A CFD Analysis of the Operating Conditions of a Multitube Pd Membrane for H₂ Purification

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Introduction

The production of hydrogen is a major process for the chemical industry as well as for the energy sector. Using palladium membranes is an economic and efficient method to purify H₂. They remove H₂ by catalyzing the dissociation of the molecule at the surface and diffusing it through the lattice of the metal. The physics and geometry involved make the behavior of multitube membrane modules difficult to predict and simulate, but necessary for the implementation of this technology. This work uses COMSOL Multiphysics 4.4 to study the operating conditions of a seven membrane module. The influence of different Reynolds numbers on both, recovery and membrane utilization, is discussed. An optimum point to maximize the efficiency of the module is presented.

Computational Methods

To simulate the fluid flow and mass transport, the following equations were used:

Equation of motion:
\[
\rho ( \mathbf{u} \cdot \nabla ) \mathbf{u} = - \nabla p + \chi ( \mathbf{u} \cdot \nabla ) \mathbf{u} + f
\]

Species continuity equation:
\[
j_i = - \left( \mathbf{D} \mathbf{w} \right)_i + \mathbf{j}_i
\]

Sieverts’ law was used as the boundary to simulate the H₂ flux across the membranes:
\[
\gamma = \frac{J_{H_2}}{n_i \left( p_{H_2} - p_{H_2} \right) / R_T}
\]

Where \( J_{H_2} \) and \( p_{H_2} \) are the H₂ permeance, H₂ partial pressure in the shell and tube side, respectively.

Results

The multitube membrane module consists of seven Pd membranes (Fig.1). Hydrogen enriched syngas is fed at the shell side while the permeated H₂ gas is collected from inside of the membrane tubes.

Simulation setup

The simulation used “Reacting Flow” as the physics. Table 1. shows the parameters used in this simulation. “Fine” mesh was used for the simulation as shown in Fig. 2 with 3,181,368 degrees of freedom.

Table 1: Operational setting of the module

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shell Pressure / atm</td>
<td>12.6</td>
</tr>
<tr>
<td>Tube Pressure / atm</td>
<td>1</td>
</tr>
<tr>
<td>H₂ Permeance / mol m⁻² Pa⁻⁰.₅</td>
<td>7.7 × 10⁻⁴</td>
</tr>
<tr>
<td>Reynolds number</td>
<td>1-300</td>
</tr>
<tr>
<td>Initial gas composition / mole %</td>
<td></td>
</tr>
<tr>
<td>H₂</td>
<td>43</td>
</tr>
<tr>
<td>N₂</td>
<td>50</td>
</tr>
<tr>
<td>CO</td>
<td>5</td>
</tr>
<tr>
<td>CO₂</td>
<td>1.5</td>
</tr>
<tr>
<td>CH₄</td>
<td>0.5</td>
</tr>
</tbody>
</table>

Conclusions

1. Low Re numbers displayed high recoveries, but the membranes were utilized ineffectively.
2. High Re numbers use the membranes more evenly and reduced concentration polarization, but H₂ recovery decreased.
3. A tradeoff between usage of the membrane and H₂ recovery was successfully depicted. An optimized Re number was presented balancing both properties.

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