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CFD Modeling of Asphaltenes Deposition from Crude Oil Through Discrete Phase Simulations

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Abstract: Crude oil fouling in processing equipment have been a major unresolved problem in petroleum industries. The underlying behavior of fouling precursors present in the crude oil have to be investigated to mitigate the deposit formations. In the present research, an attempt has been made to predict the asphaltenes deposition rate from crude oil in a heat exchanger tube through discrete phase CFD simulations. Various forces such as stochastic collision, thermophoretic, Saffman lift, coalescence and drag are applied on the particles to understand the transportation and adhesion mechanism of the asphaltenes particles. As asphaltenes have the tendency to aggregate irreversibly with different particle sizes, the transportation of asphaltenes particles is studied through varying the particles diameters. The propensity of asphaltenes particles in a Lagrangian frame is studied through the available discrete phase models in the commercial CFD Software Ansys Fluent.

Key words: Computational fluid dynamics, discrete phase, asphaltenes, crude oil, fouling

INTRODUCTION

Preheat exchanger fouling is one of the major unsolved issues in petroleum refineries. Fouling adversely affects the heat recovery and pumping capacity forcing frequent shutdowns for cleaning the heat exchangers (Deshannavar *et al*., 2010). There are several attempts to understand the fouling mechanism in order to devise fouling mitigation techniques (Srinivasan, 2008; Leontaritis and Mansoori, 1988; Jamialahmadi *et al*., 2009; Artola *et al*., 2011). The lack of complete understanding on the physical and chemical aspects of fouling has resulted in ineffective fouling mitigation. Theoretical studies assume that foulant deposits on the heat transfer surfaces are uniform across the length of the tubes in shell and tube heat exchangers. Almost all estimates of fouling in preheat trains assume this uniformity. However, in practice the deposits have been found to be more at the entrance and exit of the tube sheets rather than on the heat transfer surface of the tube itself. This industrial observation has led to the conclusion that whatever be the source of the foulant particles they get suspended in the bulk of the crude oil and deposit at locations where the flow path changes and where the velocities become very low. In order to mitigate fouling, it is important to have the basic knowledge on formation of deposits such as where and how they occur, so that necessary steps can be taken. The precursors present in the crude oil are due to various reactions of crude oil components that take place inside the heat exchanger (Emani *et al*., 2016; Haghshenasfard and Hooman, 2015; Bayat *et al*., 2012; Fontoura *et al*., 2013; Yang *et al*., 2009). On the other hand suspended particles might also be present in the crude oil without undergoing any reactions (Emani *et al*., 2016; Coletti and Hewitt, 2014). Therefore, understanding the transportation and adhesion phenomena of fouling precursors are highly essential.

Figure 1 shows the images of the tube sheet under clean and fouled conditions in an operating refinery. It is very clearly seen that there are deposits on the tube sheets in which the deposits are pronounced at the bottom portion and the upper portion of the tube sheet is relatively clean. All the existing studies do not consider any deposits on the tube sheets but assume a uniform deposition on the inner surface of all the tubes which is seldom the reality. Therefore, to understand the fouling precursor’s behavior inside the heat exchangers, it is necessary to perform a CFD study. The effect of flow velocity, bulk and surface temperatures and fluid path on the formation of deposits can be understood through CFD simulations.

Besides our Crude Oil Fouling Research Center (CROFREC), various research groups which include University British Columbia, Argonne National Labs, Heat Transfer Research Inc., a consortium of universities comprising of Imperial College, Bath University,

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Fig. 1: Photographic images of tube sheet under clean and fouled conditions

Cambridge University in association with Engineering Science Data Unit (ESDU) and other independent studies were also being carried out globally to understand the transportation and adhesion mechanisms of fouling precursors in the crude oil.

In this study, asphaltenes deposition rate from crude oil in a heat exchanger tube is predicted through discrete phase CFD simulations. To understand the transportation and adhesion mechanism of asphaltenes particles, various forces such as stochastic collision, thermophoretic, Saffman lift, coalescence and drag are applied on the particle.

MATERIALS AND METHODS

Computational studies on particle deposition: The mechanism involved in particle deposit formations can be understood from computational studies through various parameters such as particle mass deposition rate, particle velocity, heat transfer rate and fouling layer thickness. Since, it is difficult and time consuming to model all the length and time scales in the system, most of the studies considered Reynolds-averaged Naiver-stokes turbulent model to study the fluid flow behavior of particle depositions (Emani *et al*., 2016; Bayat *et al*., 2012).

