

Numerical simulations of a membrane assisted reactor concept for hydrogen production

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Highlights

- A two-fluid model was extended to simulate membrane assisted reforming in fluidized beds
- The model was used to study hydrogen extraction from a steam-methane reforming process
- Membranes near the walls perform much worse compared to their center-based counterparts
- The reaction stays far from its equilibrium near the membranes

1. Introduction

On an industrial scale, more than 80% of the hydrogen is currently produced by steam reforming (SR) of natural gas/methane, followed by a water-gas shift (WGS) reaction and a purification step (e.g. pressure swing adsorption). The main drawbacks are the thermodynamic equilibrium of the endothermic reforming reaction, and the large number of process steps that decrease the system efficiency.

To deal with these drawbacks, this project introduces a novel reactor concept for the production of ultra-pure hydrogen with integrated CO₂ capture, based on membrane-assisted chemical-looping reforming of methane. The concept consists of two interconnected fluidized bed reactors (see Figure 1). In the air reactor, a metal oxygen carrier particle (e.g. copper or nickel) is oxidized in air. The hot metal oxide (MeO) is then transported to the fuel reactor where it is reduced, generating the heat to perform the SR and WGS reactions. The produced hydrogen is separated in-situ via hydrogen perm-selective membranes, drawing the equilibrium to the product side and allowing operation at lower temperatures.

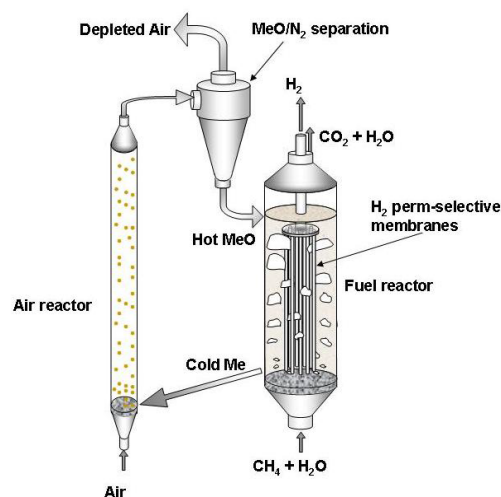


Figure 1. Chemical looping reforming reactor concept with H₂ perm-selective membranes for ultra-pure H₂ production.

Design questions arise because of the high cost of palladium-based membranes. The performance and placement of the membranes is important, because the high fluxes that can be achieved with state-of-the-art membranes can cause depletion of hydrogen near the membrane surface (a phenomenon called concentration polarization), which limits the membrane performance. This work investigates various aspects on the membrane performance in the reactor concept using numerical simulations.

2. Methods

The fluidized bed hydrodynamics is simulated using a Two-Fluid model (TFM), and Euler-Euler type model. The TFM is a Computational Fluid Dynamics model based on the OpenFOAM 2.3.0 framework. We have extended the model with chemical species transfer, chemical reactions and hydrogen extraction via the membranes, and perform extensive validation (Voncken et al., 2017a,b).

3. Results and discussion

The verified and validated model is currently used to investigate various design aspects of the fuel reactor. An important consideration is that the grid near the membranes should be refined, allowing a high-detail simulation of the mass transfer and extraction via the membranes. The performance of fluidized beds with various horizontally immersed membrane tube bank configurations were investigated with 2D simulations.

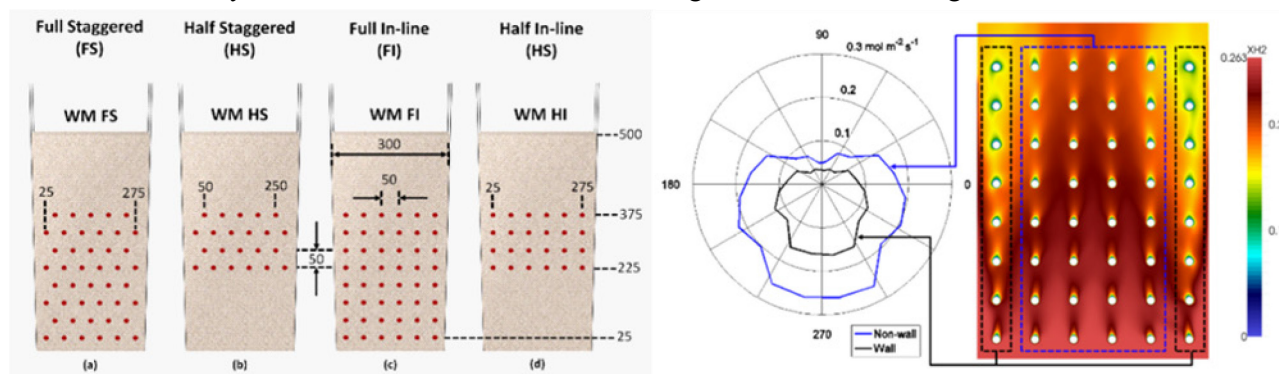


Figure 2. (left) Membrane tube bank configurations; (right) Simulation result – the polar plot indicates fluxes through the membranes, the snapshot shows the hydrogen concentration in the reactor.

We will show the influence of the membrane placement on the hydrogen extraction and reaction, and offer detailed design rules. For instance, in Figure 2 it can be seen that the membranes on the reactor sides perform much worse compared to the membranes located at the reactor center. We are also observing a strong increase in the reaction rate near the membranes due to the extraction of hydrogen in these zones. Moreover, we will extend the simulations to 3D and analyze the results. Different numbers of membranes in bundles will be inserted in the reactor, and we will relate our 2D findings to the actual 3D cases.

4. Conclusions

We show the validity of a newly extended Two-Fluid model for the simulation of membrane assisted fluidized bed reactors, and show how we can use the model to optimize the performance and design of this type of reactors.

References

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Keywords

Fluidized bed; simulation; hydrogen; membrane;