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. $CH_4+H_2O=CO+3H_2$ $\Delta H_{298}=206$ kJ/mol
  2. $CO+H_2O=CO_2+H_2$ $\Delta H_{298}=-41$ kJ/mol
  3. $CH_4+2H_2O=CO_2+4H_2$ $\Delta H_{298}=165$ kJ/mol

- CO_2 adsorption [CaO sorbent]

  $CaO + CO_2 = CaCO_3$ $\Delta H_{298}=-178$ KJ/mol

Reactions

Kinetics

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

$$R_1 = \frac{k_1}{p_{\mathrm{H_2}}^{2.5}}\left[\frac{p_{\mathrm{CH_4}} p_{\mathrm{H_2O}} - p_{\mathrm{H_2}}^3 p_{\mathrm{CO}} / K_1}{\mathrm{DEN}^2}\right] \qquad R_2 = \frac{k_2}{p_{\mathrm{H_2}}}\left[\frac{p_{\mathrm{CO}} p_{\mathrm{H_2O}} - p_{\mathrm{H_2}} p_{\mathrm{CO_2}} / K_2}{\mathrm{DEN}^2}\right]$$

$$R_3 = \frac{k_1}{p_{\mathrm{H_2}}^{3.5}}\left[\frac{p_{\mathrm{CH_4}} p_{\mathrm{H_2O}}^2 - p_{\mathrm{H_2}}^4 p_{\mathrm{CO_2}} / K_3}{\mathrm{DEN}^2}\right]$$

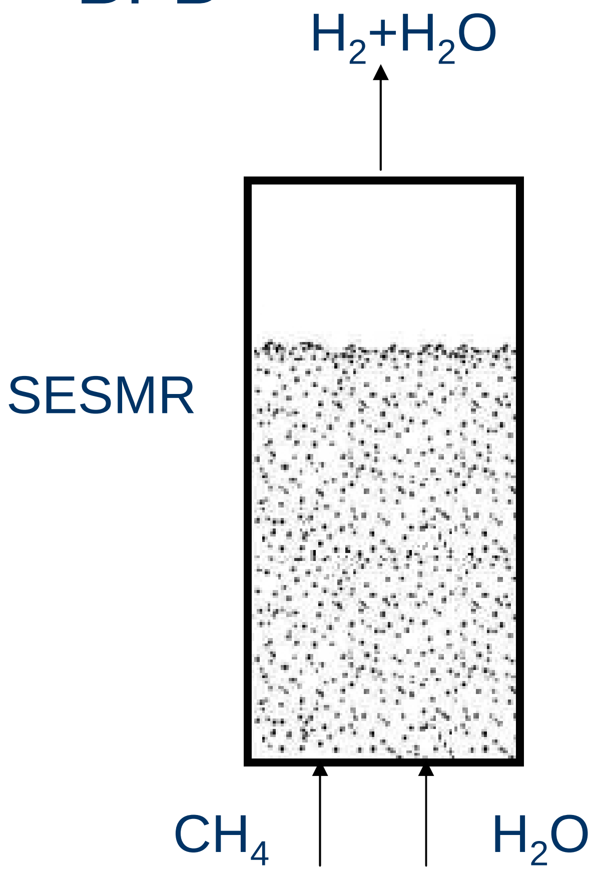
$$\mathrm{DEN} = 1 + K_{\mathrm{CO}} p_{\mathrm{CO}} + K_{\mathrm{H_2}} p_{\mathrm{H_2}} + K_{\mathrm{CH_4}} p_{\mathrm{CH_4}} + K_{\mathrm{H_2O}} p_{\mathrm{H_2O}} / p_{\mathrm{H_2}}$$

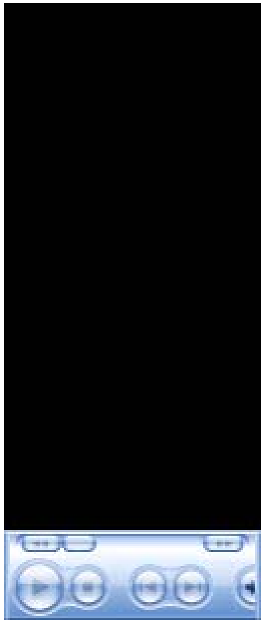
CO_2 adsorption -- [Sun et al. 2008 CES, 63, 47-56]

