CFD Simulation of Fisher-Tropsch Synthesis in Slurry Bubble Column

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Motivation & Objectives

• Internal FLUENT effort to provide guidelines and best practices for bubble column simulations with chemical reaction
• To study the effect of gas superficial velocity and slurry concentration on production rate
• 3D time dependent simulations
  – Gravity and drag are main interfacial forces acting on bubbles
• Production rate and syngas conversion was compared to 1D empirical model of C. Maretto & R. Krishna, Catalysis Today, 52, 1999
Model settings

- Euler/Euler three-phase model
- Industrial size column (H= 30 m, D= 7 m)
- Column operates in churn-turbulent regime
- Two bubble classes of 5 and 45 mm
- No coalescence/break up model assumed
- For each gas velocity two catalyst volume fractions were investigated: 20% and 35%
- Catalyst VOF defines bubble size distribution, slurry properties and CH₂ production rate
- Mesh size of ~30,000 prismatic cells
Inlet/outlet boundary zones

Inlet boundary
• Two different inlet gas velocities of 15 and 40 cm/sec
• Inlet area aerated at 50%
• Pressure at 30 bar and temperature at 240°C

Outlet boundary
• Implicit definition through degassing boundary condition with zero liquid axial velocity
• Outlet surface is velocity inlet boundary condition
• Values of all variables are defined through a UDF and extrapolated from adjacent cell center
• Gas vertical velocity is set to some value, say, 3-4 times gas superficial velocity
• Additional sources for any variable $\phi_{liq}$ in liquid phase are defined as:

$$S_{\phi_{liq}} = \phi_{liq} \left( \rho_{liq} \bar{U}_{liq} \cdot \bar{A}_{cell} / V_{cell} \right)$$
Drag law and turbulence model

- **Bubble size and drag law**
  - If bubble diameter is 1-10 mm, then
    \[ C_d = 0.666d_b \sqrt{g(\rho_{liq} - \rho_{gas})/\sigma} \]
  - If bubble diameter is larger than 1 cm, then
    \[ C_d = 2.6666 \]
  - One can also use effective single bubble size with churn turbulent regime such as it is between smallest and largest size

- **Turbulence model recommendations**
  - The following is a recommended procedure for choosing turbulence model
    - Standard k-eps model overestimates energy dissipation and results in stuck gas plume
    - RNG mixture model is recommended instead
    - If plume is stuck with RNG mixture, use RNG per phase or decrease \( C_\mu \) by factor of 10
Phase properties & numerical settings

- Slurry viscosity based on Einstein equation
  \[ \mu_{SL} = \mu_L \left(1 + 4.5 \varepsilon_S \right) \]
- Slurry density calculated as
  \[ \rho_{SL} = \rho_L \left(1 - \frac{\rho_L}{\rho_{SK}} \varepsilon_S \right) + \rho_p \varepsilon_S \]
- Density of Syngas \( \sim 7 \text{ kg/m}^3 \)

Numerical parameters
- For all simulations, a time step of \( \sim 0.01 \) was used
- For mixed and hex meshes, high UR factors and 4 iterations per time step are recommended
- All variables should be discretized with QUICK scheme
- If solution diverges during first iterations, discretize all variables with Upwind, run for 1-2 time steps, than switch back to QUICK
Chemical reaction

- Three phase model:
  - Small bubbles ~0.5 cm
  - Large bubbles ~4.5 cm
  - Slurry liquid
- Two stages Fischer-Tropsch synthesis
  - Heterogeneous:
    - \( \text{CO}_{\text{gas}} \rightarrow \text{CO}_{\text{liq}} \)
    - \( \text{H}_2\text{O}_{\text{gas}} \rightarrow \text{H}_2\text{O}_{\text{liq}} \)
  - Homogeneous
    - \( \text{CO}_{\text{liq}} + 2\text{H}_2_{\text{liq}} \rightarrow \text{CH}_2_{\text{liq}} + \text{H}_2\text{O}_{\text{liq}} \)
Reaction rates

