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Procedia Engineering 148 (2016) 1058 – 1065

Procedia Engineering

www.elsevier.com/locate/procedia

4th International Conference on Process Engineering and Advanced Materials

Effect of Shear Stress on Crude Oil Fouling in a Heat Exchanger Tube Through CFD Simulations

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Abstract

This work presents the effect of shear stress on deposit formation caused by the heavy petroleum residues in the crude oil. The investigation is based on a three dimensional study through Computational Fluid Dynamics approach. Fouling process is simulated using asphaltenes precipitation and chemical reaction routes. The asphaltenes phase deposition and coke formation rates were predicted through Volume-of-Fluid (VoF) multiphase model and thermal cracking due to chemical reactions, respectively. The aging process of the fouling layer was studied through a transient state numerical approach. Grid dependence study has been performed to confirm the accuracy of the performed mesh. It was observed that, wall shear stress enables the removal of fouling precursors and thus reduce the deposit formation.

Peer-review under responsibility of the organizing committee of ICPEAM 2016

Keywords: Crude oil, fouling, heat exchanger, Computational Fluid Dynamics

Nomenclature

v	fluid velocity [m/s]
T	temperature [K]
T_b	bulk temperature [K]
X_f	thickness of fouling layer [μm]

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Peer-review under responsibility of the organizing committee of ICPEAM 2016
doi:10.1016/j.proeng.2016.06.592

R_f	fouling resistance [$m^2K\cdot kW^{-1}$]
ρ_f	density of fouling layer [kg/m^3]
k	reaction rate coefficient [$mol\cdot L^{-1}$]
A	frequency factor [s^{-1}]
E	activation energy [kJ/mol]
m_{pq}	mass transfer from phase q to phase p [mol/s]
α	volume fraction
Y_j	mass fraction of species
D_j	mass diffusion coefficient of species [m^2s^{-1}]
r_j	intrinsic reaction rate of species
k_{eff}	Effective thermal conductivity [$Wm^{-1}K^{-1}$]

1. Introduction

Crude oil is one of the most predominant fossil fuel/energy resources in the world today. A complex mixture of hydrocarbons with various molecular weights, the crude oil, needs to be processed and fractionated into various fractions in a crude distillation unit (CDU) in refineries. The crude oil is normally preheated by recovering heat from the separated fractions and pump-around flows from the CDU in a battery of preheat exchangers. Efficient recovery of heat from the product streams is very essential in order to minimize the specific energy requirement of processing the crude oil. Nearly 6% of the total energy content of each barrel of crude oil is used in the refinery itself.

Effective recovery of heat in the preheat train suffers a major blow due to the occurrence of fouling in the heat exchangers. Fouling is the deposition of solid particles on the heat transfer surfaces which results in increased thermal resistance and reduced heat transfer. In addition, fouling reduces the cross sectional area for flow introducing additional pressure drops requiring higher pumping power. When the extent of fouling reaches the limits of operation either in the pumping capacity or in the furnace that provides the additional heat necessary, a plant shutdown becomes necessary for cleaning the heat exchangers and restoring their heat transfer efficiencies. The total cost of fouling in various refineries is estimated to be approximately USD 1.5 billion per year [1] and the annual cost for cleaning an industrial heat exchanger is about USD 40,000 to USD 50,000[2].

Asphaltenes are very large polyaromatic compounds which are classified as the major precursors of fouling [3]. High concentrations of asphaltenes might form as coke and cause deposits in the heat exchanger tubes. The prevention of asphaltenes deposition in the heat exchanger tube might help in mitigating the fouling caused. However, to maximize the usefulness of crude oil, it is highly essential to understand the formation of deposits in the heat exchangers, which requires much better understanding of the properties and reactivity of asphaltenes. Besides our CROFREC (CRude Oil Fouling REsearch Center) group, 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, Cambridge University in association with Engineering Science Data Unit (ESDU), and other independent studies were also being carried out globally to understand the physical and chemical aspects involved in crude oil fouling. Various experimental and computational studies were performed to understand the effect of shear stress on crude oil fouling on batch stirred cells [4-7] and observed that, with the influence of shear stress, deposits formed in the stirred cells can be removed/suppressed from the heated surface which eventually reduces the overall deposition. Therefore, one of the approaches to mitigate fouling was identified as enhancement of wall shear stress.