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

Reactor

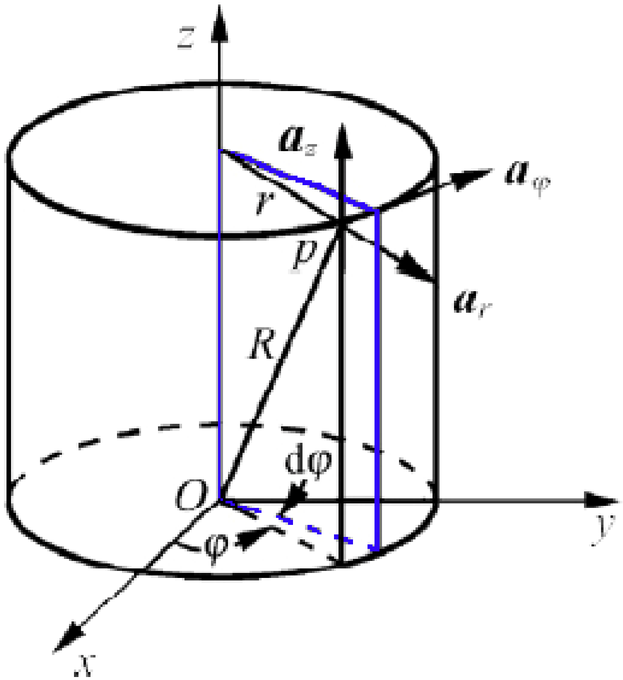
bubbling fluidized beds----BFB





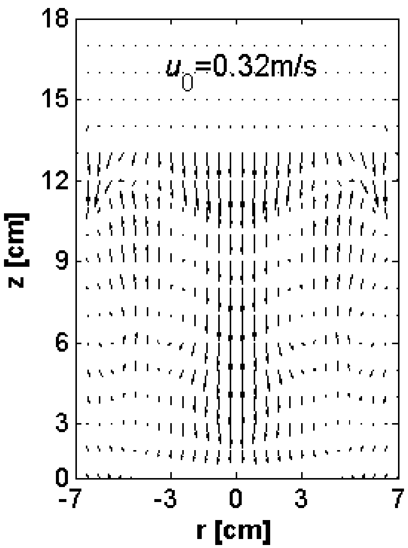
Model

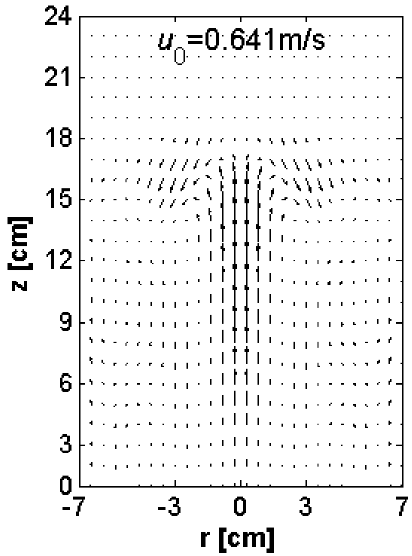
- Two-Fluid approach
- Kinetic theory of granular flow
- *k-ε* turbulent model for gas phase
- Non axi-symmetry 3D
- Cylindrical coordinates
- Reactions

