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PRELIMINARY STUDY OF FLUID FLOW AND HEAT TRANSFER IN A MICRO REACTOR USED FOR CATALYTIC UPGRADING OF HEAVY OIL AND BITUMEN

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ABSTRACT

This study presents simulation of the fluid flow and heat transfer within the tar sand reservoir during the use of the Toe-to-Heel Air Injection (THAI) enhanced oil recovery process. The Catalytic upgrading PRocess In-situ (CAPRI) process is a modification of THAI that includes an upgrading catalyst bed wrapped around the horizontal producer well. A two-dimensional (2D) reactor model has been developed to simulate the flow behaviour in a micro CAPRI reactor for heavy oil and bitumen upgrading. Computational fluid dynamics (CFD) code fluent was employed as the tool for carrying out this study. The effect of process parameters, including temperature, flow rate, feed concentration and coke deposition on the catalyst bed was investigated over a range of conditions. The simulation results showed that feed conversion and coke deposition were affected by operation conditions investigated in this work. Increase in reaction temperature caused an increase in catalyst deactivation during the catalytic upgrading process. Therefore, it is expected that the results could be useful to improve the process performance.

Keywords: Catalyst, Fluid Flow, Heat transfer, Heavy oil, Reactor, Upgrading,

INTRODUCTION

In the processing and upgrading of heavy oil and bitumen, transportation is one of the main challenges facing the process. Studies have shown that the THAI - CAPRI process suffers the same challenges especially the CAPRI concept, such as catalyst deactivation with increased contact time in reservoir [1, 2]. THAI, is an integrated reservoir-horizontal wells process, which uses air injection to propagate a combustion front from the toe-position to the heel of the horizontal

producer well [3]. CAPRI is the catalytic extension of the THAI process, incorporating an annular layer of catalyst, placed on the outside of the perforated horizontal producer well, along its whole length [4, 5].

Therefore, there is the need for investigation and understanding in order to improve the process. A new method to estimate the hydrodynamics and heat transfer is required which should also be able to predict the velocity and concentration fields in the micro CAPRI reactor for better design and scale-up applications.

CFD is a well-established technique for the analysis of systems involving fluid flow, heat transfer, and reaction and associated phenomena. There are several advantages of using CFD such as ability to study hazardous system in a safe environment and reduction in the time and cost of analysis [6]. CFD was employed to study the flow field across the micro CAPRI bed and also predict the coking behaviour in the fixed bed. In the previous studies by Shah et al [7] and Hart et al [8], it was shown that Micro CAPRI reactor enables the study of what is taking place at underground since it is inaccessible for investigation. In the aforementioned studies, Shah et al [7] and Hart et al [8], performed upgrading of heavy oil on a catalyst bed in a vertical micro CAPRI reactor. There are advantages of using Micro CAPRI reactors. The reactor scale is small. The furnace used for the heating of the reactor can be controlled somehow. This allows uniform temperature in the reactor; the gas flows downward in the reactor and through the catalyst bed. Such geometrical arrangement causes uniform flow through the reactor. The annular reactor geometry is extensively studied in literature because of its advantages [9, 10, 11]. Therefore, little is known about the hydrodynamics and associated heat and mass transfer, pressure drop for micro CAPRI reactors. Recently, White [12] reported that the essence of studying packed beds is to regulate the significant operating cost of the pressure drop through the packed bed. Kruger et al. [13], also stated that pressure drop over packed beds is the most important parameter that must be accurately predicted when designing any system that incorporates packed bed, pressure drop determines the pumping power and operating cost in a packed bed system. Mohammadikah et al. [14] studied the use of CFD in the improvement of hydrodynamics performance of Naphta catalytic reforming reactions. Their study showed that, small velocity result into small pressure drop and greater velocity lead to an increase in pressure drop across the bed. In addition, CFD modelling of gas flow in porous medium and catalytic coupling reactions from carbon monoxide