In this study, the effect of shear stress on crude oil fouling due to asphaltenes precipitation and chemical reaction is investigated in a single heat exchanger tube. The crude oil was described as a mixture of three pseudo components: petroleum, salt and asphaltenes and a three dimensional CFD simulation was performed on the heat exchanger tube using ANSYS FLUENT solver. The boundary conditions of the domain and properties of the pseudo components are detailed in Table 1 and 2. The lumped surface reaction rates and properties of the pseudo components considered by Mahmoud et al., (2012) has been used in the present work to predict the coke deposition inside the tubes [8].

The present paper is divided into five sections. The background on fouling, its effects and earlier approaches in mitigating fouling were discussed in introduction part. The simulation methodology focusing mainly on the approach used in predicting the crude oil fouling in heat exchangers through asphaltenes precipitation and chemical reaction fouling route is presented in Section 2. The CFD model with the governing equations, geometry and grid, and chemical reaction rate equations are provided in Section 3. Section 4 summarizes the results and discusses, the formation of deposits on the tube surface through asphaltenes precipitation and chemical reaction fouling routes with wall shear stress and no slip conditions.

Table 1. Boundary conditions

Surface	**Boundary conditions**
Inlet	Velocity inlet
Wall	Wall (with no slip and shear stress conditions)
Outlet	Pressure outlet

Table 2. Properties of pseudo components

Material	Density (kg m^{-3})	Viscosity (kg m^{-1} s^{-1})	Thermal conductivity (W m^{-1} K^{-1})	Heat capacity (J kg^{-1} K^{-1})
Petroleum	870	0.00164	0.145	1800
Asphaltenes	850	0.006	0.123	1500
Coke	900	150,000	1.500	1500
$Salt_b$	850	0.006	0.123	1500
$Salt_w$	900	180,000	1.500	1500

2. Simulation methodology

The fouling precursors in the crude oil can be formed due to various reactions of crude oil components that take place inside the heat exchanger [9-11]. Also, suspended particles might be present in the crude oil without any reactions, i.e. by asphaltenes precipitation [9]. Applying Computational Fluid Dynamics (CFD) to crude oil fouling appears to be quite promising to understand the phenomena of deposit formation through a series of reactions and without any reactions. The use of appropriate phase viscosities and molecular diffusion coefficients has a significant role in predicting the formation of deposits. The deposit formation in the heat exchanger tube was modeled through asphaltenes precipitation and chemical reaction fouling route as outlined in the following sections.

2.1 Asphaltenes precipitation

Heavy components dissolved in the crude oil may precipitate and adhere on the heat transfer surfaces. In the present CFD formulation, multiphase modeling was considered to understand the phase separation of heavy components in crude oil. Two phase flow problems can be solved numerically by either Eulerian-Eulerian approach or Eulerian-Lagrange approach. Volume-of-Fluid (VoF), a category of Eulerian-Eulerian approach, is mainly focused on phase interface tracking [12]. Therefore, in the present work, pressure based solver with VoF multiphase model has been implemented to track the deposit phase. Since fouling is a dynamic process, transient flow analysis has been made to predict the aging of deposit formations with time. In this work, non–asphaltenes are described as continuous phase and asphaltenes as dispersed phase. From the developed CFD methodology, asphaltenes deposition rate has been predicted from the volume fraction contours obtained through the simulations. The role of wall shear stress is observed by comparing the CFD results with no slip boundary condition.

2.2 Chemical reaction fouling

Chemical reaction fouling is described as the deposition resulting from one or more chemical reactions between reactants contained in the crude oil [13, 14] and it has been identified as the main cause of pre-heat exchanger fouling in many refineries. Chemical reaction fouling involves a two-step reaction process:

Reactant (soluble) ⟶ Precursor (sparingly soluble) ⟶ Foulant (insoluble)

Initially, a dynamic simulation was performed without activation of the considered species. Once the domain has achieved a fully developed flow, the species were activated to understand the deposition of asphaltenes due to thermal cracking. Petroleum is considered as the bulk fluid and the coke content is specified at the inlet as zero. Therefore, the first phenomenon involved to understand the fouling process through chemical reaction route is the diffusion of the species through the bulk fluid. Then, the reactions of the pseudo components on the tube surface were activated to observe the formation of fouling layer. The same simulation methodology has been considered for comparison of results with no slip condition and with shear stress of 0.05 Pa on the wall.

3. Mathematical model

3.1 Geometry and grid

A three dimensional heat exchanger tube was modeled to implement the described simulation methodology to predict the deposit formations. Fig. 1 shows the geometry domain and its boundary conditions. Table 3 provides the domain dimensions and operating conditions.