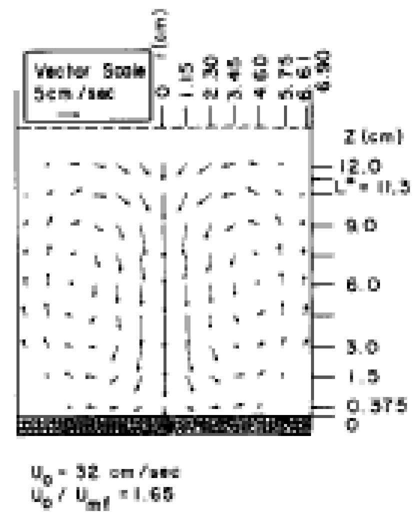


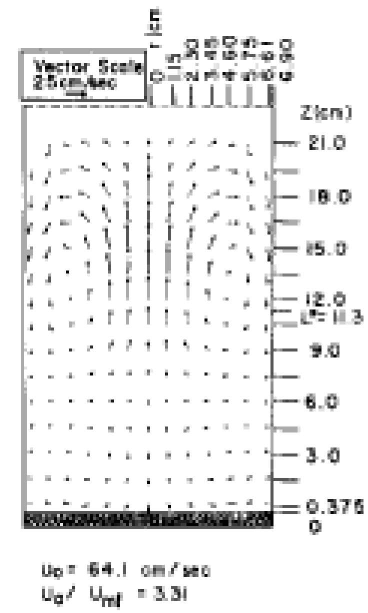
Simulation results

- Solid flow pattern









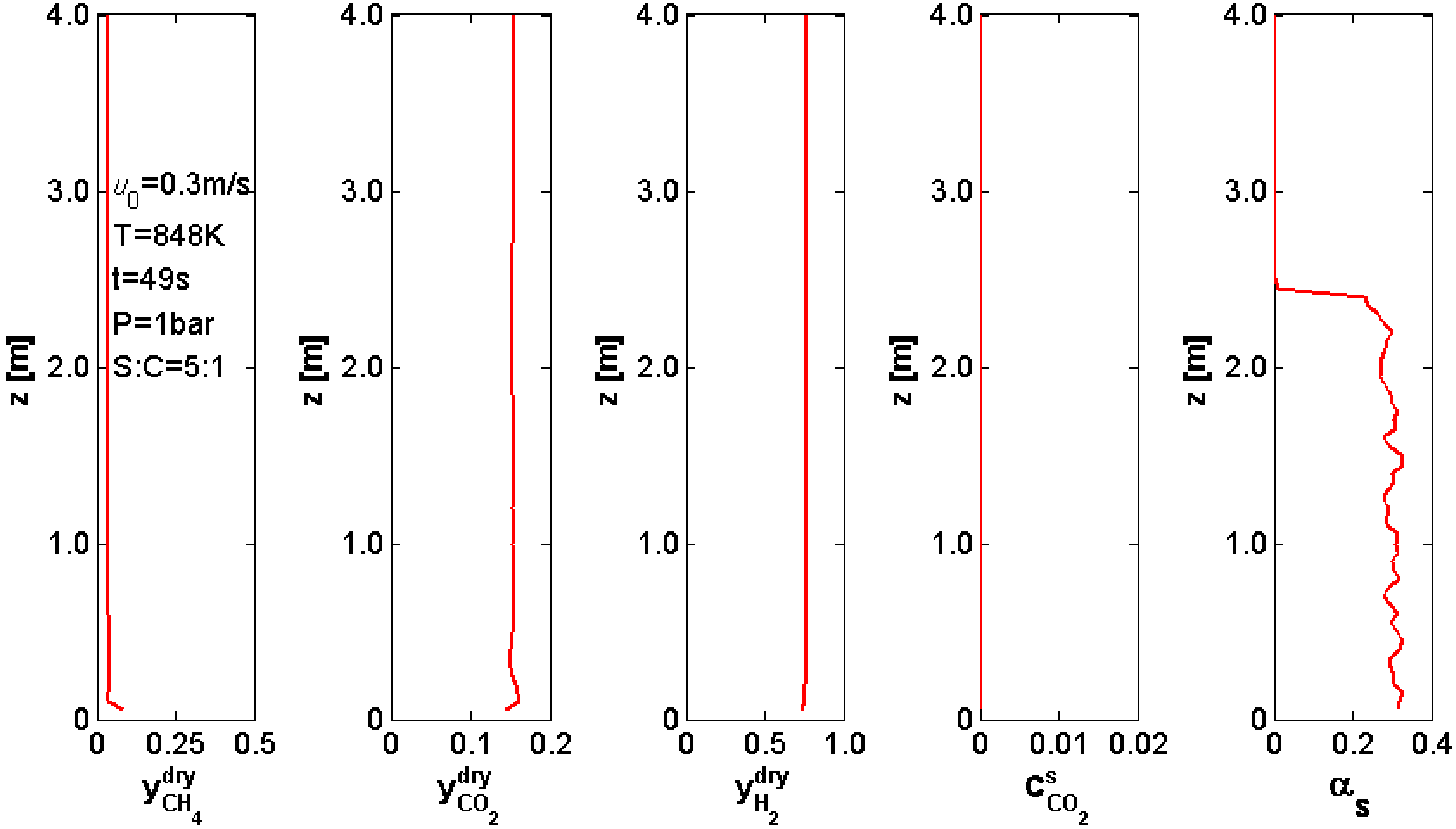
Toroidal vortex

- 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