to diethyl oxalate in fixed bed reactor has been reported by Giao et al. [15]. Their findings indicated that CFD tools are suitable for predicting the hydrodynamic of the gas – solid flow and catalytic coupling reaction of CO – DEO in a fixed bed reactor. Niaei et al. [16] used CFD to simulate catalytic oxidation of benzene on monolithic catalytic bed reactor. They concluded that CFD is the appropriate tool to study fluid regime and heat transfer and especially, concentration of species, and surface deposition along the reactor in the chemical process, especially catalytic combustion. Salari et al. [17] employed CFD to study coke deposition in a fixed bed catalytic cracking tube reactor. They observed that coke deposition is changed with variation of flow rate, steam ratio, and that stagnation points and vorticity are two important factors on coke deposition.

In this work two-dimension (2D) CFD was used to simulate fluid flow and heat transfer in a micro CAPRI reactor. It was carried out using Fluent 13.0 to simulate velocity, temperature, and concentration, coke deposition profiles during the upgrading of heavy oil in a Micro CAPRI reactor. To author's knowledge, no research has been performed to predict the hydrodynamics and heat transfer of heavy oil upgrading in Micro CAPRI reactor using CFD. The objectives of this simulation were to evaluate and predict the fluid flow hydrodynamics and heat transfer in the reactor.

CFD MODELLING

The CFD modelling and simulation was carried out through CFD code FLUENT 13.0 on the Micro CAPRI reactor. A comprehensive two-dimensional (2D) reactor model has been developed to simulate the flow behaviour in the reactor for heavy oil upgrading.

Micro CAPRI reactor for model simulation

The first step was to select a proper arrangement for the fixed bed. The dimension of the reactor was based on the previous experimental studies by Shah et al [7] and Hart et al [8]. The steel tube selected for this work was a 1/2" tubing from Swagelok, with an internal diameter and length of 10.2 mm and 400 mm, see Figure 1.

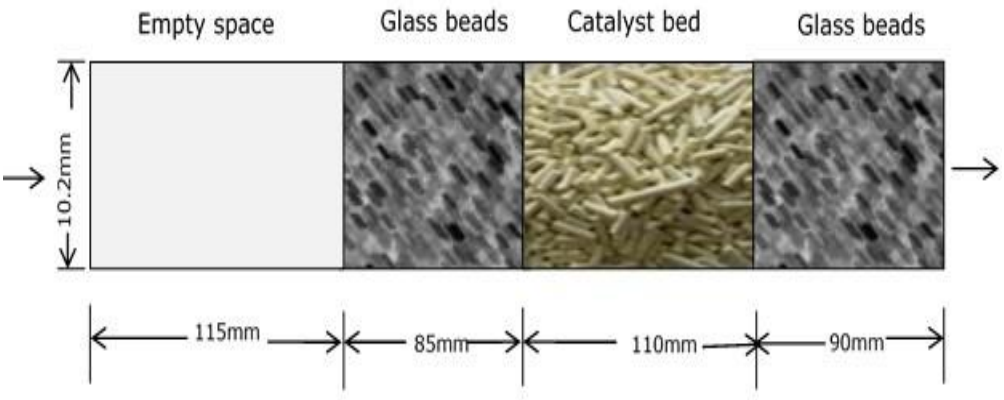


Figure 1: Model of CAPRI reactor

The catalyst bed is located within a furnace and the annular gap between the reactor tube and furnace wall is filled with marble chips to maintain thermal condition from the furnace to the reactor. Cyclooctyne (C_8H_{12}) represent the typical THAI oil from the combustion zone into the catalyst bed in the in-situ process along the horizontal producer well. The THAI oil is heated in a mixing chamber at temperature of 300 ^oC before it was fed into the reactor, with all the components in vapour state. According to Shah et al. [7] and Hart et al. [8], the reactor can be divided into Four zones. Where; Zone I = Empty space, Zone II = Glass beads, Zone III = Catalyst bed and, Zone IV = Glass beads. Zone I ensured that the flow field has become fully developed before the heated or reactor region. Zone II & IV are section of the reactor filled with glass beads to ensure effective thermal conductivity in the reactor. And finally Zone III in the middle of glass beads is the section where reaction occurs.

