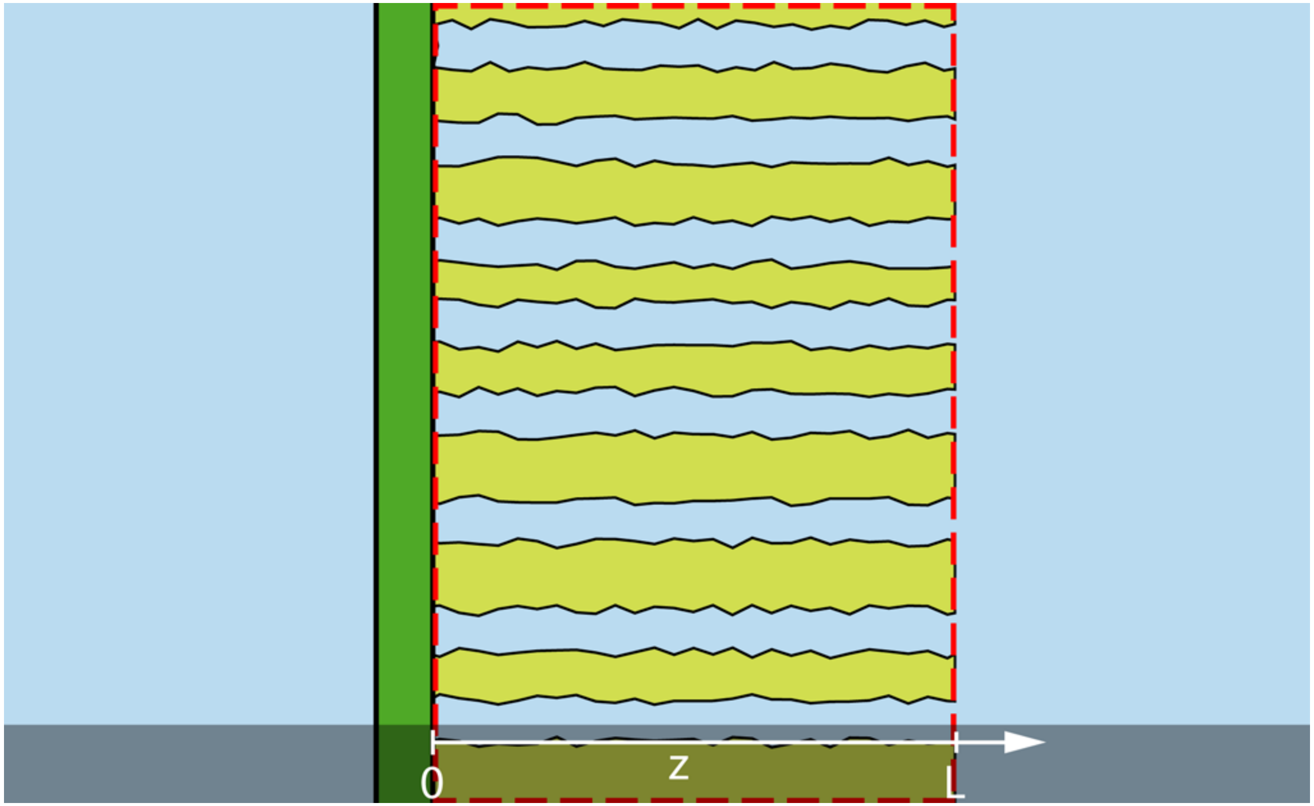
  → Substitution of reaction rates

Boundary Conditions

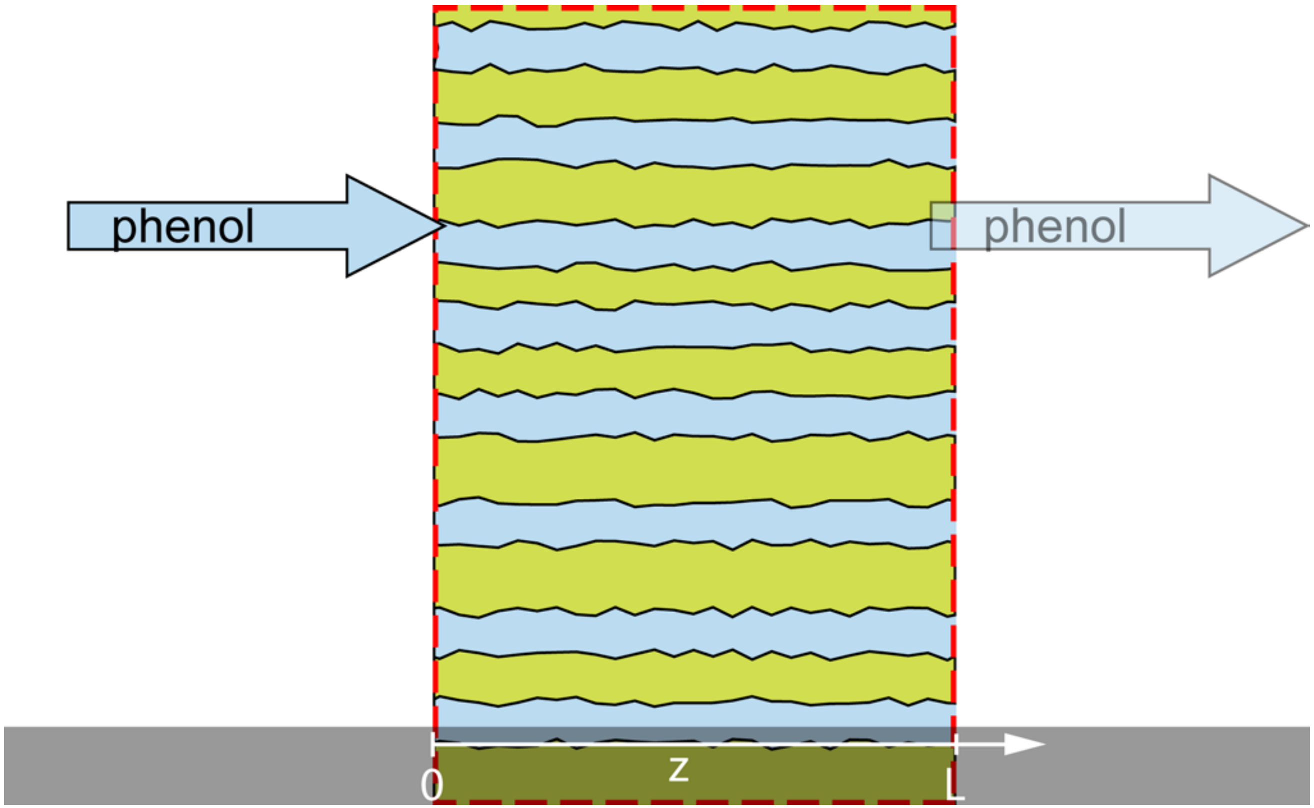
#	Bnd	Species	Condition
1	z = 0	OH	Insulation
2		Phat	Insulation
3		Phol	$\dot{n}_{Phol} = k_{mem} \cdot \Delta c_{\mathrm{Phol}}$
4	z = L	Phol	$c_{Phol}^{z=L} = c_{Phol}^{stripp}$
5		Phat	$c_{Phat}^{z=L} = c_{Phat}^{stripp}$