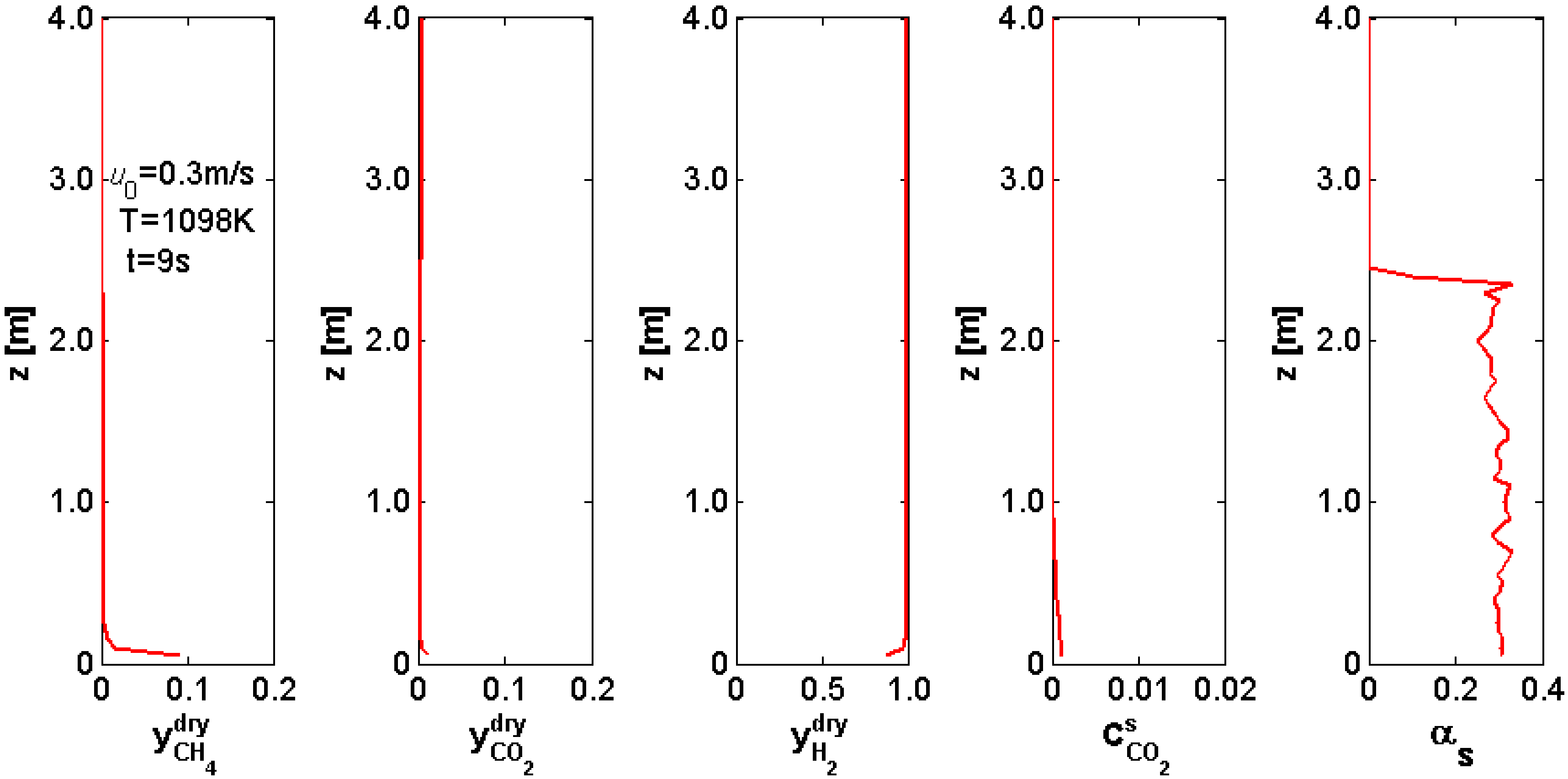


Simulation results

- SE-SMR

p=1bar, S:C=5:1

-- axial distribution of components fraction and solid fraction



Simulation results

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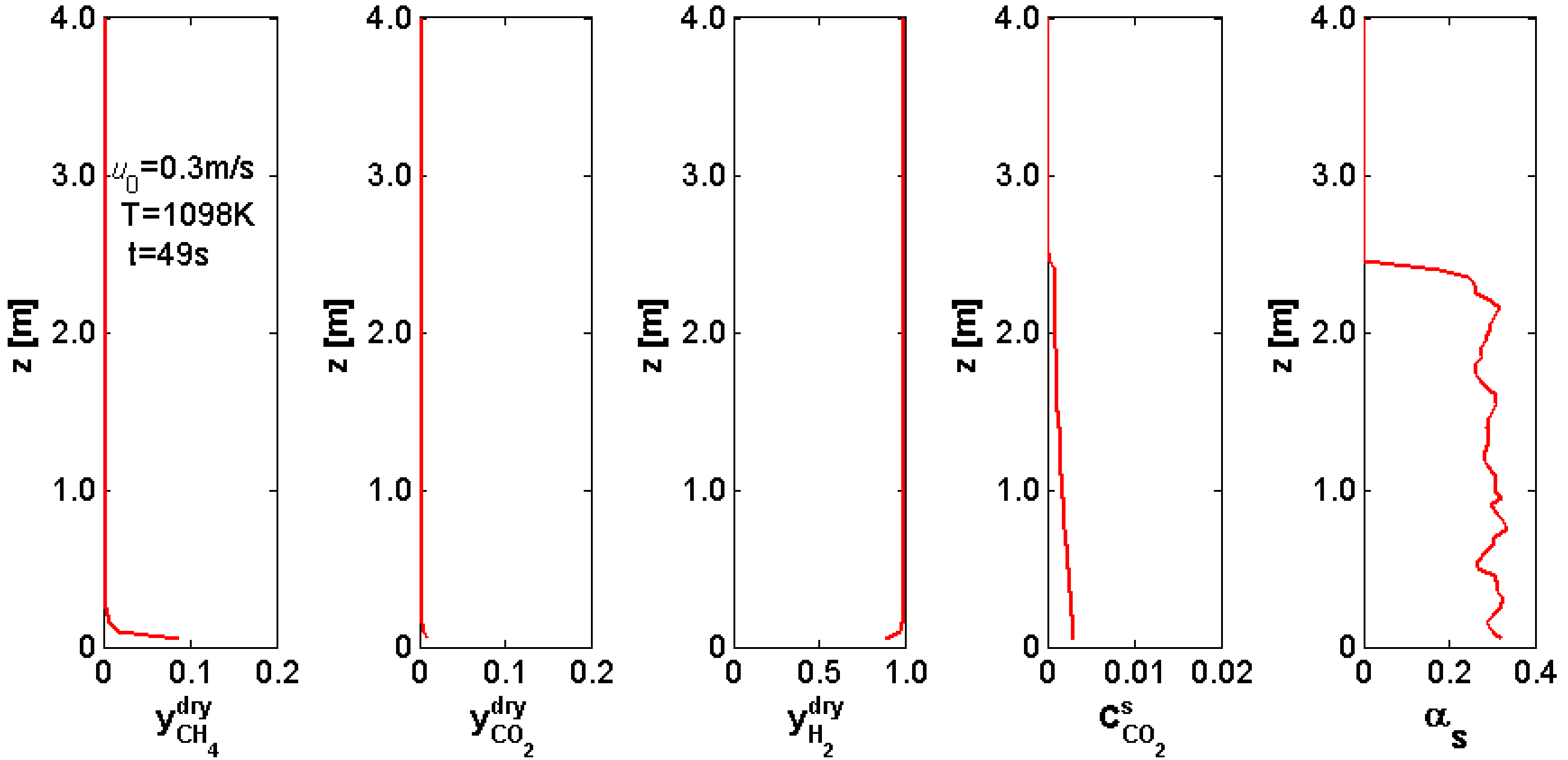