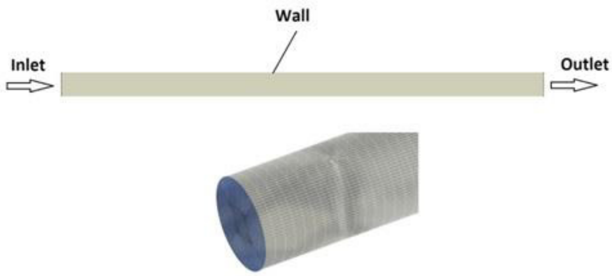

Figure 1. Geometric model and grid

Table 3. Model dimensions and operating conditions

Description	Value
Tube length	500 mm
Tube diameter	25 mm
Flow velocity	0.79m/s
Wall temperature	450 K
Bulk temperature	350 K

The domain was discretized with 0.12 quadrilateral cells and a grid independence test was performed to confirm the consistency and accuracy of the simulation results.

3.2 Governing equations

An analytical description of deposit formations can be understood from computational studies through various parameters such as mass deposition rate, fluid velocity, heat transfer rate, fouling layer thickness, and volume fraction of asphaltenes inside the domain. Since it is difficult and time consuming to model all the length and time scales in the system, the present study considered the Reynolds-Averaged Navier Stokes SST K–ω turbulent model to study the fluid flow behavior of particle depositions. The fluid flow inside the heat exchanger domain is governed by incompressible Navier-Stokes equations for mass, momentum and energy. The conservation of mass or the continuity equation can be written as:

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

Momentum conservation equation:

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

Energy conservation equation:

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

Continuity equation for the volume fraction of multiphase can be accomplished in tracking the phase interface. For q^{th} phase, interface tracking can be computed as:

$$\frac{1}{\rho_q}[\frac{\partial}{\partial t}(\alpha_q \rho_q) + \nabla.(\alpha_q \rho_q \vartheta_q) = S_{\alpha_q} + \sum_{p=1}^{n}(m_{pq} - m_{qp})] \quad (4)$$

Species transport equation for species j is given as:

$$\frac{\partial}{\partial t}(\rho Y_j) + \frac{\partial}{\partial \overline{x}}(\rho Y_j \overline{u}) = \frac{\partial}{\partial \overline{x}}\left(\rho D_j \frac{\partial Y_j}{\partial \overline{x}}\right) - r_j \quad (5)$$

The chemical reactions of the pseudo components on the heat exchanger tube surface are modelled using Arrhenius type chemical rate expression:

$$k_1 = Aexp^{-E/RT_s} \quad (6)$$

The corresponding reaction rates are shown in equations (7) and (8):

$$-r_{asph.} = 8 \times 10^{20} e^{-2e8/RT}[asph.]^{0.5} \quad (7)$$

$$-r_{salt_b} = 1.2 \times 10^{21} e^{-2e8/RT}[salt_b]^{0.5} \quad (8)$$

The described governing equations were solved through pressure based solver by finite volume method. Simple consistent pressure velocity coupling scheme is considered. As the present simulation methodology involves the transport and adhesion mechanism of heavy hydrocarbon phase, discretization of convective transport terms are performed though a high order differencing scheme *i.e.* Quadratic Upstream Interpolation for Convective Kinematics (QUICK) scheme to accurately predict the kinematics of the considered pseudo components.

4. Results and discussions

The CFD simulations successfully demonstrate the formation of deposits on a heat exchanger tube and the effect of shear stress on crude oil fouling is investigated. Wall shear stress helps in dislodging of deposits from heat transfer surface. From the observed results, bulk temperature, volume fraction and mass deposition rate profiles were studied with no slip and wall shear stress boundary conditions.

Volume fraction of asphaltenes and coke mass deposition rate profiles along the length of the tube are shown in Fig. 2 and Fig. 3. It can be observed that, with 0.05Pa wall shear stress, deposition rate is reduced compared with no slip condition on wall. The reduction in fouling is due to the increase in crude oil velocity with shear stress which helps to dislodge the asphalt phase from the location it got deposited on the tube wall. With wall shear stress on the tube surface, an increase in the initiation time for fouling is observed. The difference in asphaltenes volume fraction deposition was significantly 25-35% less pronounced with shear stress condition. It is also observed that, with wall shear stress, the rate of deposition significantly decreased throughout the tube with transient time step.

a) b)