Model governing equations

The governing equations are based on a two-dimensional, laminar, steady state flow including heat transfer and chemical reactions. In fluent the governing equations available are equations of conservation mass, momentum, energy, and species. Since the CFD modelling includes chemical and thermal effects, all four equations were solved.

The Continuity equation is: $\nabla \cdot (\rho u) = 0,$ (1)

where, ρ is density and u is the velocity of the gas mixture.

In the reactor the space filled with catalyst particles in the CAPRI reactor is assumed to be a continuous porous medium, which in CFD is modelled as a fluid region with extra terms in the momentum balance to allow for additional resistance to flow. The momentum equations were solved for both porous (catalyst bed) and fluid (gaseous mixture) zones. The effects of the porous medium were modelled through the addition of a momentum source-term to the momentum conservation equation:

$$\nabla \cdot (\rho uu) = -\nabla p + \nabla \cdot \bar{\bar{\tau}} + \rho g + \vec{S} \qquad (2)$$

Where, p is the pressure, $\bar{\bar{\tau}}$ is the stress tensor, g is the acceleration due to gravity and $\vec{S}$ is the momentum source term. The latter consists of two terms: (1) Darcy viscous loss and (2) inertial loss. For a homogeneous porous media, Si (i correspond to ith axis) assumes the following form:

$$S_i = -\left(\frac{\mu}{\kappa} ui + \frac{1}{2} C\rho uui\right) \qquad (3)$$

where, μ is the viscosity of the fluid, and κ and C are constants.

The species transport equation used for the chemical reaction that is the THAI Oil (asphaltene) decomposition is given as:

$$\nabla \cdot (\rho uyi) = -\nabla \cdot Ji + Ri \qquad (4)$$

Where, Ri is the reaction rate per volume of the species i produced by reaction; Ji is the ith species diffusion flux; yi is the mass fraction of ith species.

The reaction mechanism for coke deposition was based on the fact that THAI Oil are the main coke precursors undergo decomposition and reaction subsequently. Hence, for this study, it was assumed that coke precursor or THAI Oil compounds are lumped as C_nH_{2n-4}. The reaction adopted assumed that decomposition of THAI oil during CAPRI catalytic reaction was first order. Therefore, the reaction below was considered.

$$C_8H_{12} \rightarrow 8C + 6H_2 \qquad (5)$$

The laminar finite rate model was used and the rate constant was expressed in Arrhenius form:

$$K_V = Ae^{-(E_r / RgT)} \quad (6)$$

For the first order reaction,

$$R_{C8H12} = K_V C_{C8H12} \quad (7)$$

When the pre-exponential factors and activation energy are substituted as adopted from [18]. As a result, eqn (6) can now be written as follows:

$$K_V = 2.512e^{+08} \times \exp^{(1.674e+05/RgT)} \quad (8)$$

Mesh generation and Boundary conditions

Structured meshing method done in ANSYS Workbench was used for meshing the geometry. The 2D geometry of micro CAPRI reactor with mesh generated using ANSYS Meshing software. To confirm that the CFD results are independent of the mesh size, the simulations of the system with 5 x 50, 10 x 100, 20 x 200, 30 x 300 and 40 x 400 grids (radial x axial) are performed feeding cold gas mixture. At the inlet, a uniform velocity inlet and a constant inlet temperature 300 ^{o}C were assigned at the reactor inlet. Other components of the reactor inlet can be calculated based on the boundary conditions of the reactor inlet. Furthermore, for the inner wall of the reactor, the fluids are assumed to obey the no slip boundary condition at the wall, where both velocity components were set to zero at that boundary i.e, Vr =Vx = 0. A constant temperature is applied in the reactor. At the outlet, the pressure outlet was specified.