Simulation results

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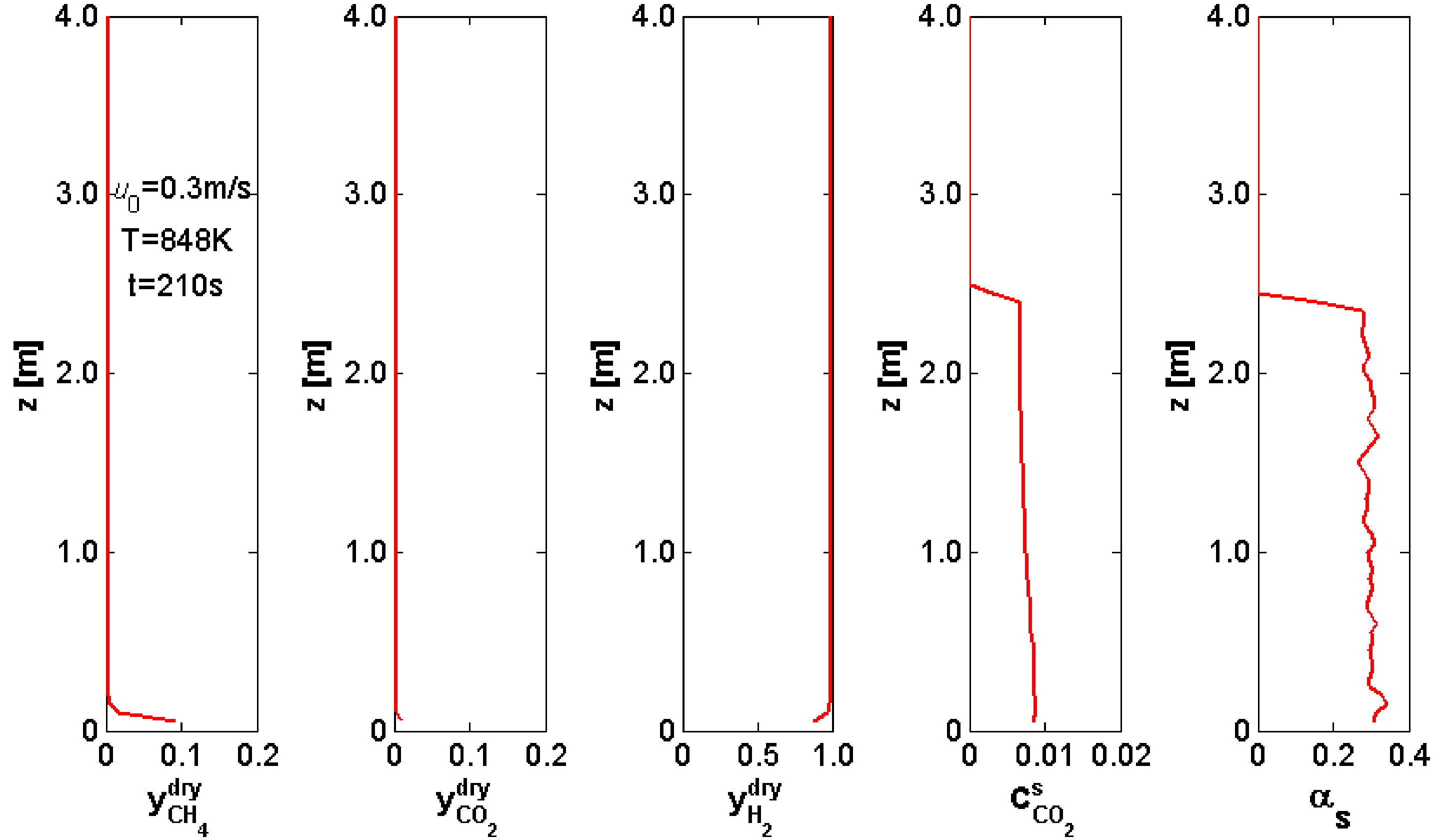
p=1bar, S:C=5:1

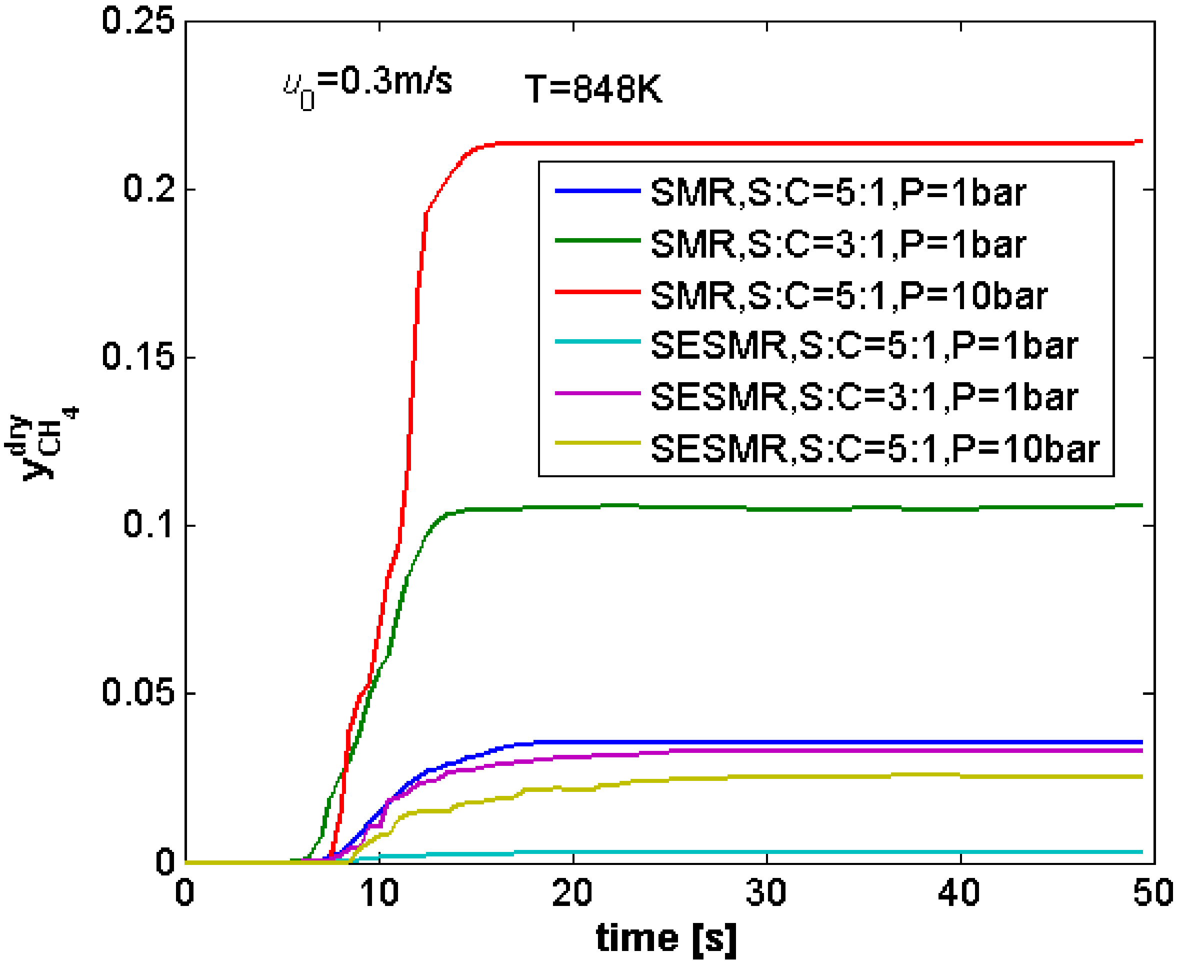
-- axial distribution of components fraction and solid fraction



