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# A generic approach to evaluate the performance of membrane reactor configurations

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September 2012

MTG

# Introduction

- How to obtain products from equilibrium limited reactions?

$k_f$

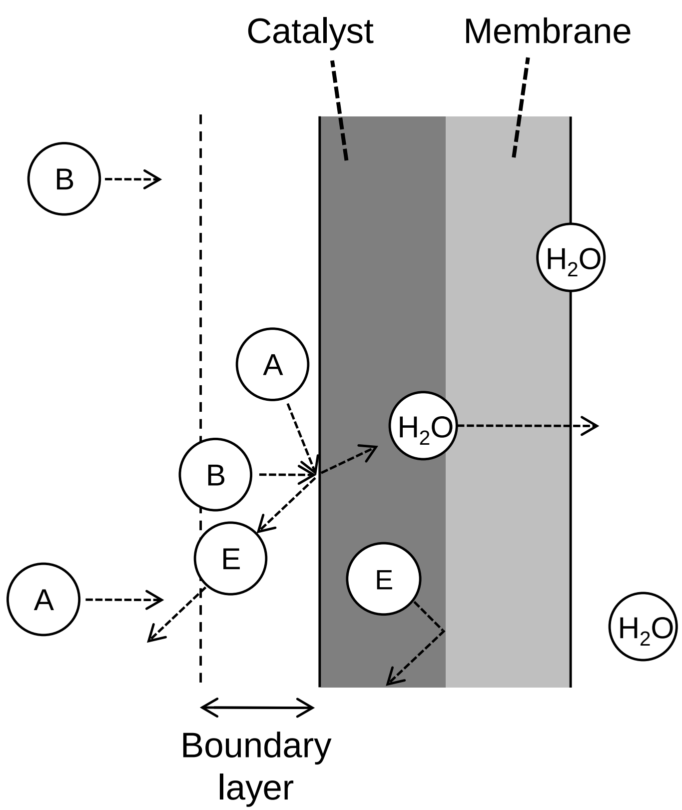
$k_b$

$$K_{eq} = \frac{k_f}{k_b} = \frac{[E][H_2O]}{[A][B]} \quad < \quad 1$$

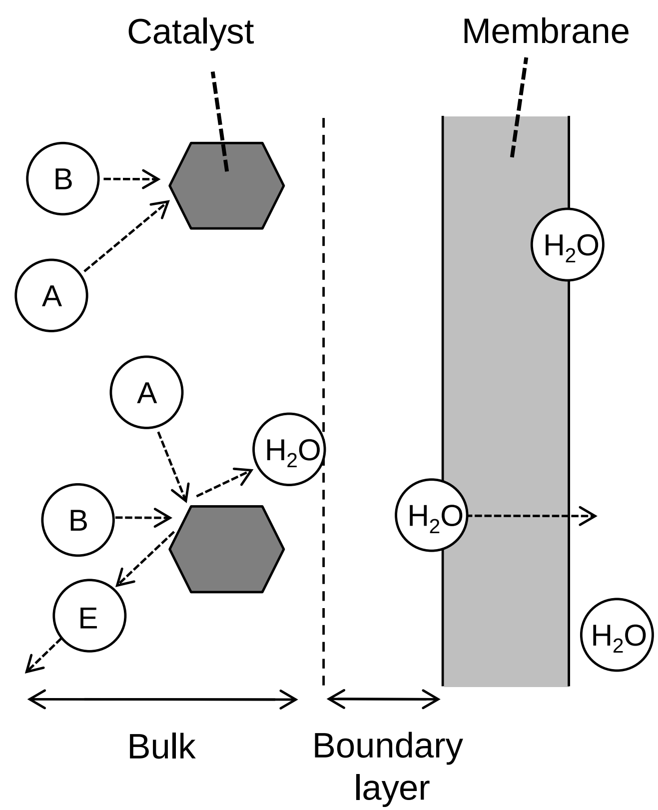
- **Solution:** membrane reactors
  - Remove one of the products selectively

# Introduction

## Catalytic membrane reactor (CMR)




## Inert membrane reactor (IMR)



# Theory

## Model

- Reaction

- Bulk membrane reactor: CSTR

- Mass transport: Maxwell Stefan

$$\Delta x_i = \sum_{i \neq j} \frac{\left( \bar{x}_j N_i - \bar{x}_i N_j \right)}{k_{bl} \bar{c}}$$