Various CFD simulation studies to understand the particle deposition through one way coupling Lagrangian tracking method have been reported (Zhang and Li, 2008; Landry *et al*., 2012). In order to understand the particle behavior in a practical approach, various forces such as inertial, lift, drag, gravity were activated and their influences on particle depositions were studied. A lagrangian stochastic model is activated to understand the particle tracking phenomenon. The lagrangian approach cleaves the particle phase into a group of individual particles and tracks each particle separately inside the flow domain.

It has been noted that the number of particles getting trapped on the walls will be high if the particle flow velocity is extremely low. Nevertheless with high fluid velocities, particles might promote shear stress and carry forward even if they stick on the surface (Landry *et al*., 2012).

Asphaltenes precipitation fouling route: Heavy components such as asphaltenes which are dissolved in the crude oil can be precipitated and formed as deposits on the heat transfer surfaces. The formation of deposits through crude oil on a batch stirred cell's heated test probe has been investigated (Yang *et al*., 2009). In order to understand the physical phenomenon of crude oil fouling on the batch stirred cell through CFD simulations, shear stress, surface temperature and fouling layer thickness profiles were observed. Fouling layer thickness has been observed to be maximum at locations where the surface temperature is maximum. Therefore with a relatively constant shear stress, fouling behavior entirely depends on the surface temperature of the test probe.

Asphaltenes precipitation fouling route has been also studied through large eddy and direct numerical simulations in a cylindrical pipe (Sileri *et al*., 2009). Volume-of-Fluid Multiphase model has been chosen to predict the asphaltenes deposition rate. Volume fraction and viscosity profiles were observed to understand the aging effects of fouling layer thickness occurred due to asphaltenes. From the analysis, it is noted that a complete flow blockage can happen inside the pipe with a gradual increase in fouling layer thickness with time. Therefore, there is a need to understand the hydrodynamic interactions of solid particles with bulk phase to achieve better deposits removal efficiency. Various studies were performed to understand the fluid dynamics and phase behavior of crude oil in a closed-end heat-exchanger (Emani *et al*., 2016; Yang *et al*., 2015). The deposition process associated with fouling is observed by two approaches: asphaltenes precipitation and chemical reaction fouling routes. Deposit formations through asphaltenes precipitation have been investigated through various SAFT models (Yang *et al*., 2015). A high fouling rate has been observed due to chemical reaction fouling compared with asphaltenes precipitation fouling route. Asphaltenes deposition rate and coke formation from crude oil have been investigated in a vertical pipe using species transport model (Haghshenasfard and Hooman, 2015). Various parameters such as Reynolds number, surface temperature, surface roughness and

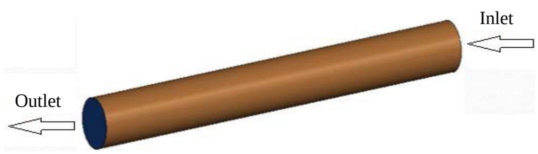

Fig. 2: Geometry model

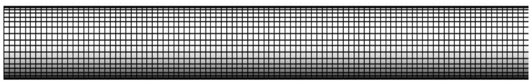

Fig. 3: Grid

Table 1: Asphaltenes particle properties

Descriptions	Values
Density	1200 (kg/m^3)
Diameter	0.01-0.1 (mm)
Thermal conductivity	0.756 (W/m/K)
Heat capacity	1500 (J/kg/K)

Table 2: Boundary conditions

Surfaces	Boundary conditions
Inlet	Velocity inlet
Wall	Wall with no slip condition
Outlet	Outflow

asphaltenes concentration on asphaltenes deposition rate, thermal resistance and heat transfer coefficient were discussed. Nevertheless, the transportation and adhesion mechanism of asphaltenes particles still remain unclear. Therefore, the present work focusses on the transportation and adhesion mechanism of the asphaltenes particles through discrete phase CFD simulations. The present discrete phase CFD predictions attempt to compare with the asphaltenes deposition rate estimated by Haghshenasfard *et al.* (2015) and with the experimental work performed by Jamialahmadi *et al.* (2009).

