A generic approach to evaluate the performance of membrane reactor configurations

Harro Mengers, Nieck Benes, Kitty Nijmeijer
Introduction

- How to obtain products from equilibrium limited reactions?

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

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

Catalytic membrane reactor (CMR)

Inert membrane reactor (IMR)

![Diagram of Catalytic Membrane Reactor (CMR)]

![Diagram of Inert Membrane Reactor (IMR)]
Theory

Model

- Reaction

- Bulk membrane reactor: CSTR

- Mass transport: Maxwell Stefan

\[ \Delta x_i = \sum_{i \neq j} \left( \frac{x_j N_i - x_i N_j}{k_{bl} c} \right) \]

- Only H₂O permeates through the membrane

- No mass transport limitations in IMR to reach catalyst particles
### Assumptions material and process conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{\text{in, overall}}$</td>
<td>100</td>
<td>mol/m$^3$</td>
<td>$A/V$</td>
<td>1000</td>
<td>1/m</td>
</tr>
<tr>
<td>$T$</td>
<td>150</td>
<td>°C</td>
<td>$k_f$</td>
<td>$10^{-2}$</td>
<td>(m$^3$)$^2$/mol$^2$·s</td>
</tr>
<tr>
<td>$x_{\text{in, A}}$</td>
<td>0.67</td>
<td>-</td>
<td>$k_{bl}$</td>
<td>$10^{-4}$</td>
<td>m/s</td>
</tr>
<tr>
<td>$x_{\text{in, B}}$</td>
<td>0.33</td>
<td>-</td>
<td>$P_{H2O}$</td>
<td>$10^{-6}$</td>
<td>mol/m$^2$·s·Pa</td>
</tr>
<tr>
<td>$V$</td>
<td>1</td>
<td>m$^3$</td>
<td>$P_A=P_B=P_E$</td>
<td>0</td>
<td>mol/m$^2$·s·Pa</td>
</tr>
<tr>
<td>$\tau$</td>
<td>100</td>
<td>s</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Theory

- **CMR**

- **IMR**
Results

![Graph showing the relationship between ζ [%] and log(K_{eq}) [-] with three regions marked as 1, 2, and 3. The graph also labels CMR and IMR.]
Results

\[ k_f \cdot C_A^2 \cdot C_B \ll \frac{k_f \cdot C_E \cdot C_{H2O}}{K_{eq}} \]
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 ($k_{bl}$)

![Graph showing CMR as a function of log($K_{eq}$) for different values of $k_{bl}$: $k_{bl} = 10^{-2}$, $k_{bl} = 10^{-4}$, $k_{bl} = 10^{-6}$.

Diagram illustrating a flow system with labeled components: Boundary layer, Catalyst, Membrane, and water flow paths.]
Results – Mass transfer coefficient ($k_{bl}$)

$\log(K_{eq})$ [-]

$\xi$ [%]

$IMR$

$k_{bl} = 10^{-2}$

$k_{bl} = 10^{-4}$

$k_{bl} = 10^{-6}$

Catalyst

Bulk

Boundary layer

Membrane

$H_2O$

$H_2O$
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$_2$O ($P_{H_2O}$)

\[
\begin{align*}
\frac{1}{k_{tot}} &= \frac{1}{k_{mem}} \\
\frac{1}{k_{tot}} &= \frac{1}{k_{mem}} + \frac{1}{k_{bl}}
\end{align*}
\]
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))