- Only $H_2O$ permeates through the membrane

- No mass transport limitations in IMR to reach catalyst particles

# Theory

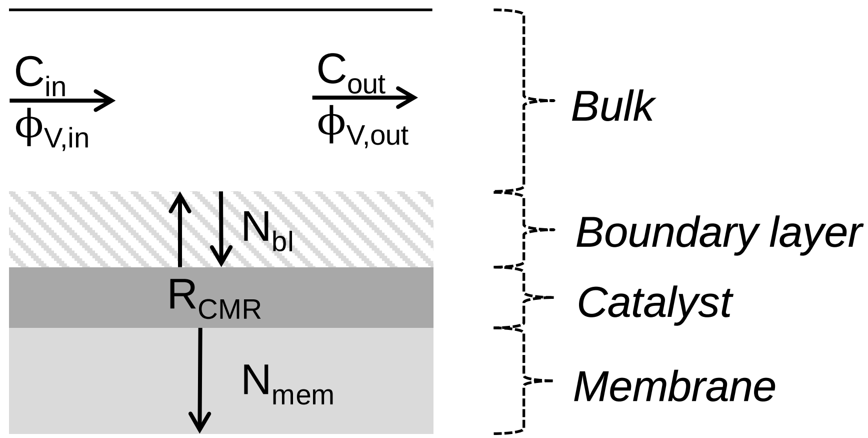
## Assumptions material and process conditions

| Parameter | Value | Unit |
|---|---|---|
| $C_{in, overall}$ | 100 | $mol/m^3$ |
| T | 150 | $^oC$ |
| $x_{in, A}$ | 0.67 | - |
| $x_{in, B}$ | 0.33 | - |
| V | 1 | $m^3$ |
| $\tau$ | 100 | s |

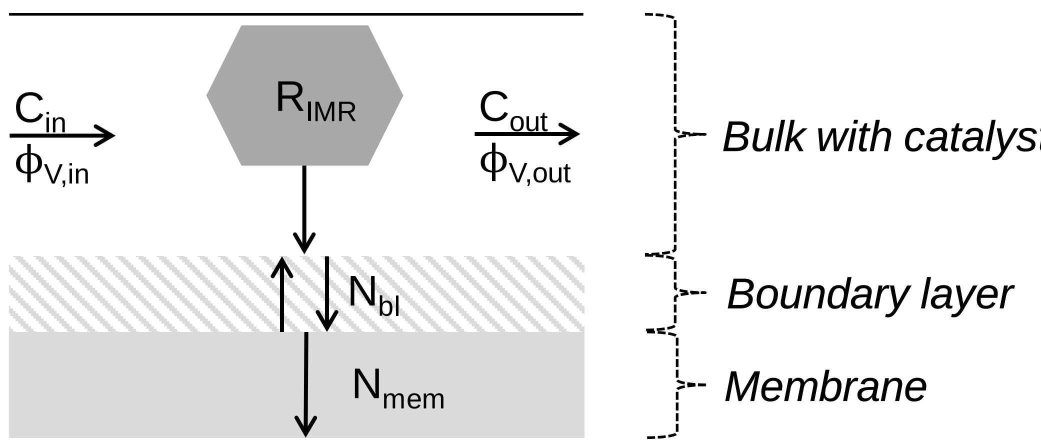
| Parameter | Value | Unit |
|---|---|---|
| A/V | 1000 | 1/m |
| $k_f$ | $10^{-2}$ | $(m^3)^2 /mol^2 \cdot s$ |
| $k_{bl}$ | $10^{-4}$ | m/s |
| $P_{H2O}$ | $10^{-6}$ | $mol/m^2 \cdot s \cdot Pa$ |
| $P_A=P_B=P_E$ | 0 | $mol/m^2 \cdot s \cdot Pa$ |

