Computational Fluid Dynamic Studies of Autothermal Spiral Reactor

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Abstract. This research applied the fundamental concept of spiral heat exchanger to design a new reactor for autothermal coupling endo- and exothermic reactions. The autothermal coupling endo- and exothermic reactor can be used when heat have to be removed from exothermic reactions (heat source). Such heat is then used for endothermic reactions (heat sink) that requires high operating temperature. This brings various benefits in terms of energy saving, economics and environment. In this study, the Computational Fluid Dynamics (CFD) was utilized to predict the performance of the spiral heat exchanger. The optimal operating conditions i.e. pressure drop, velocity and temperature distribution were studied. Low fluid velocity was observed without dead and hot spot zone along the radius flow of the channel and good temperature distribution was noticed.

1. Introduction

Process integration (PI) is considered as the most significant methodologies in chemical process engineering. It combines several processes to reduce the consumption of energy and materials or environmental emissions [1]. It can also reduce size of equipment by several orders of magnitude resulting in substantial savings of capital cost or improvement of intrinsic safety. The study on PI started in the late 1970s and early 1980s [2] including hierarchical design methods, knowledge-based systems, numerical and graphical techniques and pinch analysis [3].

Pinch analysis is used to design chemical processes to minimize energy consumption and enhance energy efficiency especially in the reactor which is the core of chemical process technologies [4]. The best field of using multifunctional reactors is the combination of endothermic and exothermic reactions. In this technique, exothermic reactions produce the source of heat to drive endothermic reactions. The difference between heat source and heat sink regions is a main point in the pinch analysis [3]. Moreover, the auto-thermal multifunctional reactors can be used with co- and counter-current flow in the reaction zone [5]. The thermal efficiency of these reactors can be improved and is investigated using reactor model [6].

Spiral heat exchangers have evinced significant interest owing to their compact size, large heat transfer surface area per unit volume, high heat transfer rates, lower fouling, operational flexibility and ease of maintenance [7]. This research focused on the design of the autothermal spiral reactor using both methane combustion and steam methane reforming reactions. The computational fluid dynamics
was used to study the effect of various parameters for the reactor design i.e., momentum (pressure drop and velocity) and heat transfer (temperature distribution).

2. Computational approach
COMSOL MULTIPHYSICS 3.5a software was employed in this research to observe the hydrodynamic and heat transfer characteristics i.e., pressure, velocity distributions and temperature profile. The autothermal system of spiral reactor was created via a symmetrical 3D model with Momentum Transport equations and Energy Transport equations. In the simulations, the following assumptions were made:
- Flow and reaction are in a steady state and isothermal.
- Flow is asymmetric and laminar
- Flow and temperature and pressure are uniform at the inlet

The hydrodynamics and heat transfers of gas phase were governed by the incompressible Navier-Stokes equation coupled with the convection-conduction equation as indicated in equation (1) and (2), respectively:

\[ \rho \frac{\partial u}{\partial t} - \nabla \cdot (\eta (\nabla u + (\nabla u)^T)) + \rho (u \cdot \nabla)u + \nabla p = 0 \]
\[ \nabla \cdot u = 0 \]  
\[ \rho C_p \frac{\partial T}{\partial t} + u \cdot \nabla T = \nabla \cdot (k \nabla T) + Q \]

where \( \eta \) = dynamic viscosity [kg/m·s], \( u \) = velocity vector [m/s], \( \rho \) = effective density [kg/m³], and \( p \) = pressure of the mixed gas [Pa]

\[ T \] = temperature [K], \( C_p \) = heat capacity [J/kg·K], \( k \) = thermal conductivity of the mixed gas [W/m·K], and \( Q \) = heat generation rate from the SMR and MC [W/m³]. The governing equations were discretized and solved numerically to provide the results in terms of the hydrodynamics and thermophysical parameters.

The spiral reactor was presumably made as detailed in table 1. The inlet and outlet feed patterns of SMR and MC at steady state condition were shown in figure 1. The reactor consists of Steam Methane Reforming (SMR) channels and Methane Combustion (MC) channels. The physical and transport properties were also summarized in figure 1. Figure 2 shows a mesh size for the case of 3D-models. According to the computational limitation, the velocity, pressure and temperature profiles were determined for a single channel of spiral reactor. Several reactions taking place during the autothermal reforming of methane were listed in equation (3)-(7) [7].

Steam Reforming: \( \text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2, \Delta H_{298K} = +206\text{kJ/mol} \) (3)
Partial Oxidation: \( \text{CH}_4 + \frac{1}{2}\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2, \Delta H_{298K} = -36\text{kJ/mol} \) (4)
Dry Reforming: \( \text{CH}_4 + \text{CO}_2 \rightarrow 2\text{CO} + 2\text{H}_2, \Delta H_{298K} = +247\text{kJ/mol} \) (5)
Methane Combustion: \( \text{CH}_4 + 2\text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2\text{O}, \Delta H_{298K} = -802\text{kJ/mol} \) (6)
Partial Combustion: \( \text{CH}_4 + \text{O}_2 \rightarrow \text{CO}_2 + 2\text{H}_2, \Delta H_{298K} = -71\text{kJ/mol} \) (7)
### Table 1. The physical and transport properties of model used.

