Theoretical comparison of micro-structured packed bed and fluidized bed membrane reactors for water gas shift reaction
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Abstract title: THEORETICAL COMPARISON OF MICRO-STRUCTURED PACKED BED AND FLUIDIZED BED MEMBRANE REACTORS FOR WATER GAS SHIFT REACTION

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1. Background

Water Gas Shift (WGS) is a well-known reaction step in the process of synthesis gas production which is used for upgrading H2 to CO ratio of the product. Due to the fact that the reaction is reversible and moderately exothermic, industrial WGS process is performed in multiple stages following by a Pressure Swing Adsorption (PSA) unit, where H2 is separated from other gases. During last few years more attention has been paid on hydrogen perm-selective membrane reactors which can integrate WGS reaction and in situ extraction of ultra-pure H2 in one-stage and accordingly shift the equilibrium and thus intensify the process.

2. Aims

Recently, micro-structured packed bed and fluidised bed membrane reactors have been introduced because of their superior heat and mass transfer characteristics as they can be used effectively for small scale hydrogen production. However, detail theoretical studies on the performance of these reactors have not been exploited yet for WGS reaction. Therefore, objective of this study is detail performance analysis of a micro-structured fluidized bed membrane reactor and a packed bed membrane reactor while quantitative comparison of these two reactor concepts for WGS reaction will be done through a modeling approach.

3. Methods

To model a packed bed membrane reactor the same continuum models available for packed bed reactors was used by considering permeation through the membrane as a source/sink term in 1 dimensional (1D) models. A 1D two-phase phenomenological model was developed for the simulation of a fluidized bed membrane reactor. It was assumed that WGS reaction takes place only in the emulsion phase. Hydrogen extracted through membranes from both bubble phase and emulsion phase while the amount of gas which is extracted from the emulsion phase is instantaneously replaced by bubble phase. Temperature is considered to be uniform through the whole fluidized bed reactor with no heat loss to the surroundings and without any heat transfer limitation between two phases.

4. Results

Table 1 shows preliminary comparison on mass transfer limitations between different reactor concepts while Figure 1 demonstrates more general comparison at 400 °C for different catalyst type and particle sizes inside a packed bed membrane reactor.

5. Summary / Conclusions

Results show that intrinsic rate of reaction, external diffusion limitation, the mass transfer resistance through the membrane and also diffusion limitation from bed to wall should be taken into account to be able to find the rate limiting phenomenon inside the membrane reactor. The same analysis was performed for micro-scale packed bed and fluidised bed membrane reactors where it will be discussed in detail later in the full paper.

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Images
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Reference equation</th>
<th>Value (1/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intrinsic rate of reaction</td>
<td>Regression</td>
<td>0.58</td>
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<tr>
<td>External mass transfer rate for packed bed</td>
<td>Thoenes &amp; Kramers</td>
<td>45.60</td>
</tr>
<tr>
<td>External mass transfer rate for fluidized bed</td>
<td>Froessling</td>
<td>560.33</td>
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<tr>
<td>External mass transfer rate for wall coated micro-channel</td>
<td>P. Van Male et al.</td>
<td>64.71</td>
</tr>
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Table 1. Preliminary comparison of mass transfer resistance
Fig 1. Comparison between mass transfer and kinetics at 400 °C.