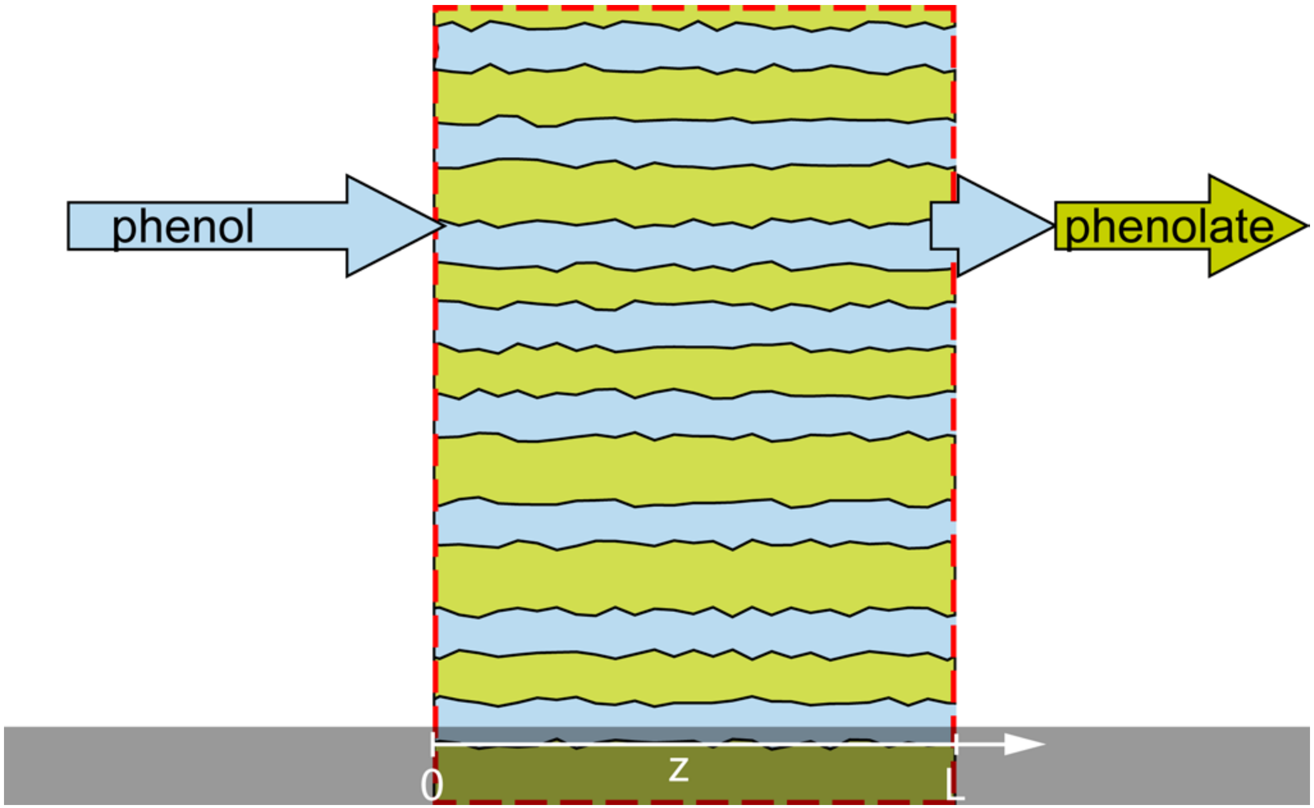
Boundary Conditions



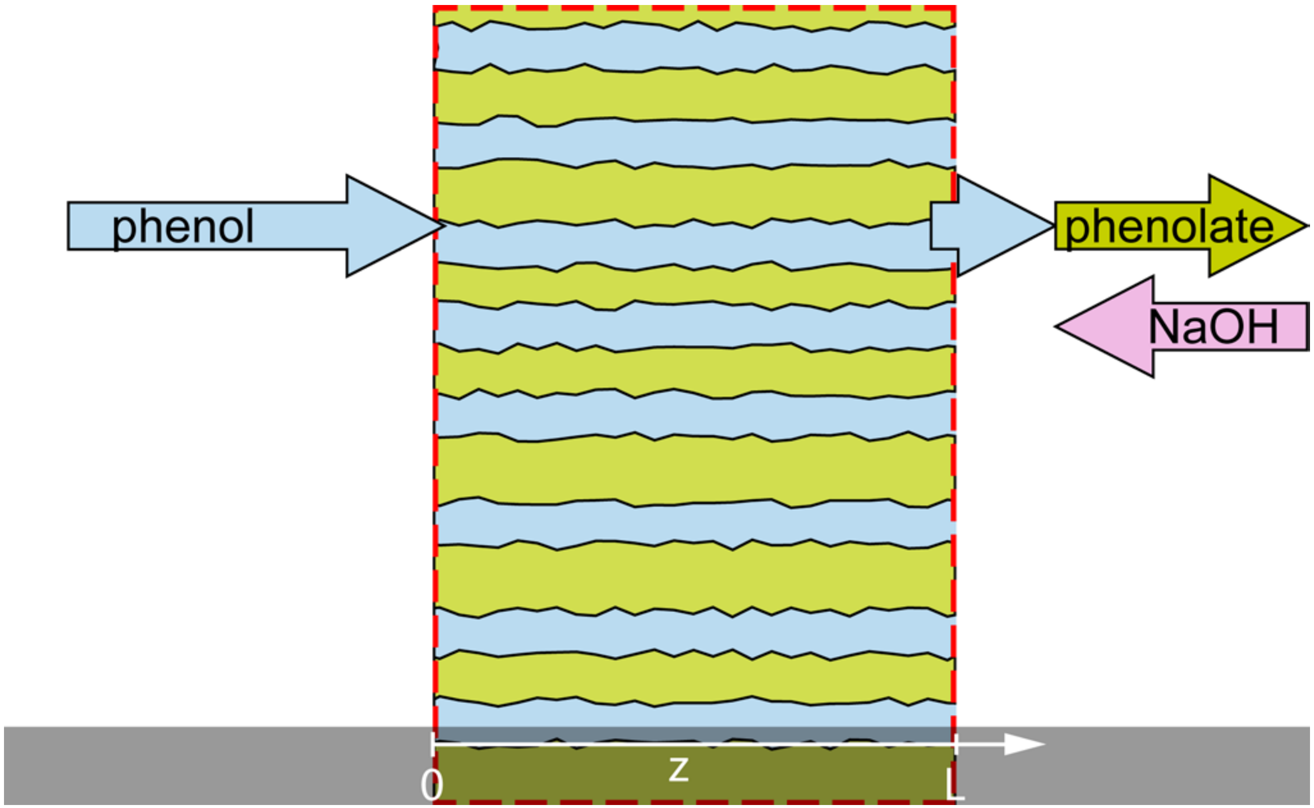
Boundary Conditions



Boundary Conditions



Boundary Conditions



- 6th boundary condition:

$$\boxed{\boxed{k_{mem}\left(c_{Phol}^{Feed} - c_{Phol}^{z=0}\right)}\frac{c_{Phat}^{z=L}}{c_{Phol}^{z=L} + c_{Phat}^{z=L}}} = \boxed{D_{OH}\frac{\partial c_{OH}^{z=L}}{\partial z}}$$

Numerical models and analytical solution (Olander)