# Theory

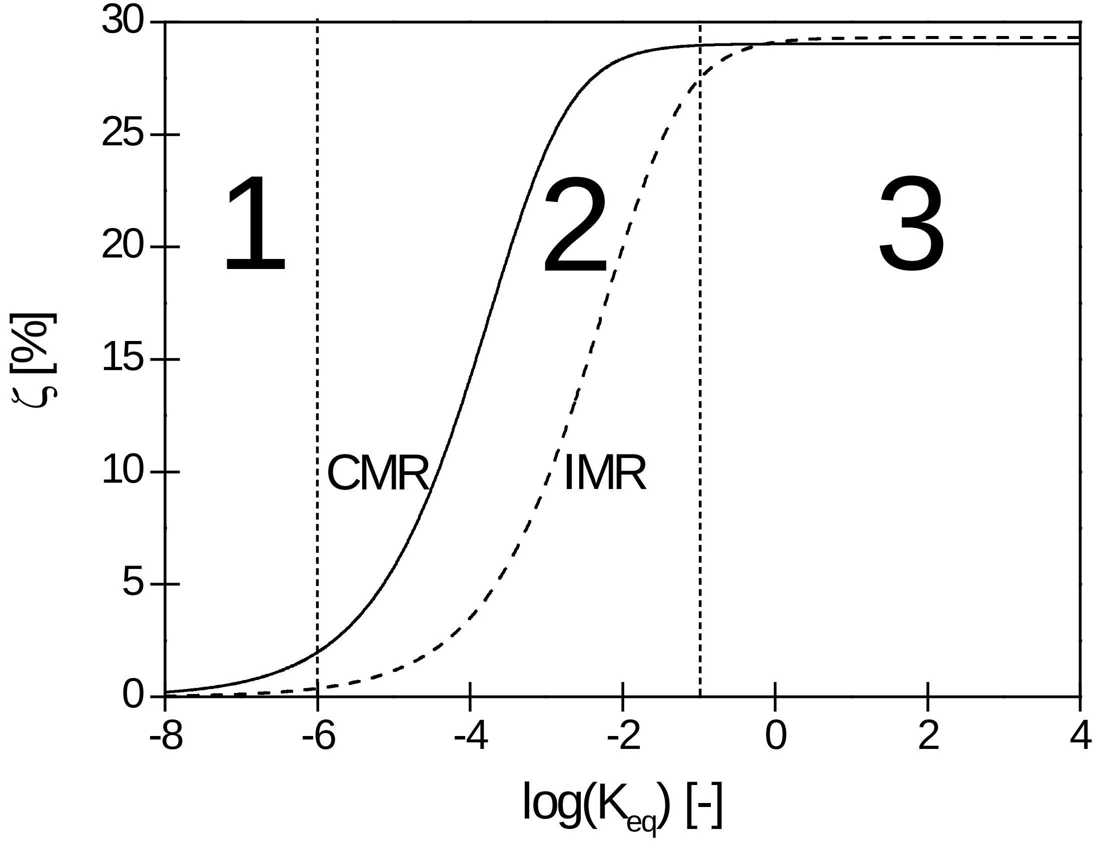
- CMR



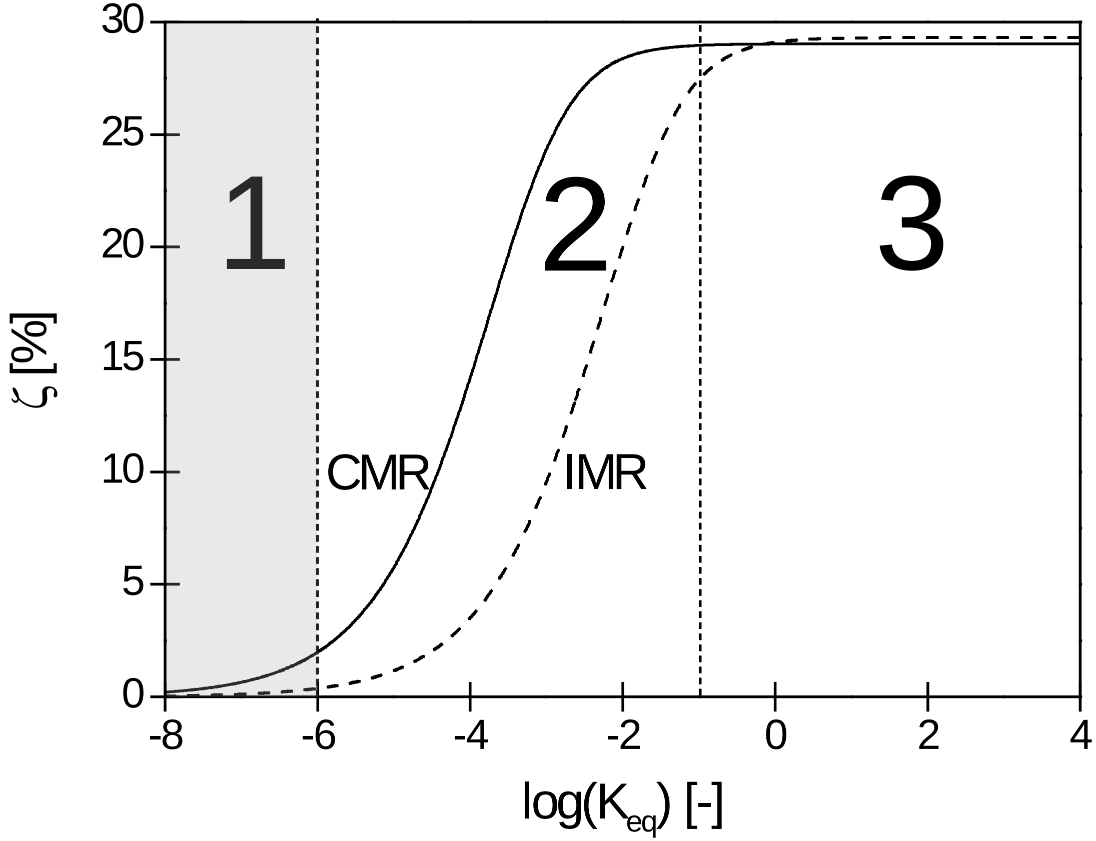

- IMR



# Results