In the present study, the behavior of the asphaltenes particles is studied in a three dimensional heat exchanger tube. All the particles are injected from the inlet surface with diameters of 0.01-0.1 mm. DPM-CFD simulations required a high computational power to expound the particles behavior. Therefore, simulations were performed by activating the enhanced wall treatment effects with K-epsilon turbulence model. The domain is discretized with 0.15 million quadrilateral cells and mesh independence test has been performed to validate the consistency and accuracy of the simulation results. Figure 2 shows the geometry domain of the heat exchanger tube and Fig. 3 shows the grid created for the geometry. Table 1 provides the asphaltenes particle properties and Table 2 provides the boundary conditions of the heat exchanger tube.

In the present simulation, one way coupling with unsteady particle tracking has been considered with particle forces such as gravity, drag, thermophoretic, saffman lift and stochastic collision. A second order upwind momentum spacial discretization method has been used with Semi-Implicit Method for Pressure Linked Equations (SIMPLE) solution method for a better convergence. Initially, a dynamic simulation was performed without activation of the discrete phase models. Once, the fully developed flow is observed in the domain, DPM was activated to study the stick, spread, rebound and splash behavior of the asphaltenes particles.

Crude oil has been described as the bulk fluid and asphaltenes are described as discrete phase particles. As asphaltenes have the tendency to aggregate in an irreversible fashion with different particle diameters, the transportation of asphaltenes is modelled with various particles sizes. The fluid dynamics inside the heat exchanger tube is governed by incompressible Navier-stokes Eq. 1 for mass, momentum and energy. The continuity equation can be written as:

$$\frac{\partial \rho}{\partial t} + \Delta \cdot \left(\rho \overline{v}\right) \rho = 0 \tag{1}$$

pv

Momentum conservation (Eq. 2):

$$\frac{\partial \left(\rho \overline{v}\right)}{\partial t} + \Delta \cdot \left(\rho \overline{vv}\right) = -\Delta p + \Delta \cdot \left(\overline{\tau}\right) + \rho \overline{g} \tag{2}$$

Energy conservation (Eq. 3):

$$\frac{\partial \left(\rho E\right)}{\partial t} + \Delta \cdot \left(v\left(\rho E + p\right)\right) = \Delta \cdot \left(k_{eff} \Delta T + \left(\overline{\tau_{eff} v}\right)\right) \tag{3}$$

The trajectory of the asphaltenes particles inside the heat exchanger tube is calculated from Eq. 4:

$$\frac{du_p}{dt} = F_D\left(u - u_p\right) + \frac{g_i\left(\rho_p - \rho\right)}{\rho_p} + F_i \tag{4}$$

Where:

u_p = The particle velocity
F_D = The drag force
p = The density
ρ = The gravity force

The particles drag force is estimated as:

$$F_D = \frac{18\mu}{\rho_p d_p^2} \frac{C_D R_e}{24} \tag{5}$$

Where:

$$C_D = \frac{24}{Re}\left(1 + b_1 Re^{b_2}\right) + \frac{b_3 Re}{b_4 + Re} \tag{6}$$

$$Re = \frac{\rho d_p |u_p - u|}{\mu} \quad (7)$$

Where:

C_D = The drag coefficient of asphaltenes particles
Re = The Reynolds number
b_1-b_4 = Constants

The $b_1 = 0.186$; $b_2 = 0.653$; $b_3 = 0.437$; $b_4 = 7178.74$. The particles lift due to the shear is calculated by Saffman's lift force as given in Eq. 8:

$$\vec{F} = \frac{2Kv^{1/2}\rho d_{ij}}{\rho_p d_p (d_{lk} d_{kl})} \left(\vec{v} - \vec{v_p}\right) \quad (8)$$

where, K = 2.594 and d_{ij} are the deformation tensors. The asphaltenes particle accumulation rate is computed as Eq. 9:

$$R_a = \sum_{p=1}^{Np} \frac{m_p}{A_f} \quad (9)$$

Where:

m_p = The mass of the particles
A_f = The projection area of particle on the wall

RESULTS AND DISCUSSION

The CFD simulations successfully demonstrate the transportation and adhesion behavior of asphaltenes particles inside the heat exchanger tube. The stick, spread, rebound and splash behavior of the asphaltenes particles were studied successfully from the discrete phase CFD simulations. From the results obtained, asphaltenes mass deposition rate, deposition film thickness can be estimated to further mitigate the fouling.

From Fig. 4, the deposition of asphaltenes particles can be observed. Due to the force of gravity, asphaltenes particles are deposited on the bottom portion of the tube. The particles that are colored red were suspended from the bulk and deposited on the heat transfer surface. Other colored particles indicate that they are splashed, rebounded and finally deposited on the heat transfer surface. A film spreading of deposited particles can also be observed from Fig. 4.