CFD solution

The equations above were solved by the CFD code ANSYS Fluent 13.0. The governing equations are discretized in a non-uniform structural mesh by a finite volume method. Grid independency has been executed for some mesh points and finally a 300 × 30 non-uniform mesh is selected. Pressure and the velocity are coupled by the SIMPLE algorithm. The dilute approximation was used to calculate the diffusion flux. Thermo-physical properties of each species are temperature dependent and those of the gas mixture were calculated using the standard mixing law for ideal

gas. A second order upwind scheme was used to discretize the transport equations of momentum, heat and mass. Assuming incompressible flow, a pressure-based solver was used to linearize and solve the governing momentum (Navier–Stokes) equation. Appropriate reaction rate kinetics was included in the species-conservation equation. Details of the numerical algorithm and procedure are available [19]. A convergence criterion of $1 \times 10{-}3$ was applied to the residuals of continuity, momentum, energy, and species balance equations. All simulations were performed under the steady state conditions and calculation was continued till the convergence-criterion was achieved. In order to simulate the practical case, the results of the flow field without the reaction at a steady state are first obtained. Then the reaction was further added into the flow field, simultaneously. The model validation was carried out in the present work to evaluate CFD modelling of hydrodynamics at different flow velocities of 0.051, 0.082, and 0.102 m/s.

RESULTS AND DISCUSSION

The hydrodynamics of any reactor is characteristic of its overall performance and it helps to evaluate the nature of flow patterns in the reactor. The model validation was carried out by simulating the effect of various parameters on the flow properties over a range of conditions. The CFD simulations of Micro CAPRI reactor operating at flow velocities of 0.051, 0.082, and 0.102 m/s were performed. And it was also performed at different operating temperatures of 673K, 723 and 773 K. The CFD modelled variation in axial velocity with respect to radial distance within the reactor at various flow velocities have been shown in Figure 2. The results correspond to the line (x=0.15 m) of the reactor length before the catalyst bed. The velocity distribution depicted by CFD simulations along the micro CAPRI reactor space is parabolic. This is characteristic of laminar flow in agreement with Bird et al [20]. The results show that velocity is minimum at the walls and maximum near the middle region, this is consistent with literature.

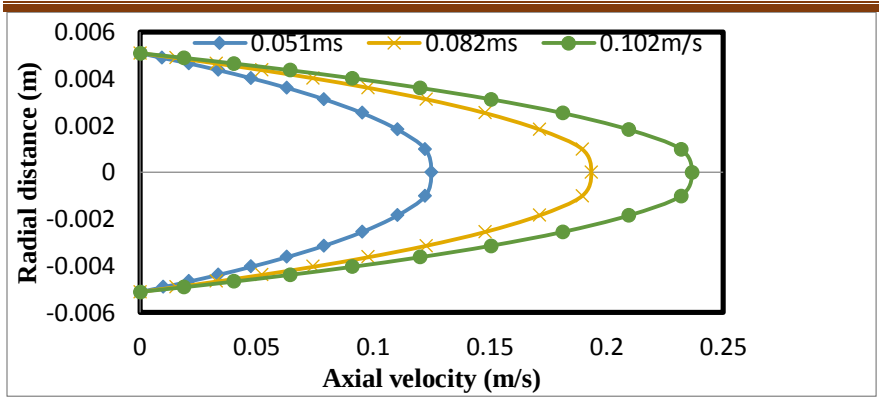
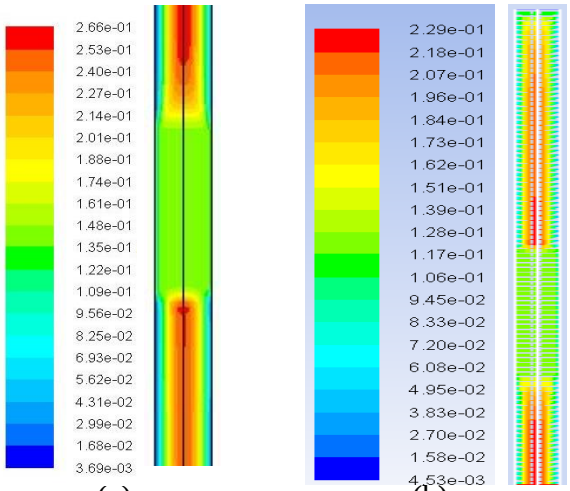