Simulation results

- Steam-to-carbon ratio and pressure

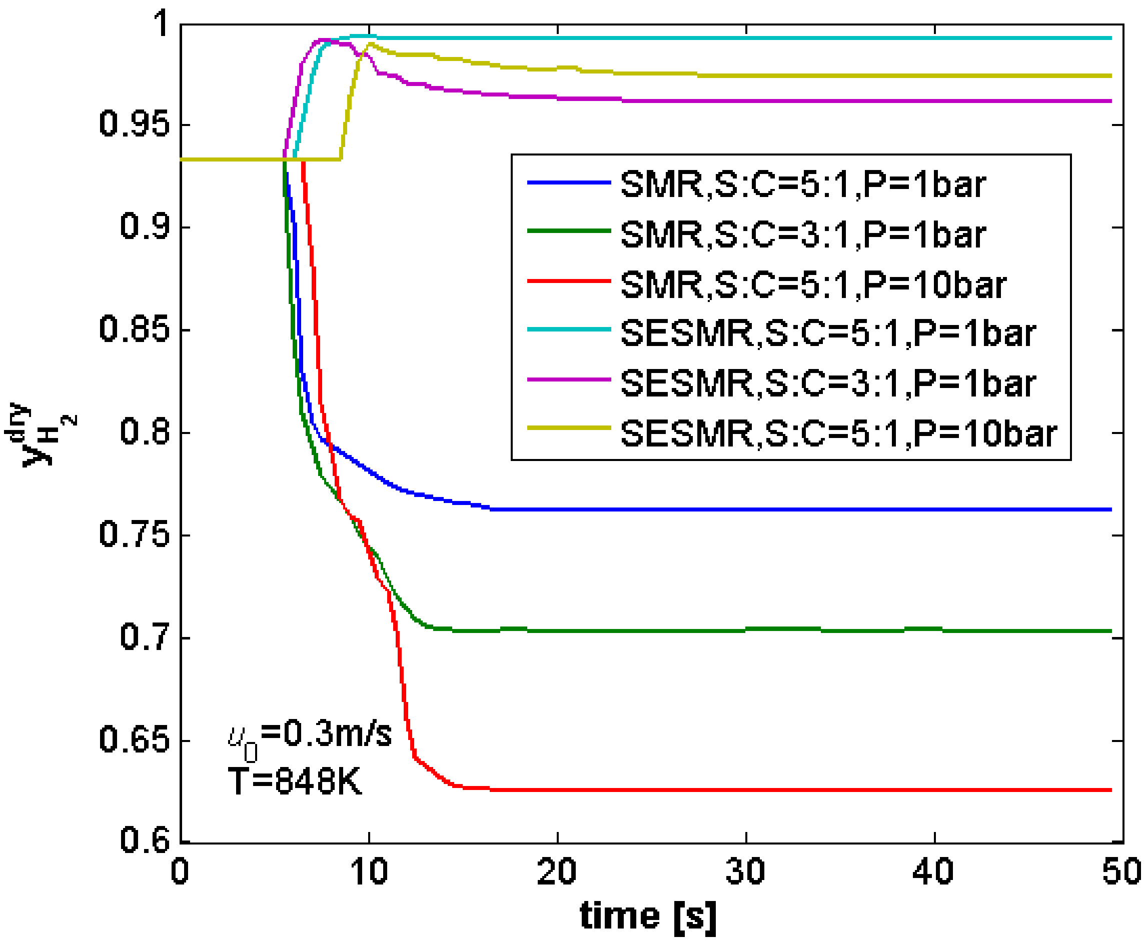
-- outlet CH_4 fraction



Simulation results

- Steam-to-carbon ratio and pressure

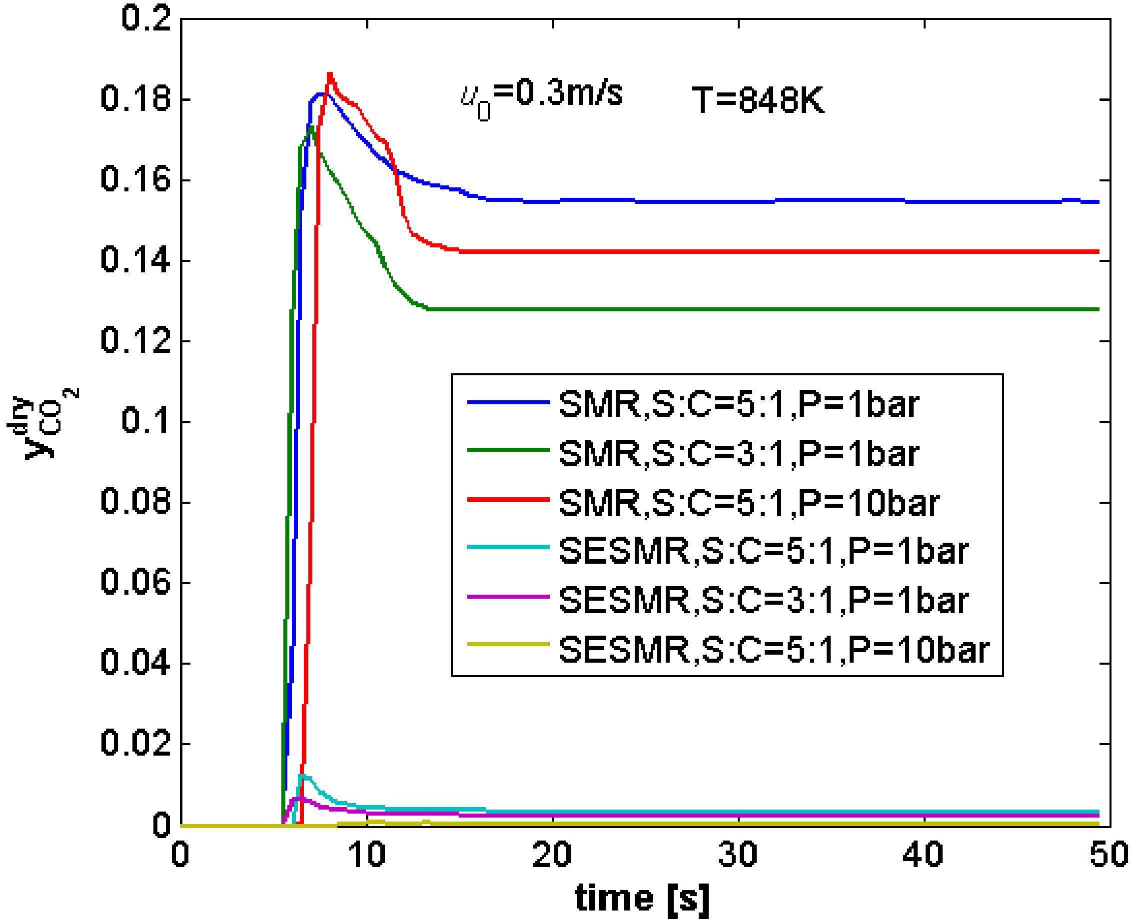
  -- outlet H_2 fraction



Simulation results

- Steam-to-carbon ratio and pressure