Figure 5 shows the contour plot of the fouled tube. As the particle deposition is only on the bottom portion of the tube, the upper portion is seen to be relatively clean. The mass of the deposited particles and fouling layer thickness is observed from Fig. 6 and 7. Further, the deposited asphaltenes particles will be subjected to ageing process and hardens the deposit which might be difficult to remove. The particles transportation with

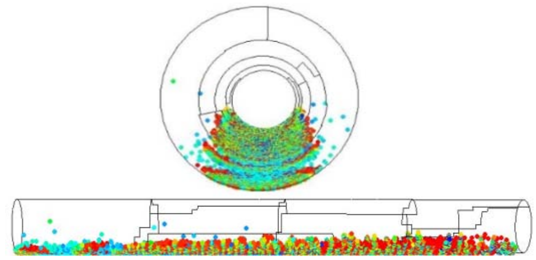

Fig. 4: Asphaltenes particle deposition on the tube surface

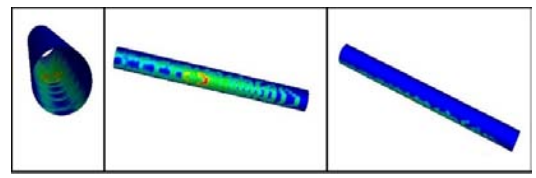

Fig. 5: Fouled tube

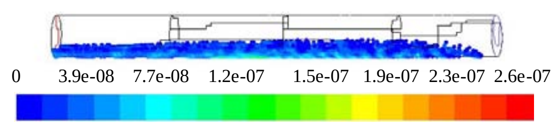

Fig. 6: Asphaltenes deposition mass (kg)

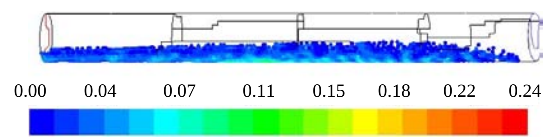

Fig. 7: Fouling layer thickness (mm)

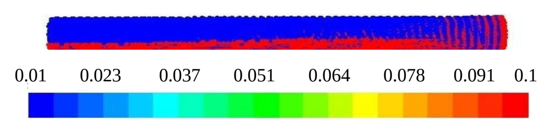

Fig. 8: Asphaltenes particle size profile (mm)

various sizes is observed from Fig. 8. Due to the activated Saffman lift force, smaller particle diameters are gaining a shear force which stimulates the particle momentum and particles with larger diameter are getting deposited on the heat transfer surface.

Figure 9 shows the graphical representation of asphaltenes deposition rate at various crude oil velocities predicted through the discrete phase CFD simulations. It is observed that at low fluid velocity conditions, asphaltenes particles will have a higher deposition rate compared with the high fluid velocity conditions. The present simulation results were impressively correlated with the existing experimental data.

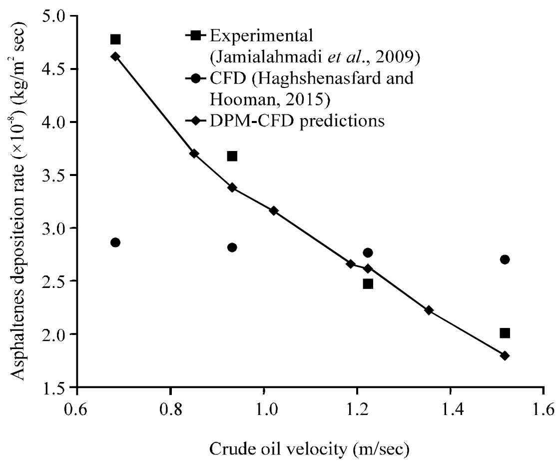

Fig. 9: Asphaltenes deposition rate vs. velocity

CONCLUSION

A three dimensional discrete phase CFD study has been performed to predict the asphaltenes deposition rate from crude oil. From the obtained results, the asphaltenes particle velocity is observed to have a high impact on mitigation of fouling. The discrete phase CFD simulation results clearly forecasts the asphaltenes particle deposition location in the tube, deposition mass and fouling layer thickness. Therefore, the non-symmetric fouling behavior of crude oil can be modelled using the available computational techniques, through which the susceptible regions of concern can be predicted in the shell and tube heat exchangers. More computational research is required to understand the fouling behavior of crude oil in pre-heaters and necessary operating condition modifications are in need to mitigate the fouling.

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