• Homogeneous reaction rate in liquid is:
  • \( \text{CO}_{\text{liq}} + 2\text{H}_2_{\text{liq}} \Rightarrow \text{CH}_2_{\text{liq}} + \text{H}_2\text{O}_{\text{liq}} \)

\[
\dot{R}_{\text{hom}}^{\text{small/large}} = a\alpha_{\text{liq}} c_{\text{CO,liq}} c_{\text{H}_2,\text{liq}} \left( 1 + b c_{\text{CO,liq}}^2 \right)^{-1} \rho_{\text{cat}} \alpha_{\text{cat}}
\]

- Reaction constants
- Density and VOF of catalyst

• Heterogeneous reaction rate for CO is:
  • \( \text{CO}_{\text{gas}} \Rightarrow \text{CO}_{\text{liq}} \)

\[
R_{\text{het}}^{\text{small/large}} = \alpha_{\text{small/large}} \left( k_L a \right)_{\text{small/large}} \left( \frac{c_{\text{CO,small/large}}}{m_{\text{CO}}} - c_{\text{CO,liq}} \right)
\]

- Reduction of CO concentration at gas-liquid interface

CREL meeting 2004
Volume fraction evolution

Time evolution of VOF before and after reaction start-up

![Graph showing volume fraction evolution over flow time with different labels for large, small, large reaction, and small reaction.](graph.png)
Overall gas volume fraction

<table>
<thead>
<tr>
<th></th>
<th>J_{gas}, cm/s</th>
<th>15</th>
<th>15</th>
<th>40</th>
<th>40</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_{cat}$, %</td>
<td>20</td>
<td>35</td>
<td>20</td>
<td>35</td>
<td></td>
</tr>
<tr>
<td>VOF of small</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>bubbles [%]</td>
<td>0.94</td>
<td>3.16</td>
<td>0.7</td>
<td>2.5</td>
<td></td>
</tr>
<tr>
<td>Without reaction</td>
<td>0.045</td>
<td>0.21</td>
<td>0.07</td>
<td>0.46</td>
<td></td>
</tr>
<tr>
<td>With reaction</td>
<td>13</td>
<td>14</td>
<td>24</td>
<td>24</td>
<td></td>
</tr>
<tr>
<td>Overall gas</td>
<td>1.3</td>
<td>1.0</td>
<td>7.9</td>
<td>4.7</td>
<td></td>
</tr>
<tr>
<td>holdup [%]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Without reaction</td>
<td>13</td>
<td>14</td>
<td>24</td>
<td>24</td>
<td></td>
</tr>
<tr>
<td>With reaction</td>
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<td>7.9</td>
<td>4.7</td>
<td></td>
</tr>
</tbody>
</table>

Catalyst volume fraction strongly affects small bubble volume fraction but not overall holdup
VOF of large bubbles

• Results for $J_{gas}=40$ cm/sec, $\alpha_{cat}=20\%$ and $\alpha_{cat}=35\%$
VOF of small bubbles

- Results for $J_{\text{gas}} = 40$ cm/sec, $\alpha_{\text{cat}} = 20\%$ and $\alpha_{\text{cat}} = 35\%$

$\alpha_{\text{cat}} = 20\%$  \hspace{2cm} $\alpha_{\text{cat}} = 35\%$
Homogeneous reaction rates

- Results for $J_{\text{gas}} = 40$ cm/sec, $\alpha_{\text{cat}} = 20\%$ and $\alpha_{\text{cat}} = 35\%$

\[
\alpha_{\text{cat}} = 20\% \\
\alpha_{\text{cat}} = 35\%
\]
Comparison of production rate of CH₂

Time averaged values
\( \alpha_{cat}=20\% \) and 35%

Influence of catalyst concentration on production rate
p. rate(\( \alpha_{cat}=35\% \))/ p. rate(\( \alpha_{cat}=20\% \))
Syngas conversion ratio comparison

- At lower gas flow rate, conversion is almost independent of slurry concentration
- Conversion decreases with gas flow rate
Conclusion

- Bubble column simulation should be 3D and time dependent to capture essential dynamics.
- Turbulence model is essential to capture bubble plume movement.
- RNG k-eps per phase or mixture appears to ensure plume dancing, but it is very far from clear whether they predict turbulence field in liquid correctly.
- Two bubble size model with realistic chemistry appears to adequately predict main trends in real production size bubble column.
- Additional improvement can include bubble-bubble interaction with population balance.