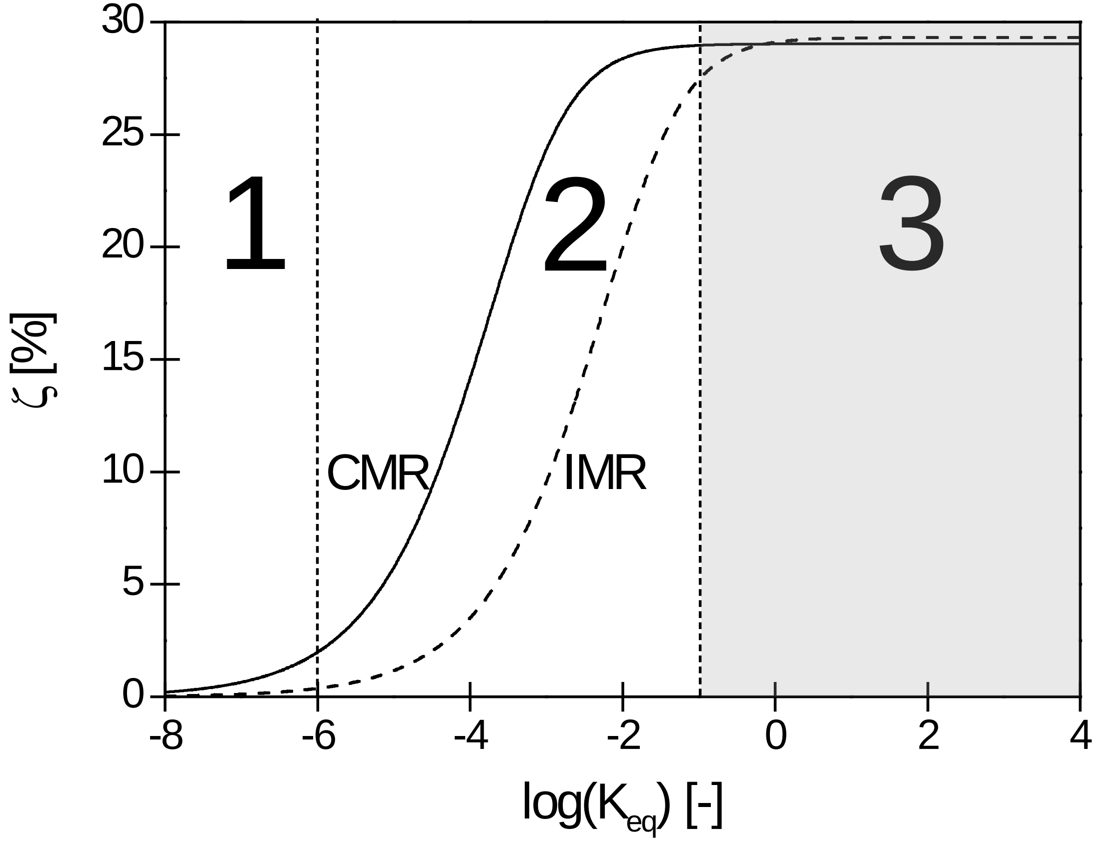


# Results



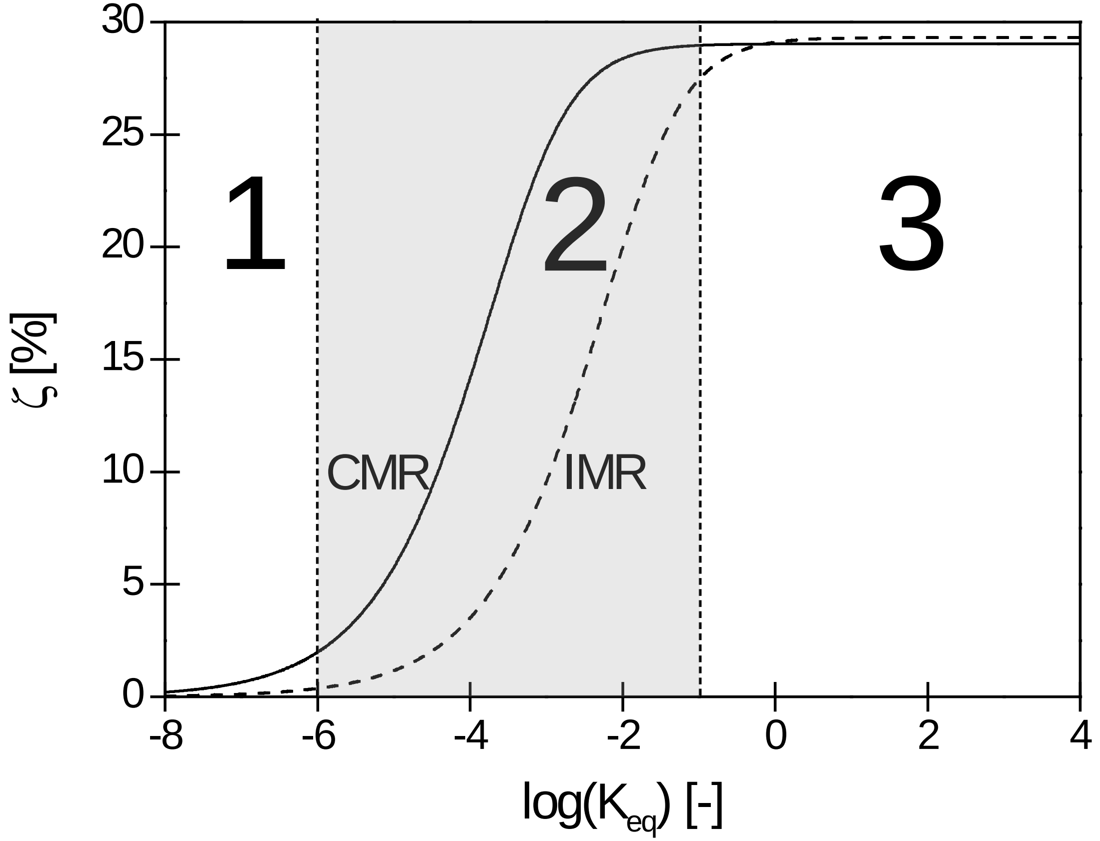

$$k_f \cdot C_A^2 \cdot C_B << \frac{k_f}{K_{eq}} \cdot C_E \cdot C_{H2O}$$

