Modelling of carbon dioxide methanation in radial flow reactor

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Highlights

- MCN model proposed for sorption-enhanced CO_2 methanation in a radial reactor.
- Ni-Ce/13X kinetics and H_2O adsorption were implemented in dynamic simulations.
- Water adsorption delayed breakthrough, and MCN trends agreed with the PBR.

1. Introduction

Power-to-Gas routes can valorize captured CO_2 by hydrogenation to synthetic methane. Because CO_2 methanation is strongly exothermic and transport-sensitive, radial flow reactors are attractive owing to low pressure drop and better heat-management potential. This work develops a preliminary sorption-enhanced radial-reactor model using a bifunctional Ni-Ce/13X catalyst and compares it with an equivalent tubular packed-bed reactor.

2. Methods

A dynamic, pseudo-homogeneous two-dimensional mixing cell network (MCN) represented the radial packed bed as interconnected stirred cells. CO_2 methanation kinetics for the Ni-based catalyst were coupled with H_2O adsorption on zeolite 13X through a linear driving force model. Simulations were isothermal and compared to a tubular packed-bed reactor of equal bed volume using the same operating and kinetic parameters. The radial reactor was discretized as a 10×10 grid, with cell-to-cell outflow splitting described by a constant ratio.

3. Results and discussion

The MCN reproduced the expected sorption-enhanced behavior: water breakthrough was delayed by adsorption, and CO_2/H_2 conversion to CH_4 was favored during the pre-breakthrough period. Cellwise concentration profiles showed stronger CO_2 depletion near the inlet-side region, consistent with equilibrium shifting toward products as H_2O was removed from the gas phase.

Compared with the tubular packed-bed reactor, the radial model predicted a slightly shorter enhancement period and a delayed post-saturation steady state. These deviations were attributed to residence-time distribution and numerical diffusion caused by cell-to-cell flow splitting. Overall, the agreement supports the MCN framework as a feasible first approximation for radial sorption-enhanced methanation.

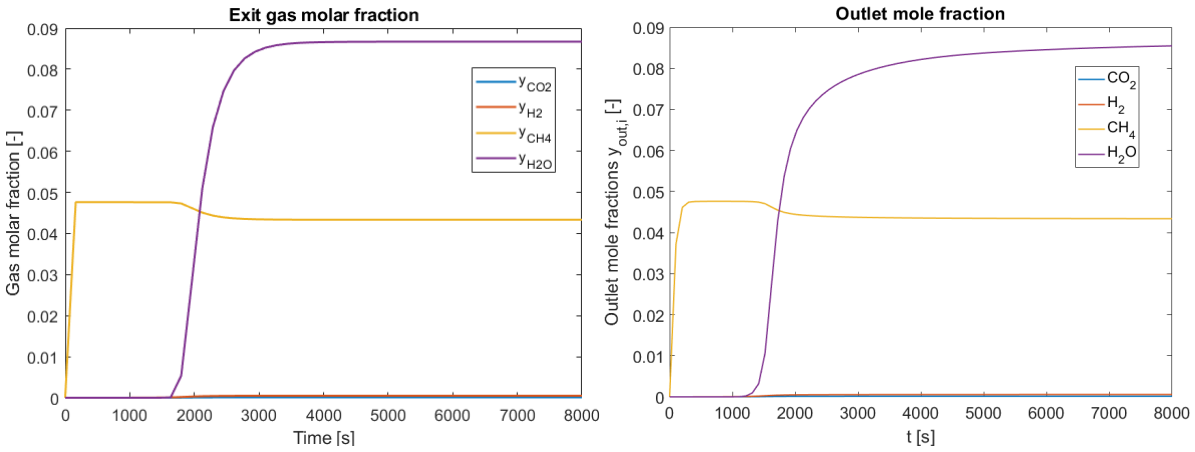

Figure 1 *Outlet molar fractions of the participant to the reaction versus time in tubular packed bed reactor (left) and radial flow reactor (right); the inert (helium) was excluded for reading purposes.*

4. Conclusions

The proposed MCN framework successfully integrates methanation kinetics and water adsorption for sorption-enhanced CO_2 methanation in a radial flow reactor. Preliminary results are consistent with tubular-PBR trends while better preserving the radial-reactor topology.

References

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Keywords

Radial flow reactor; CO_2 methanation; Sorption-enhanced methanation; Mixing cell network