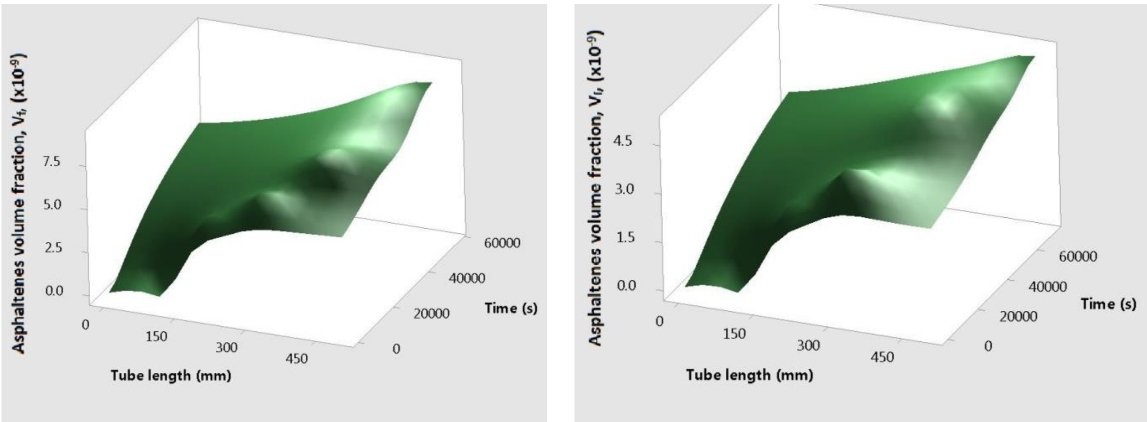

Figure 2. Asphaltenes volume fraction on tube length w.r.t time, a) no slip condition b) wall shear stress condition

a) b)

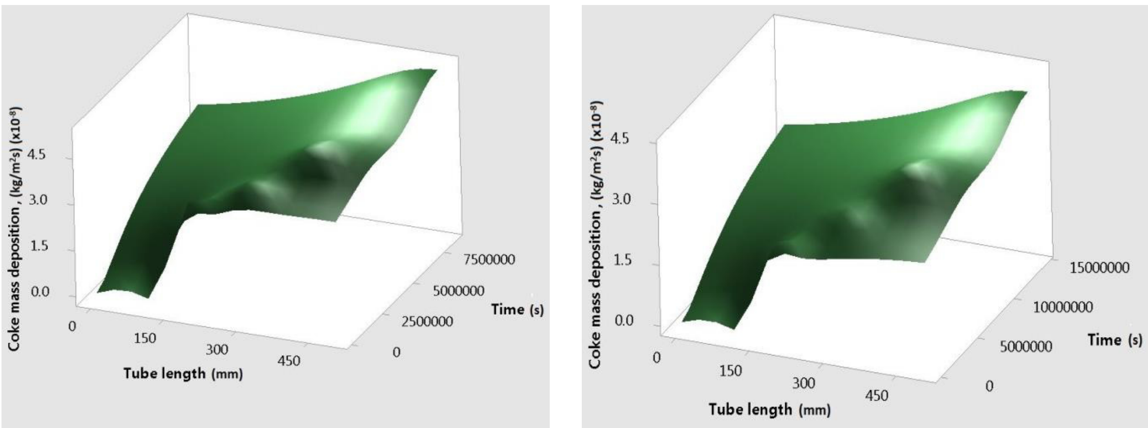

Figure 3. Coke mass deposition on tube length w.r.t time, a) no slip condition b) wall shear stress condition

a) b)

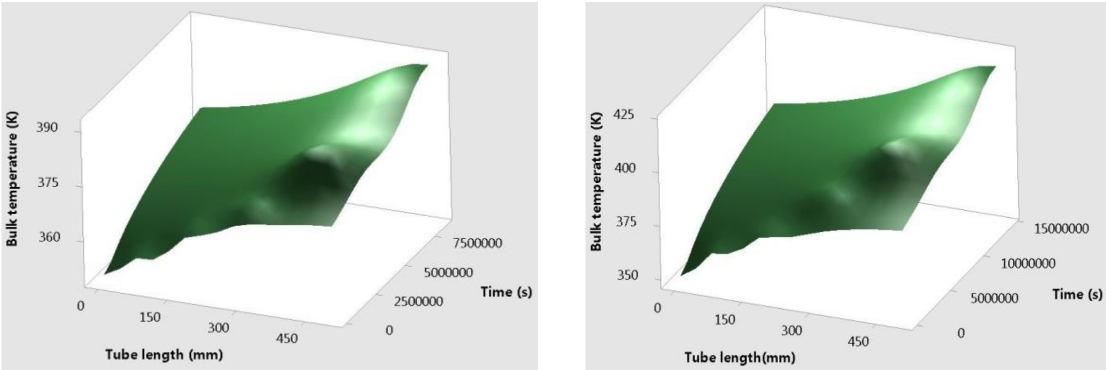

Figure 4. Bulk temperature on tube length w.r.t time, a) no slip condition
b) wall shear stress condition

Fig. 4 shows the bulk temperature profile along the tube with no slip and wall shear stress boundary conditions. It can be observed that with wall shear stress, heat transfer tends to increase when compared with no slip condition on wall. From the observed results and discussions, it can be said that, high fouling rate conditions can be controlled with increase in wall shear stress.

