

An interdigitating integrated reformer-combustor reactor design based on space-filling curves

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1. Introduction

Several strategies are being adopted worldwide to tackle the environmental problems arising from the use of fossil fuels. Developing energy efficient systems is one of them. This work proposes a novel reactor design for more efficient reforming of Methanol to generate hydrogen that can be utilized in on-board or stationary fuel cell (FC) system.

We consider the case of a Methanol steam reformer (MSR) for hydrogen generation that will be used in a low temperature PEM fuel cell. High temperature gradients inside the reformer reactor lead to lower energy efficiency and higher levels of undesirable CO [1]. Folded sheet, shell & tube, concentric cylinder and other types of reformer designs have been explored in the literature. In these designs packed bed reactors were used and temperature difference across the walls of over 100 degree C has been reported [1]. We propose a novel reactor architecture based on space filling curves [2] that aims to reduce this temperature difference considerably. Intimate contact between the two streams is ensured by the interdigitation of the wall in such a way that a high wall surface is created. Figure 1 shows the details of the novel reactor in which Hilbert's 3rd order space filling curve describes the shape of the wall within the enclosed cross-section. The wall divides the reactor into the reforming side and the combustion side in which two streams can flow without mixing. Due to temperature difference between the combustion side wall interface and the reforming side, heat is transferred across the wall to sustain the endothermic reforming reaction. The thin metal wall offers much less resistance to and provides more surface area for heat flow than a packed bed of catalyst particles.



Figure 1. Hilbert 3rd order reactor (42.4×41.6×300 mm) geometry: (a) frontal view of the inlet or outlet; (b) isometric view of the reactor, and (c) schematic illustration of catalyst coating on wall interfaces.

2. Methods

To demonstrate the concept of heat integrated reformer-combustor reactor, a 5 kWe FC system was chosen. Thermodynamic analysis was performed using Aspen Plus simulation. Operating parameters and molar composition of hot and cold side streams were derived from this analysis. CFD simulations were then carried out in ANSYS FLUENT simulator to determine the temperature profiles and Methanol conversion. An ideal reactor design would give complete conversion with no excess heat in the reformate, which is possible only with uniform temperature distribution in the reformer. Reaction kinetics were referred from literature [3, 4]

and suitably adapted to this configuration. Co-current flow was employed in the reactor where reaction takes place on the interface wall surface both in reformer and combustor zone. The external faces of the reactor were rendered adiabatic. Steel wall of thickness 0.8 mm was specified. Hot and cold side velocities were 2.34 and 2.88 m/s respectively. 50% excess air was sent in the combustor to prevent overheating of the reformer zone. The flow was laminar with Re ~ 1500 on both the sides. In reformer, Steam to Carbon mole ratio of 1.1 was chosen. Reforming was carried out at a temperature of 250 °C and 1 atm pressure. Structured mesh was created in the CFD software ANSYS with body sizing (0.25 mm element size) and sweep method, resulting in about 3.3 million cells. The 'SIMPLE' solver was used to solve continuity, energy and species balance equations with specified overall reaction kinetics for the catalytic reactions [5].

3. Results and discussion

Combustion was carried out in outer fluid zone with three external surfaces and reforming in inner one with one external surface, to maximize Methanol conversion. A peak temperature of 1334 K was reached inside the reactor. As the highly exothermic reaction on combustion side of the wall creates driving force for heat transfer to the reforming side, heat is readily conducted into the endothermic reforming zone through the metal wall. The temperature contour plots are presented in Figure 2. The average temperature on reformer inlet and outlet faces is 563 K and 946 K respectively, whereas that on combustion inlet and outlet faces is 392 K and 812 K respectively. Higher velocity on combustor side explain lower temperature in the zone.

Near-complete Methanol conversion (96.15%) is achieved at the outlet of the reformer. However, it is observed that about 94.2% of Methanol is converted just in half the length of the reactor, indicating that reactor is currently oversized. There is further scope for optimization in that the temperature in the reformer can be reduced by either sending further excess air or restricting the reaction by feeding less than stoichiometric amount of air in the combustor. Lower Methanol conversion near external face can be rectified by surrounding the reformer zone completely by the outer combustion zone. Further calculations, with a higher-order Hilbert curve are in progress along these lines.



Figure 2. (a) Temperature and (b) Methanol mole fraction contour plots at inlet, outlet and sweep surface(s) at intermediate locations.

4. Conclusions

A novel integrated combustor-reformer reactor design based on space filling curves has been proposed. Steam reforming of Methanol and combustion of fuel cell anode off-gas was successfully simulated on respective interfacial wall surfaces using a commercial CFD software. Near-complete Methanol conversion with reasonable combustion temperatures was achieved. Further optimization studies are being carried out to supply just the required amount of heat from combustor to reformer while maintaining uniform temperature in the reformer channels.

References

- [1] Morillo, A. Freund, C. Merten, Ind. Eng. Chem. Res., 43 (2004) 4624-4634.
- [2] H. Sagan, Space-Filling Curves, Springer, New York, 1994.
- [3] H. Purnama, T. Ressler, R.E. Jentoft, H. Soerijanto, R. Schlögl, R. Schomäcker, Applied Catalysis A : General, 259 (2004) 83-94.
- [4] V. N. Nguyen, R. Deja, R. Peters, L. Blum, D. Stolten, Int. J. Hydrogen Energy, 43 (2018) 17520-17530.
- [5] S. Jayanti, Computational Fluid Dynamics for Engineers and Scientists, Springer, Dordrecht, 2018.