- Model for transmembrane phenol flow

$$\dot{n}_{Phol} = \left(c_{\mathrm{Phol}}^{\mathrm{Feed}} - c_{\mathrm{Phol}}^{\mathrm{Perm}}\right) \frac{1}{\frac{1}{\mathrm{k_{act}}} + \frac{1}{\mathrm{E\,k_{por}}}}$$

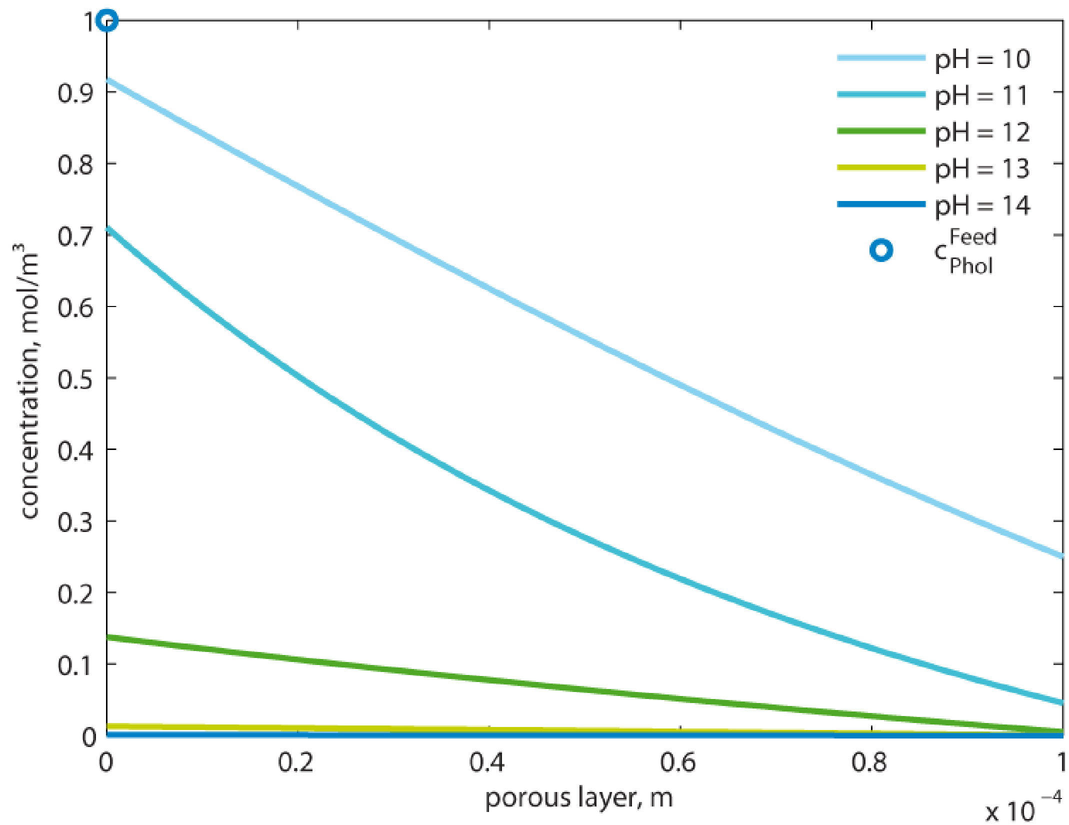
- Enhancement factor E dependent on chemical reaction
- Can range from
  - 1, no improvement of extraction
  - ∞, chemical reaction eliminates influence of porous structure