Figure 2: Axial velocity within the micro CAPRI reactor

Figures 3 a & b. shows velocity vector and magnitude for reactor at a flow velocity of 0.102 m/s. These results represent the entire length of entire reactor. Similar velocity vectors and magnitude contours were obtained in the simulations at other flow velocities and hence not shown here. As shown in Figure 3., the velocity vector and magnitude field along the reactor is uniform and it varies parabolically in radial direction. The flow is fully developed throughout the reactor. The fluid velocity in the reactor increases as the fluid approaches the porous region. The velocity is maximum just before the porous zone, and decreases as the fluid passes through the porous zone. The flow pattern shows that as the fluid passes through the porous zone, it decelerates and straightens out, and exhibits a more uniform flow distribution. The simulation results for the other different velocity were characteristically the same. The results correspond to the entire reactor length.

Figure 4 depicts the radial temperature distribution obtained for a flow velocity of 0.102 m/s and temperature of 773K.. The wall temperature of reactor was set equal to the furnace temperature. The temperature profile shows that the wall temperature is higher than the gas inlet temperature. Therefore, energy is transferred from the wall and reactor to the gas. As expected, temperature of fluid increases along the length of reactor and temperature varies in radial direction, but became steady in the porous zone. This shows the temperature profile at different positions along the radial direction of the reactor.



(a) (b)

Figure 3: Velocity (a) vector field coloured by velocity magnitude and (b) velocity magnitude contour within the reactor for flow velocity of 0.102 m/s.

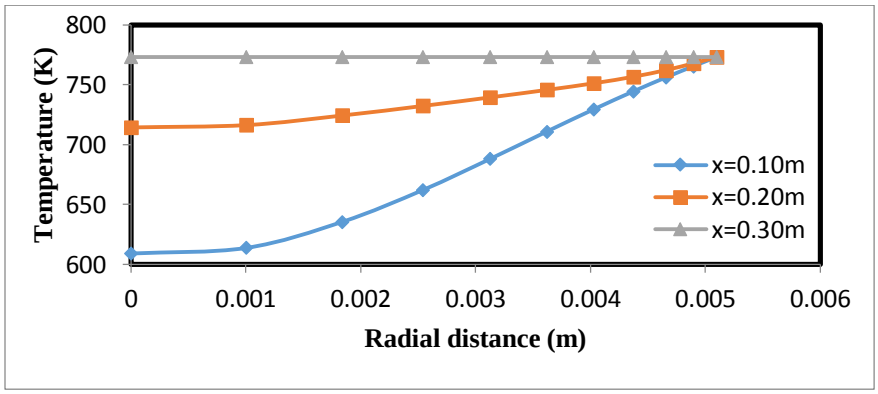


Figure 4: Radial temperature distribution in the reactor

The different temperature distribution curve along the axial direction of the reactor have been shown in Figure 5. It can be seen that the temperature of fluid increases from the entrance zone up to the porous zone, after which the temperature become uniform.