5. Conclusions

A three dimensional Computational Fluid Dynamic study has been performed to investigate the effect of shear stress on crude oil fouling and to predict the asphaltenes deposition and coke formation in a heat exchanger tube. Crude oil has been described with three pseudo components: petroleum, asphalt and salt. With the available multiphase and species transport models, heavy hydrocarbons deposition on the heat exchanger tube wall has been predicted through asphaltenes precipitation and chemical reaction fouling routes. From the obtained results, it can be said that wall shear stress have a high impact on mitigation of fouling. Further, the developed CFD methodology can be employed to understand the transportation and adhesion behavior of fouling precursors in an industrial heat exchanger.

Acknowledgements

Authors of the study greatly acknowledge the support and facilities provided by Universiti Teknologi PETRONAS.

References

[1] I. Wiehe, Petroleum fouling: causes, tools, and mitigation methods, Soluble Solutions, Gladstone, NJ, 2006.
[2] C.B. Panchal, E.P. Huang-Fu, Effects of mitigating fouling on the energy efficiency of crude-oil distillation, Heat Transfer Eng., Vol. 21, pp. 3-9, 2000.
[3] G.A. Mansoori, Modelling of asphaltenes and other heavy organic depositions, Journal of Petroleum Science and Engineering, Vol. 17, pp. 101-111, 1997.
[4] A. Young, S. Venditti, C. Berrueco, M. Yang, A. Waters, H. Davies, S. Hill, M. Millan, and B.D. Crittenden, Characterization of crude oils and their fouling deposits using a batch stirred cell system, Heat Transfer Engineering, 32 (3-4), pp. 216-227. 2011.
[5] Y. Mengyan, Y. Andrew and B.D. Crittenden, Use of CFD to correlate crude oil fouling against surface temperature and surface shear stress in a stirred fouling apparatus, Proceedings of International Conference on Heat Exchanger Fouling and Cleaning VIII, 2009.
[6] Y. Mengyan, Z. Wood, B. Rickard, B.D. Crittenden, M. Gough, P. Droegemueller, T. Higley, Effect of turbulence enhancement on crude oil fouling in a batch stirred cell, Chemical Engineering Transactions, Vol. 29, 2012.
[7] M. Yang, A.O. Meara, B.D. Crittenden, Determination of crude oil fouling thresholds, Proceedings of International Conference on Heat Exchanger Fouling and Cleaning, 2011.
[8] M. Bayat, J. Aminian, M. Bazmi, S. Shahhosseini, K. Sharifi, CFD modelling of fouling in crude oil pre-heaters, Energy Conversion and Management, Vol. 64, pp. 344-350, 2012.
[9] J. Yang, G. Maria, J. Serratos, D.S.F. Arole, E.A. Muller, O.K. Matar, Crude Oil Fouling: Fluid Dynamics, Reactions and Phase Change,

Procedia IUTAM, Vol. 15, pp. 186–193, 2015.
[10] M. Haghshenasfard, K. Hooman, CFD modelling of asphaltenes deposition rate from crude oil, Journal of Petroleum Science and Engineering, Vol. 128 , pp. 24-32, 2015.
[11] X.G. Li, L.U. Zhang, R.Y. Zhang, X. Li, CFD modeling of phase change and coke formation in petroleum refining heaters, Fuel Processing Technology, Vol. 134, pp. 18-25, 2015
[12] D.V.R. Fontoura, E.M. Matos, J.R. Nunhez, A three-dimensional two-phase flow model with phase change inside a tube of petrochemical pre-heaters, Fuel, Vol. 110, pp. 196-203, 2013.
[13] A.P. Watkinson, D.I. Wilson, Chemical reaction fouling: a review, Exp. Therm. Fluid Sci., Vol. 14, pp. 361–374, 1997.
[14] B.D. Crittenden, S.T. Kolackzkowski, D.Z. Phillips, Chemical reaction fouling, In: Bott, E.F.C. (Eds.), Proc. Int. Conf. on Understanding Heat Exchanger Fouling and its Mitigation, Italy. pp. 91–103, May 1997.