→ Analytical solution for the calculation of E available

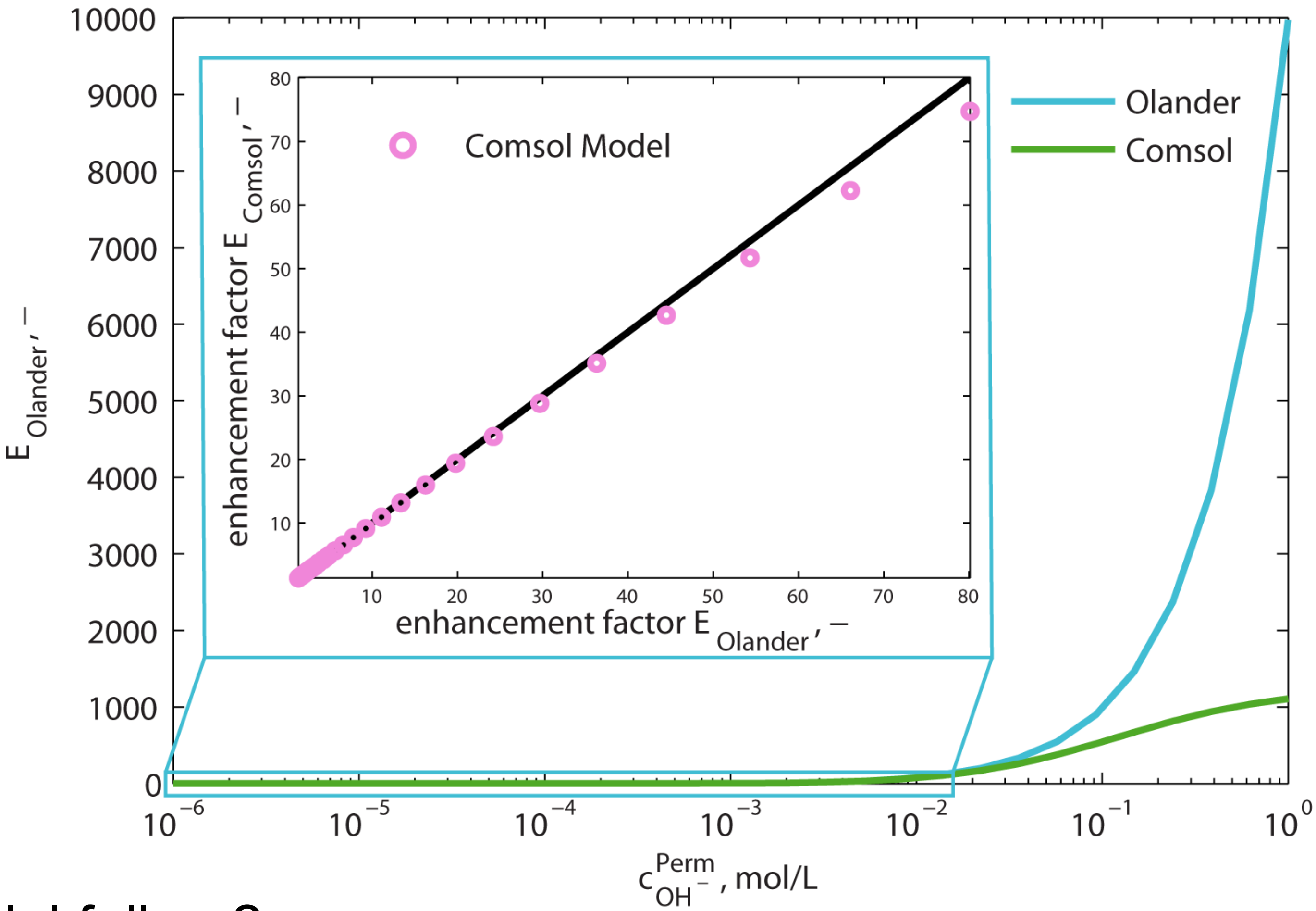
→ Olander‘s solution acts as benchmark for Comsol