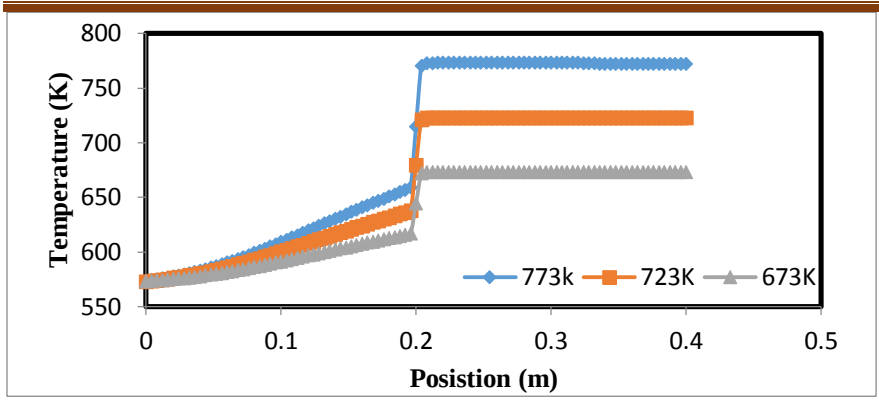


Figure 5: Axial temperature distribution in the reactor

At the entrance of the catalyst bed there was a jump in temperature. This suggests that there was a thermal reaction on the glass beads in the reactor which has caused the jump in temperature, and consequently initiating the catalytic reaction on the bed.

Considering the simulation in Figure 6, it was carried out for different temperatures, keeping all other remaining conditions same. It shows the mass concentration distribution of C_8H_{12} at various reaction temperatures. The mass concentration starts decreasing at the entrance to the porous zone (x=0.2 m) due to it decomposition on the surface of catalyst. It can be seen that the decomposition or consumption increases with temperature. As observed the rate of consumption of C_8H_{12} increase with reaction temperature, showed clearly the temperature effect as the slope of the distribution curve developed from gentle to steep slope.

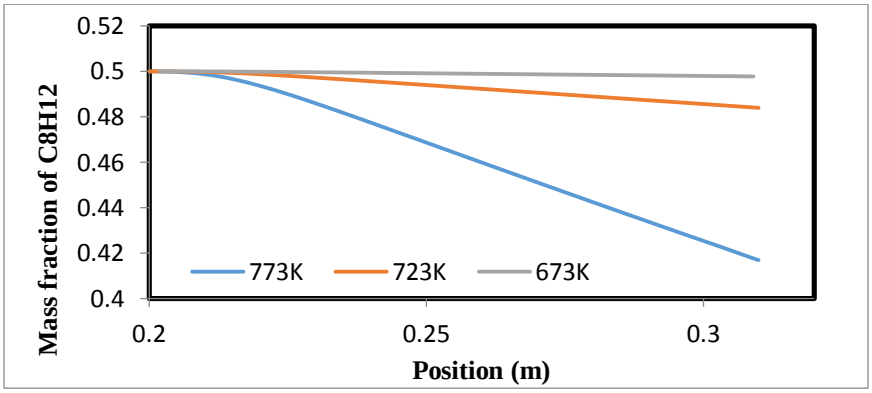


Figure 6: Mass fraction concentration of C_8H_{12} at different reaction temperature

The dependence of pressure on flow velocity was shown in Figure 7. It can be observed that pressure drop increase as fluid velocity increases. Furthermore, for a constant Reynolds number the rate of pressure drop remain unchanged. The pressure decreased gradually from the entrance point of the porous zone to the end. It can be seen that pressure drop occurs mainly in the porous zone where reaction occurs. Moreover, the increasing pressure drop was found with increasing velocity. The average coke deposition rates at different temperatures were plotted in Figure 8. It shows that the average coke deposition over a cross-sectional area along the porous zone at various temperatures increased with increase in reaction temperature. The maximum average coke deposition rate is 1.23e-03 kg/m2-S at 773 K while the minimum average coke deposition rate is 3.157e-05 kg/m2-S at 673 K. Coke deposition was found to vary with temperature.