# Results



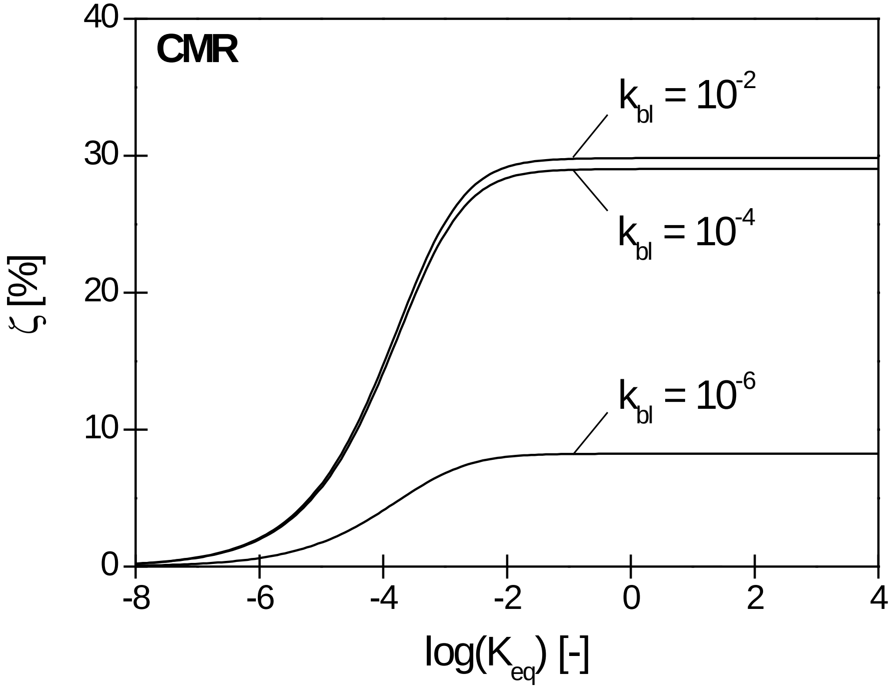

$$k_f \cdot C_A^2 \cdot C_B >> \frac{k_f}{K_{eq}} \cdot C_E \cdot C_{H2O}$$