|                          | Combustion side | Reforming side |
|--------------------------|-----------------|----------------|
| **Geometry**             |                 |                |
| Flow channel width (m)   | 1×10^{-3}       | 1×10^{-3}      |
| Flow channel high (m)    | 1×10^{-3}       | 1×10^{-3}      |
| Stainless steel thickness (m) | 5×10^{-5}     | 5×10^{-5}      |
| Surface area (m$^2$)     | 1.38×10^{-4}    | 1.13×10^{-4}   |
| **\(\alpha\)-alumina (Substrate)** |                 |                |
| Catalyst layer thickness (m) | 6×10^{-5}    | 6×10^{-5}      |
| Thermal conductivity (W/m·K) | 35             | 35             |
| Permeability (m$^3$) [8-10] | 1×10^{-8}     | 1×10^{-8}      |
| **Gaseous phase**        |                 |                |
| Flow rate (ml/min)       | 500             | 500            |
| Density (kg/m$^3$)       | 0.38            | 0.24           |
| Viscosity (Pa·s)         | 4.2×10^{-5}     | 3.1×10^{-5}    |
| Heat capacity (J/kg·K)   | 1335.20         | 3642.91        |
| Thermal conductivity (W/m·K) | 0.80        | 0.11           |

**Figure 1.** Autothermal spiral reactor used for SMR (blue channel) and MC (pink channel) with 2 patterns feed flow (a) Co-current and (b) Counter current.
A simplified process scheme, depicted in figure 3, shows that exothermic reactions is fed to the reactor, producing the desired higher temperature, and endothermic reactions is led to a steam reforming channel. The excess reaction heat from exothermic reactions is consumed by the steam reforming reactions. In this simulation, the enthalpy of exothermic reaction was represented in term of the equivalent functions of temperature, and applied as one of the thermal boundary conditions. For comparison and design purposes, the velocity and temperature profiles were determined for both the co-current and counter-current in spiral reactor under the inlet volumetric flow rate of the gas mixture of 300 ml/min and 500 ml/min (MC and SMR at 873K). The removal of heat flux at porous layer of MC and SMR are $1.614 \times 10^3$ and $0.246 \times 10^3$ W/m², respectively.

3. Results and discussion

Flow Fields of Gaseous Phase: For co-current and counter-current operation, the three dimensional velocity fields can be plotted as shown in figure 4(a) to 4(f). Figure 4(g) and 4(h) illustrate the pressure profiles of the mixed gases for co-current and counter-current, respectively.

Simulation results of fluid flow showed that the combustion gas and reforming gas flowed along the channel. Both gases were change in radial and tangential direction. There was no velocity distribution throughout the flow channel. This means that there was no dead spot. Both radial and tangential flow were observed throughout the flow channel [11]. The velocity vectors indicated by red arrows were mainly in the radial direction. The spanwise velocity profiles presented in figure 4(a) and 4(b) and figure 4(c) to 4(f) illustrated the velocity contours of the gas mixture along each reactor channel. This profiles showed the flow velocity in the free-flow region (axial velocity) that was lower than the radial velocity. The friction causes the streamwise velocity to decrease towards the wall from
the center of the channel. The thickness of boundary layer for the low Reynolds number regime, and the porosity of the catalytic layer were completely eliminates. This could imply that the reacting flow is convectively dominated in the free flow, whereas it is diffusively dominated in the porous layer. Even though, the flow velocity within the free-flow region quite differs from that within the porous wall, the pressure gradient in the radial direction is rather insignificant. However, the pressure gradient seems to be stronger in the streamwise direction as shown in figure 4(g) and 4(h).
Figure 4. Hydrodynamics of the gas mixture within the single channel (a) Fully developed velocity vector in radial, (b) tangential direction, (c) velocity profile of co-current, (d) velocity profile of counter current, (e) velocity profile of co-current in z-x direction, (f) velocity profile of counter current in z-x direction, (g) pressure profile of co-current and (h) pressure profile of counter current.

Figure 5. Temperature distribution of SMR/MC gases in autothermal spiral reactor at the volumetric flow rate of the gas mixture was 300 ml/min at 600°C (a) co-current and (b) counter current.

Figure 6. Temperature distribution of SMR/MC gases in counter current spiral reactor at 600°C (a) volumetric flow rate of the gas mixture was 300 ml/min and (b) volumetric flow rate of the gas mixture was 500 ml/min.
The autothermal reactor concepts could be applied for endothermic high temperature reactions if both endothermic reactions and exothermic reaction are taken place at the similar time. Different flow patterns of co-current and counter current of each reaction of endothermic and exothermic reactions were considered in the following. The heat of combustion was consumed for preheating of the reforming reaction and for supplying of its reaction. During reforming and combustion, the total oxidation with complete oxygen consumption was observed at the first section of reaction zones and subsequent (endothermic) reforming section was then observed [12].

The heat transfers within the catalyst layer of each reactor design were mainly as the result of conduction-convection process among the wall-coated reactor, the wall of vessel, and the mixed gas. For the temperature profiles of SMR and MC gases, the simulation results were shown in figure 5 with the highest temperature in the vicinity of catalyst layer. This is because the exothermic enthalpy released from the MC reaction as described previously in equation (6), and was lower in the outlet flow. A certain amount of generated heat was then consumed by the reactant (mixed) gas itself during the on-going reactions while the rest was removed through the wall of vessel by SMR (negative heat flux set up at the wall-coated of catalyst layer boundary).

At different volumetric flow rates of the gas mixtures as shown in figure 6, the simulation result showed that temperature difference at 300 ml/min is lower than that of 500 ml/min. Temperature fields exhibit a well distribution within each microchannel and overall heat transfer occurs from the temperature difference between combustion gas and reforming gas. Fluid dispersion can increase mass transfer and heat transfer [13-15]. Moreover, the complete flow pattern throughout the flow channel of fluid was observed in the spiral heat exchanger.

4. Conclusion
Low fluid velocity was found in the radius flow of the channel without dead and hot spot zone. Good temperature distribution was observed in the spiral heat exchanger. Moreover, the research results could be used to improve and design the spiral reactor in case of mass and heat transfer. It could also be used to scale up the current spiral reactor for industrial applications.

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