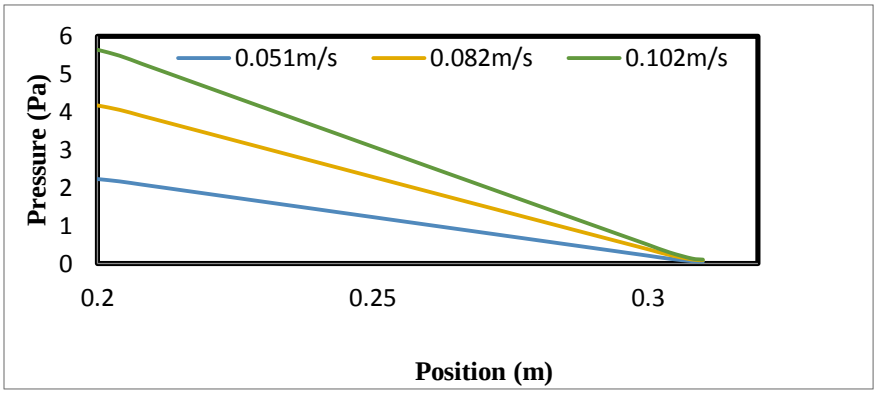


Figure 7: Axial pressure distribution for different flow velocity

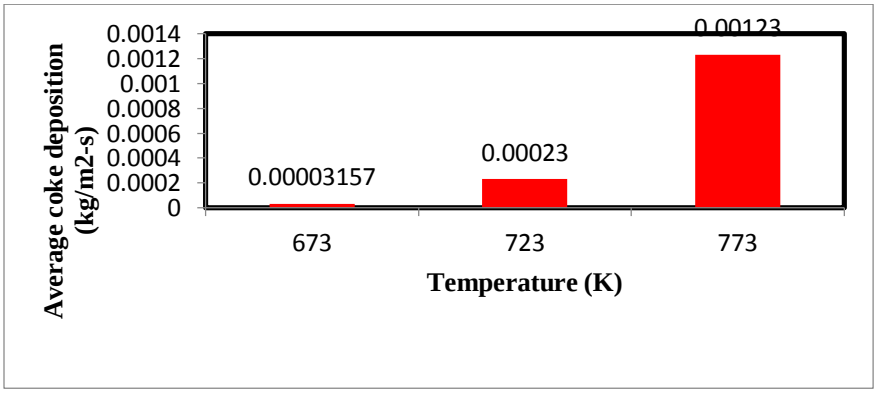


Figure 8: Average coke deposition at different reactor temperature

CONCLUSION

The hydrodynamics of the reactor system have been studied in terms of temperature, pressure, velocity distribution, average velocity, velocity vector and magnitude contours. Temperature varied axially before the bed, but becomes uniform in the porous zone. The velocity profile was parabolic in all zones except in the porous zone where it was uniform. The pressure drops across the bed increased with increase in velocity. CFD model with surface reaction was also applied to predict coke deposition in micro reactor from coke-based precursor. The simulation results revealed that approximately uniform velocity, temperature and concentration profile existed in the catalyst bed. The average rate of coke deposition and catalyst deactivation are highly dependent on temperature and amount of coke precursor.