Comsol results, concentration profile

- Rising pH leads to reduced phenol-levels in the porous structure
- Higher phenol-difference across the dense layer with increased pH
- Caustic soda effectively reduces apparent thickness of porous layer

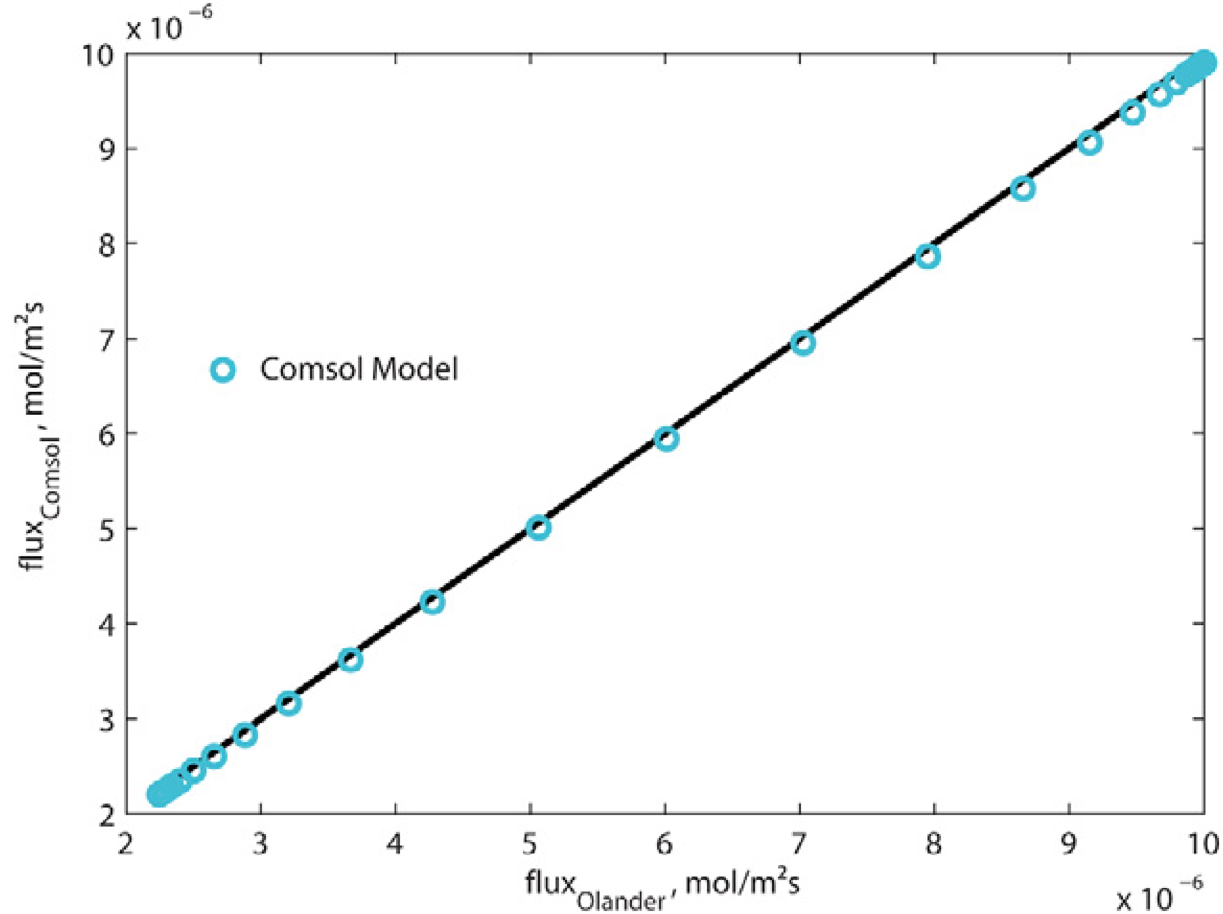


Model verification: Enhancement factor



→ Model failure?

Model verification: mass flow



→ Comsol model sufficiently accurate

→ E-factor of limited use

Summary and Outlook

- Lessons learned
  - Modeling of instantaneous reaction
    → shift from reaction rates to chemical equilibrium constant
  - Choice of boundary conditions
    → calculation of sodium hydroxide flow into the porous layer
  - Validation criteria
    → not as easy as it seems, validation by flow

- Outlook
  - Application of the model for the investigation of system parameters
  - Extension of the model to cover aspects like concentration polarization

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Thank you!

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