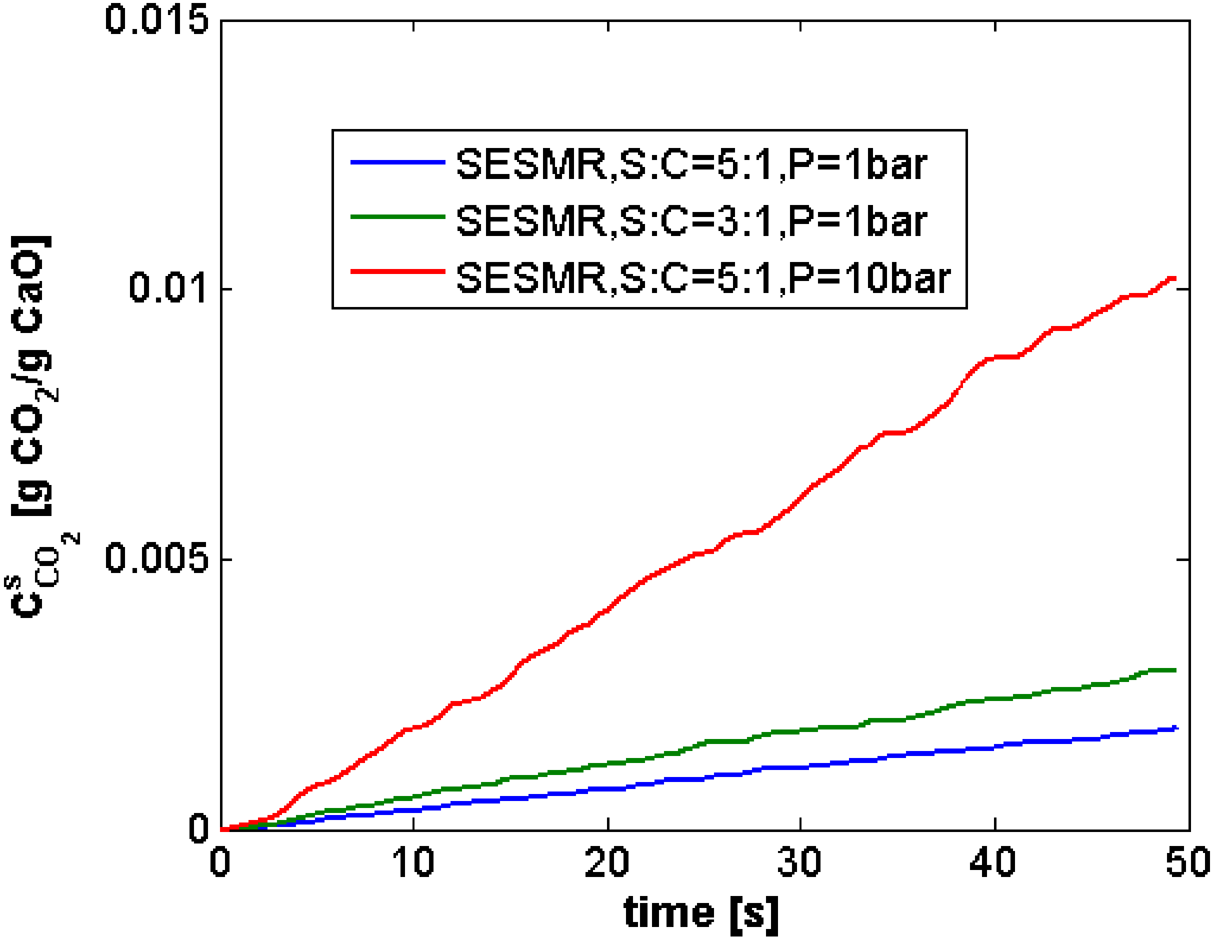
  -- outlet CO_2 fraction



Simulation results

- SE-SMR

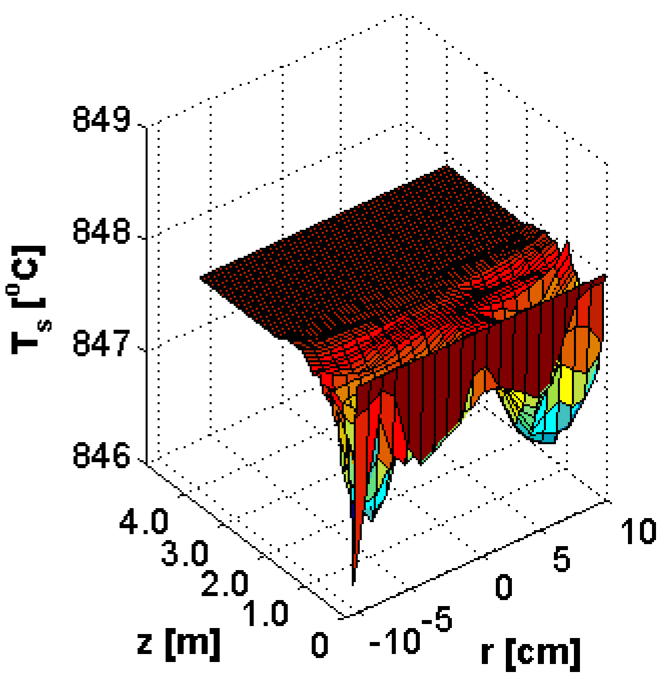
-- adsorption of CO_2 by sorbent

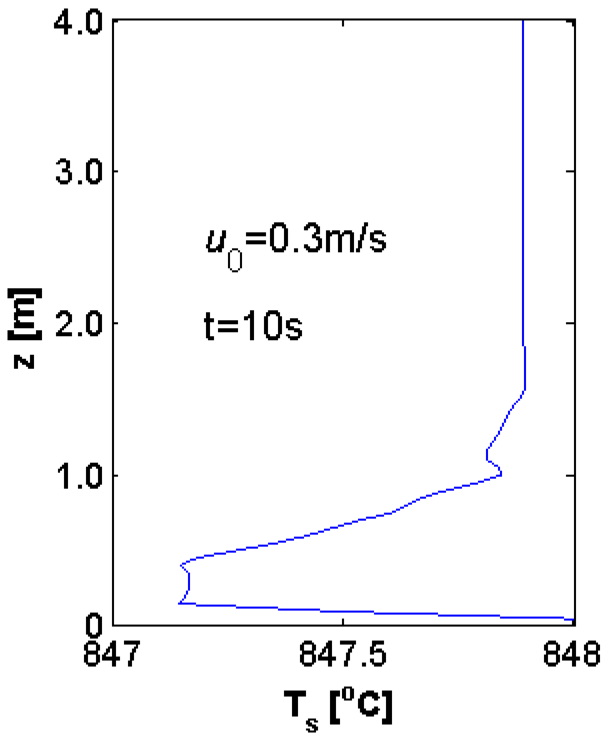


Simulation results

- SE-SMR

-- Temperature distribution (vertical cross sectional and averaged axial)





Conclusion

- This model can depict the main characteristics of solid flow patterns obtained experimentally in bubbling fluidized bed.
- The integration of CO_2 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 CO_2 faster.
- CO_2 can be adsorbed by CaO sorbents near totally under the simulated conditions of SE-SMR process.

Thank you!