REFERENCES

1. Greaves, M., Ayasse, C. & Turta, A.T. (2008). In Situ Upgrading potential of the CAPRI™ Process. World Heavy Oil Congress, Edmonton, Alberta, pp. 330-338.
2. Greaves, M. & Xia, T.X. (2004). Downhole catalytic process for upgrading heavy oil: Produced oil properties and composition. *Journal of Canadian Petroleum Technology*, 43, pp. 25-30.
3. Xia, T. X., Greaves, M., Turta, A. T. & Ayasse, C. (2003). THAI—A 'Short-Distance Displacement' In Situ Combustion Process for the Recovery and Upgrading of Heavy Oil. *Chemical Engineering Research and Design*, 81, pp. 295-304.
4. Greaves, M., El-Saghr, A. & Xia, T. X. (200). CAPRI horizontal well reactor for catalytic upgrading of heavy oil. Preprints - American Chemical Society, Division of Petroleum Chemistry, 45, pp. 595-598.
5. Xia, T., Greaves, M. & Turta, A. (2002). Injection well - Producer well combinations in THAI 'Toe-to-heel air injection'. SPE/DOE Thirteenth Symposium on Improved Oil Recovery. Tulsa, OK, United States.
6. Mohseni, M. & Taghipour, F., (2004). Experimental and CFD analysis of photocatalytic gas phase vinyl chloride (VC) oxidation. Chemcal Engineeering Science, 59, pp. 1601–1609.
7. Shah, A., Fishwick, R.P., Leeke, G.A., Wood, J., Rigby, S.P. & Greaves, M. (2011). Experimental optimization of catalytic process in situ for heavy-oil and bitumen upgrading. *Journal of Canadian Petroleum Technology*, 50, pp. 33-47.
8. Hart, A., Shah, A., Leeke, G., Greaves, M. & Wood, J. (2013). Optimization of the CAPRI process for heavy oil upgrading: Effect of hydrogen and guard bed. *Industrial and Engineering Chemistry Research*, 52, pp. 15394-15406.

9. Vianna, A.S. Jr.& Nichele J. (2010). Modelling an annular flow tubular reactor. Chemical Engineering Science, (65), pp. 4261–4270.
10. Vincent, G., Schaer, E., Marquaire, P.M. & Zahraa, O. (2011). CFD modelling of an annular reactor, application to the photocatalytic degradation of acetone. Process Safety and Environment, 89, pp. 35–40.
11. Kumar, J. & Bansal, A. (2012). CFD modelling of hydrodynamics and mass transfer of Rhodamine B in annular reactor. Heat Mass Transfer, 48, pp. 2069-2077.
12. White, J. (2016). CFD Simulation and Microscopic study of a Solitary Spherical Porous Adsorbent. School of Engineering Journal, 2-15, doi:10.20944/preprints201608. 0023.v1.
13. Kruger, J. H., Toit, C. G. D & Vander-merwe, W. J. S. (2015). Numerical validation packed beds. 11th international Conference on CFD in the mineral and process industries, 1-7.
14. Mohammadikah, R., Abghari, Z., Sorrod, G., & Ahmadi., M. M. (2014). Improvement of Hydrodynamics performance of Naphta Catalytic Reforming Reactors using CFD. *Journal of Research Institute of Petroleum Industry* (RIPI), 33 (3), 63-76.
15. Gao, X, Zhu, Y, & Luo, Z. (2011). CFD modelling of gas flow in porous medium and catalytic coupling reactions from carbon monoxide to diethyl oxalate in fixed bed reactors, *Chemical Engineering Science*, 66, 6028 – 6038.
16. Niaei, A, Salari, D, & Hosseini, S.A., (2009). CFD Simulation of Catalytic Combustion of Benzene, *Iranian Journal of Chemical Engineering*, 6 (4) (Autumn), pg.: 34-43.
17. Salari, D, Niaei, A, Yazdi, P.C., Derakhshani, M & Nabavi, S.R. (2008). CFD Flow and Heat Transfer Simulation for Empty and Packed Fixed Bed Reactor in Catalytic Cracking of Naphtha, *World Academy of Science, Engineering and Technology*, 13, pg:362-365.
18. Benson, S.W. & Shaw, R. (1967). Kinetics and mechanism of hydrogenolyses. The addition of hydrogen atoms to propylene, toluene, and xylene. Journal of Chemical and Physical Science, 47, pp. 4052–5.
19. Fluent-Inc., Fluent 13.0 User's Guide UK, 2014.
20. Bird, R., Stewart, W., & Lightfoot E., Transport phenomena, 2nd edn. Wiley, New York, 2002.