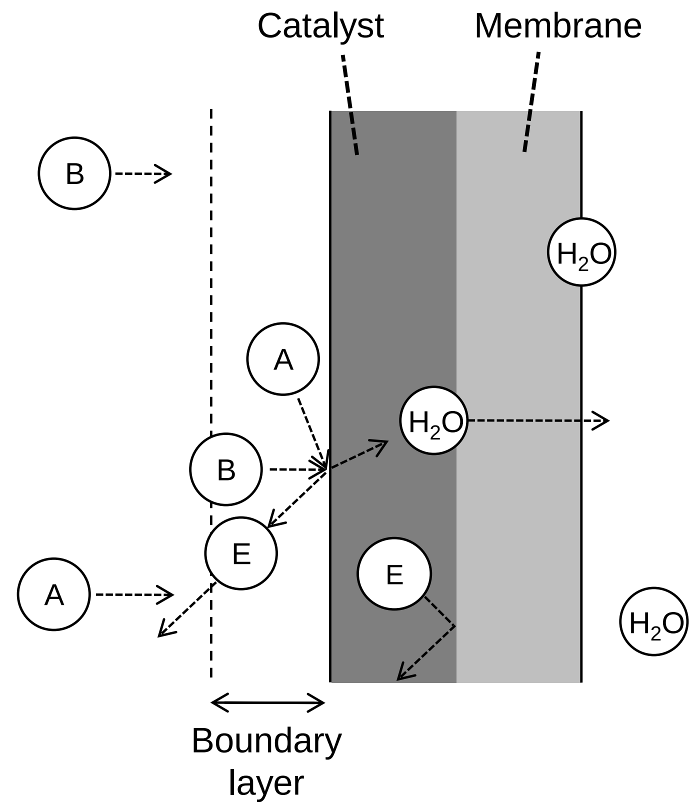
# Results



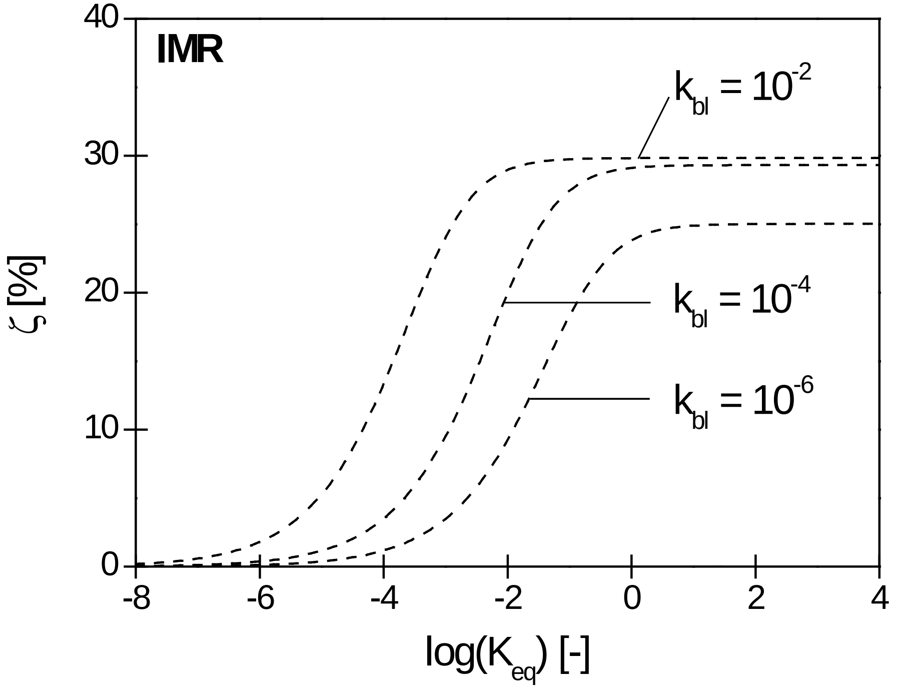

$$k_f \cdot C_A^2 \cdot C_B \approx \frac{k_f}{K_{eq}} \cdot C_E \cdot C_{H2O}$$

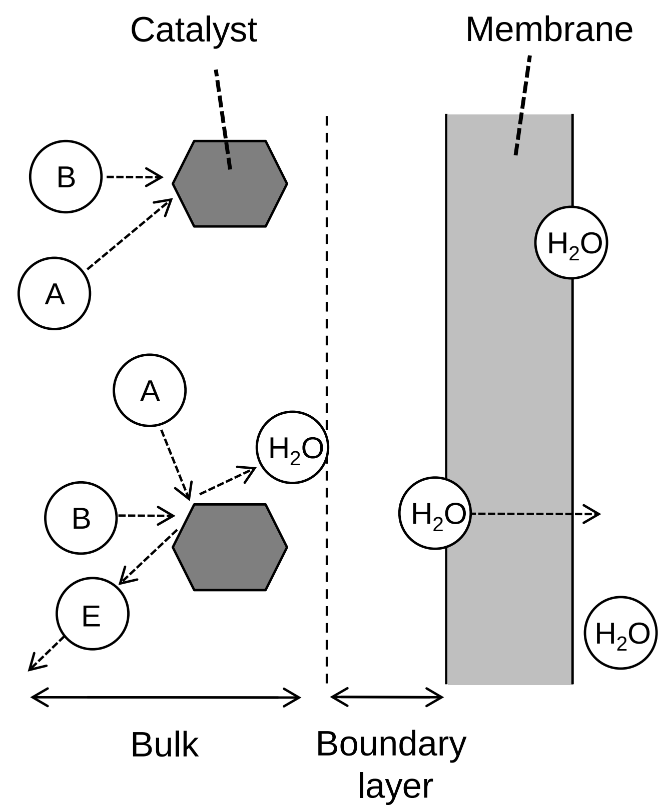
# Results – Mass transfer coefficient ($k_{bl}$)



