Modelling of methane partial oxidation in an asymmetric multilayered membrane reactor

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INTRODUCTION

- Dense O₂ permeable Mixed Ionic Electronic Conductors (MIEC) ceramic membranes have great potential for catalytic high-temperature processes.
- Permeability, however, may become limited by bulk diffusion, if the membrane becomes too thick.
- A promising approach is the consecutive deposition of MIEC nanocomposite layers with graded porosity and chemical composition on a robust macroporous substrate.
- In the framework of the OCMOL project asymmetric MIEC supported membranes are designed aiming at the separation of O₂ from air.
- In the current work, a mathematical model of a multilayered membrane reactor is developed and validated with previously reported experimental data.

COMPARISON OF SIMULATED AND EXPERIMENTAL RESULTS

Effect of CH₄ inlet flow rate

- Increase of CH₄ flow rate leads to a decrease of its conversion.
- Increase in syngas production due to the higher participation of reforming reactions over combustion.
- Adequate prediction of methane conversion.
  - O₂ flux through the membrane predicted correctly by the model.
  - Selectivity in CO and H₂ follows the experimental trends.

Effect of CH₄ inlet concentration

- CH₄ conversion satisfactorily predicted.
  - Slight drop due to the changing balance between the O₂ that diffuses through the air side and the available CH₄ at the reaction side.
  - Change in balance leads to a higher production of syngas, which is adequately reproduced by the model.

Effect of air side flow rate

- Experimental decrease in CH₄ conversion attributed to the possible oxidation of the catalyst due to the low saturation of CH₄.
- Simulations show, as expected based on the simple kinetic scheme implemented, an increase in CH₄ conversion.
- Experimentally observed drop in CO and H₂ due to higher fraction of oxidation over reforming reactions is predicted by the model, although less pronounced in order.

CONCLUSIONS

- A CH₄ partial oxidation membrane reactor model has been constructed assuming diffusion through meso- and micro-porosities layers deposited on top of the dense layer.
- The model has been validated against experimental data, obtaining a good qualitative agreement.
- The model could be further enhanced by:
  - including more detailed kinetic models
  - accounting for oxygen adsorption on and transport through the dense layer

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http://www.ocmol.eu
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