3D Simulation of Bubbling Fluidized Bed Reactors for Sorption Enhanced Steam Methane Reforming Process

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Reactions

SE-SMR:
Sorption Enhanced Steam Methane Reforming

- SMR [Ni-based catalyst]
  1. $\text{CH}_4 + \text{H}_2\text{O} = \text{CO} + 3\text{H}_2 \quad \Delta H_{298} = 206 \text{ kJ/mol}$
  2. $\text{CO} + \text{H}_2\text{O} = \text{CO}_2 + \text{H}_2 \quad \Delta H_{298} = -41 \text{ kJ/mol}$
  3. $\text{CH}_4 + 2\text{H}_2\text{O} = \text{CO}_2 + 4\text{H}_2 \quad \Delta H_{298} = 165 \text{ kJ/mol}$

- CO$_2$ adsorption [CaO sorbent]
  $\text{CaO} + \text{CO}_2 = \text{CaCO}_3 \quad \Delta H_{298} = -178 \text{ KJ/mol}$
Reactions

Kinetics

SMR -- [Xu and Froment, AIChE J. 1989, 35, 88-96]

\[
R_1 = \frac{k_1}{p_{H_2}^{2.5}} \left[ \frac{p_{CH_4} p_{H_2O} - p_{H_2}^3 p_{CO}}{DEN^2} \right] \\
R_2 = \frac{k_2}{p_{H_2}} \left[ \frac{p_{CO} p_{H_2O} - p_{H_2}^2 p_{CO_2}}{DEN^2} \right] \\
R_3 = \frac{k_1}{p_{H_2}^{3.5}} \left[ \frac{p_{CH_4}^2 p_{H_2O} - p_{H_2}^4 p_{CO_2}}{DEN^2} \right]
\]

\[DEN = 1 + K_{CO} p_{CO} + K_{H_2} p_{H_2} + K_{CH_4} p_{CH_4} + K_{H_2O} p_{H_2O} / p_{H_2}\]

\[CO_2\] adsorption -- [Sun et al. 2008 CES, 63, 47-56 ]

\[
R = \frac{dX}{dt} = 56 k_s \left(1 - X\right) \left(P_{CO_2} - P_{CO_2,eq}\right)^n S
\]
Reactor

bubbling fluidized beds---BFB

H₂+H₂O

CH₄  H₂O

SESMR
Model

- Two-Fluid approach
- Kinetic theory of granular flow
- $k$-$\epsilon$ turbulent model for gas phase
- Non axi-symmetry 3D
- Cylindrical coordinates
- Reactions
Simulation results

- Solid flow pattern

Toroidal vortex

- AWDC----ascending near the wall and descending at the center
- ACDW----ascending at the center and descending near the wall
Simulation results

- Standard SMR

-- axial distribution of components fraction and solid fraction

\[ y_{CH_4}^{dry}, y_{CO_2}^{dry}, y_{H_2}^{dry}, c_{CO_2}^S, \alpha_s \]
Simulation results

- **SE-SMR**
  
p=1bar, S:C=5:1
  
  -- axial distribution of components fraction and solid fraction
Simulation results

- **SE-SMR**
  
  \[ p = 1 \text{bar}, \ S:C = 5:1 \]

  -- axial distribution of components fraction and solid fraction

\[
\begin{align*}
\nu_0 &= 0.3 \text{m/s} \\
T &= 1098 \text{K} \\
t &= 49 \text{s}
\end{align*}
\]
Simulation results

- **SE-SMR**

  \[\text{p}=1 \text{bar}, \ S:C=5:1\]

  -- axial distribution of components fraction and solid fraction

\[\begin{align*}
\nu_0 &= 0.3 \text{m/s} \\
T &= 848 \text{K} \\
t &= 210 \text{s}
\end{align*}\]
Simulation results

- Steam-to-carbon ratio and pressure

  -- outlet CH₄ fraction

\[ \nu_0 = 0.3 \text{m/s} \quad T = 848 \text{K} \]
Simulation results

- Steam-to-carbon ratio and pressure

  -- outlet $H_2$ fraction

![Graph showing outlet $H_2$ fraction over time for different steam-to-carbon ratios and pressures.]

- $v_0 = 0.3 \text{ m/s}$
- $T = 848 \text{ K}$

Legend:
- SMR, S:C = 5:1, P = 1 bar
- SMR, S:C = 3:1, P = 1 bar
- SMR, S:C = 5:1, P = 10 bar
- SESMR, S:C = 5:1, P = 1 bar
- SESMR, S:C = 3:1, P = 1 bar
- SESMR, S:C = 5:1, P = 10 bar
Simulation results

- Steam-to-carbon ratio and pressure
  -- outlet CO$_2$ fraction

\[ u_0 = 0.3 \text{ m/s} \quad T = 848 \text{ K} \]
Simulation results

- SE-SMR
  -- adsorption of CO\textsubscript{2} by sorbent
Simulation results

- SE-SMR
  - Temperature distribution (vertical cross sectional and averaged axial)
• This model can depict the main characteristics of solid flow patterns obtained experimentally in bubbling fluidized bed.

• The integration of CO₂ sorption to the SMR process can increase the methane conversion to about 100% and make more effective energy utility, which results in the more uniform temperature distribution within the bed.

• High pressure and low steam-to-carbon ratio will decrease the conversion of methane. But the high pressure makes the adsorption of CO₂ faster.

• CO₂ can be adsorbed by CaO sorbents near totally under the simulated conditions of SE-SMR process.
Thank you!