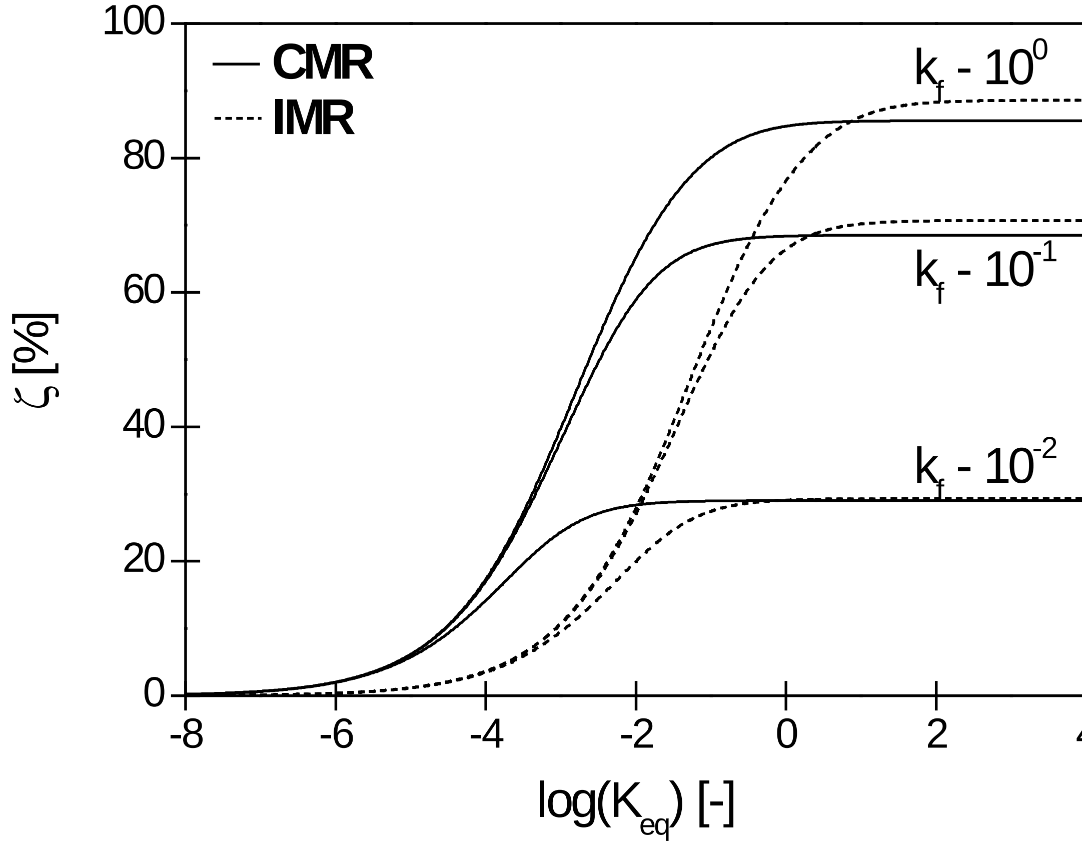



# Results – Mass transfer coefficient ($k_{bl}$)



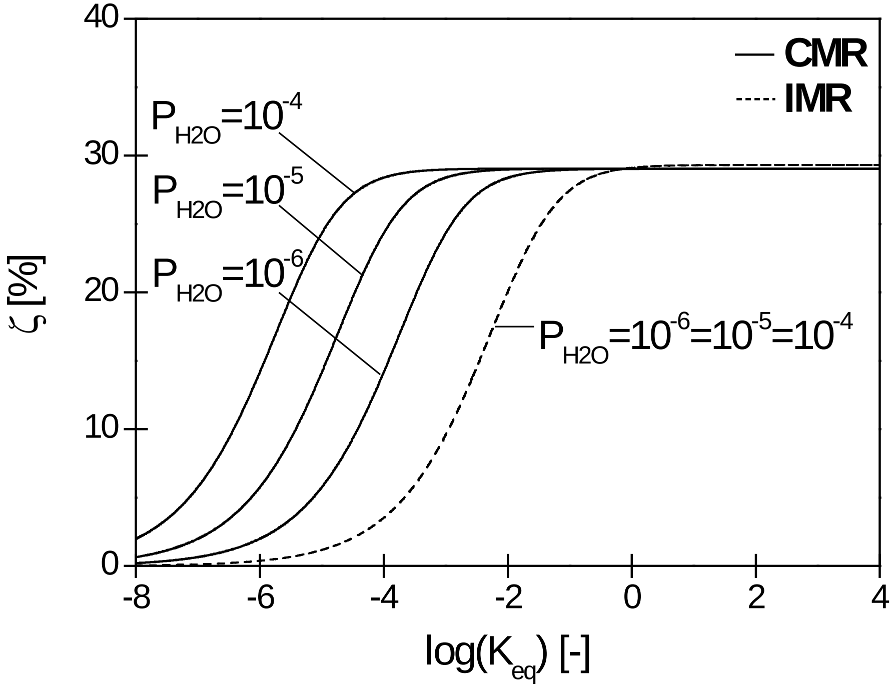



# Results – Reaction rate constant ($k_f$)




$$R = k_f \cdot C_A^2 \cdot C_B - \frac{k_f}{K_{eq}} \cdot C_E \cdot C_{H2O}$$

# Results – Permeance of $H_2O$ ($P_{H2O}$)




**CMR**

$$\frac{1}{k_{tot}} = \frac{1}{k_{mem}}$$

**IMR**

$$\frac{1}{k_{tot}} = \frac{1}{k_{mem}} + \frac{1}{k_{bl}}$$

# Conclusions

- Model made based on Maxwell Stefan principles
  - Easy selection tool
- Selection membrane reactor depends on equilibrium
  - Low $K_{eq}$ – CMRs?
  - Intermediate $K_{eq}$ – CMR
  - High $K_{eq}$ – IMR
  - Process and material parameters have a strong influence on results

# Acknowledgement

This research is financially supported by the European Union (FP7-NMP-2010-Large-4 (CARENA))

CARENA