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Fouling Modelling and Mitigation for Crude Oil Heat Exchanger Networks using Reconciled Operating Data

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In crude oil refineries, fouling in heat exchangers and heat exchanger networks represents one the most complex and challenging issues. Its occurrence produces major impacts in thermal, hydraulic and economic performance on every heat transfer process. Increasing in fuel consumption, pressure drop and CO_2 emissions across heat exchangers are examples of a wide series of consequences that are attributed to fouling in different petro-chemical process industries.
Predictive models for fouling deposition have become a useful tool for analysing thermal performance on heat exchanger networks. A wide range of semi-empirical models have been reported in the literature considering different types of crude oil. Most of these models present a series of parameters that need to be fitted using experimental data. However, there is an uncertain relation between field and laboratory conditions, compromising the quality of predictions and greatly affecting further simulation and optimisation of heat exchanger networks.
The proposed approach presents an alternative method for determining fouling models using reconciled operating data. Data reconciliation is included in order to account for the effect of measurement errors and presence of faulty instruments within a given set of measurements. Depending on the available redundancy, further analysis can take place regarding feasibility of the data reconciliation problem, along with process variable classification. Once the data have been reconciled, the specific set of fouling model parameters can be fitted and implemented into the framework for operational optimisation for fouling mitigation, or optimisation of cleaning schedules. Different sets of cleaning actions can be analysed and further optimised by minimising the total operating cost, once the specific fouling models are successfully determined, resulting and economic and environmental savings.

1. Introduction

Mitigation of fouling deposition is a complicated task. Formation and removal rates depend on several operating conditions that can change constantly throughout the refining of any specific crude. The wide range of consequences fouling carries with its occurrence have been mentioned in the past (Smith and Loyola-Fuentes, 2017) and current efforts attempt to mitigate its effect by considering the application of fouling models for prediction and assessment of fouling monitoring and mitigation.
Several approaches have been developed for determining fouling models. Attention has been driven to the use of operating data for regressing fouling models by applying different types of methodologies. In the work proposed by Coletti and Macchietto (2011), existing data was used for determining fouling conditions on a single heat exchanger within a crude oil preheat train. Another application was proposed by Ishiyama et al. (2013), where a cleaning schedule problem is formulated for a crude oil Heat Exchanger Network using operating data. On both approaches, the input data was pre-treated in order to mitigate or eliminate any faulty measurements, only considering the effect of random noise and no identification of systematic errors were implemented. Also, fouling is only considered on the tube side of each heat exchanger. However, if no bias is found, and if each exchanger presents a rather low severity of fouling, both approaches have presented a high level of applicability for industrially-relevant cases.

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When using operating data for Data reconciliation purposes, it is necessary to consider the number of observations and process states, which will define the system redundancy. Unmeasured variables can be estimated using the physical relations among streams and equipment, which directly depend on the system redundancy (Narasimhan and Jordache, 1999). If enough redundancy is not found, increase in observations by means of instrumentation is needed. Thus, redundancy analysis and variable classification is paramount as it sorts the amount of information in the most meaningful way for further reconciliation steps.
This work proposes an integrated methodology that considers the effect of measurement error as random and gross error for determining fouling models on both sides of each heat exchanger within a crude oil preheat train. A simulation scheme is applied, which minimises the level of required redundancy on the network and can be updated to include the effect of fouling dynamics and temperature dependent physical properties. Each element contained within the network is considered in this scheme, where process-to-process heat exchangers are specified by area, whereas hot and cold utilities are by heat duty. Fouling models are determined by minimising the difference between reconciled fouling resistances and the ones obtained from a set of selected fouling models for each side of each heat exchanger.

2. Methodology

The proposed methodology comprises of three main parts. The first part consists on the management of input data. Operating data is replicated by using a rigorous simulation scheme, based on the approach proposed by Ochoa-Estopier et al. (2015), where a specific time range is simulated. Mass flow rates and outlet temperatures of each heat exchanger within the network are calculated and random noise and/or bias are added into the simulated data. This last step is implemented in order to account for the effect of measurement error within the data. The second part involves the use of the noisy simulated data into a Data Reconciliation (DR) algorithm. This algorithm minimises the measurement error by using Nonlinear Programming (NLP) techniques. Mass and energy balances are set as process constraints and biased measurements are found using a combinatorial approach (Sánchez et al., 1999). The last part of this methodology consists on the parametric fitting of fouling models using the reconciled data. A hybrid optimisation scheme is applied to minimise the error between fitted and reconciled fouling resistances. The fitted fouling parameters are then used for predicting outlet conditions and fouling behaviour throughout the network. Further applications can be implemented; examples of these are the optimisation of cleaning schedules and operational optimisation for fouling mitigation.

2.1 Heat Exchanger Network simulation

All the interactions among streams and heat exchangers within an existing HEN are contained in this simulation approach, firstly developed by de Oliveira Filho et al. (2007) and then modified by Ochoa-Estopier et al. (2015) for temperature-dependent physical properties. On this simulation model, input data (supply stream temperatures, flowrates, number of heat exchanger, etc.) set the problem into a linear system of equations, which contains both mass and energy balances for each heat exchanger, splitters and mixers. This simulation scheme has been extended to consider the aspects described below.

Fouling resistance updating using fouling rate models

Fouling can be dynamically updated from a time step n to (n+1) using a fouling rate model as it is defined in Eq(1). A time step is selected, and each dynamic step is calculated using an explicit Euler integration method.

$$R_f\Big|_{n+1} = R_f\Big|_n + \Delta t \left.\frac{dR_f}{dt}\right|_n \tag{1}$$

Where R_f is the fouling resistance and t is time. The main advantages of this approach are the simplicity for its formulation and the fact that each heat exchanger is defined by area, which improves the capability for assessing heat transfer during any existing network optimisation scheme (Ochoa-Estopier et al., 2016).

Inclusion of hot and cold utilities

Based on the same matrix formulation, hot and cold utilities are added into the simulation approach. For this part, each utility is specified based on their heat duty, rather than heat exchanger area as it is case for process-to-process heat exchangers. Fouling developing is not considered for hot and cold utilities since most of these equipment use steam and cooling water as utility streams, which compared to crude oil and distillation side products, present relatively lower fouling coefficients. Process-to-process heat exchangers will present fouling, which will affect the outlet conditions for each cold and hot utility on the crude oil (and side products) side.

2.2 Data Reconciliation and Gross Error Detection

A measurement error ε is defined as the difference between the measured (y) and true value (x) of a specific state variable, as shown in Eq(2). At the same time, this measurement error can also be described as the sum of random (r_ξ) and systematic errors (or Gross Error, g_ξ), as shown in Eq(3).

$$\varepsilon = y - x \tag{2}$$

$$\varepsilon = r_\varepsilon + g_\varepsilon \tag{3}$$

Random errors are defined as random events that can cause disruptions within the data. They are produced by changes in the environment, power fluctuations, etc. Gross errors are produced by non-random events such as miscalibrations or instrumental malfunctions. Their magnitudes are often higher compared to random errors, thus it is important to mitigate their effect before reconciling any type of data (Narasimhan and Jordache, 1999).

Nonlinear Data Reconciliation

Most of chemical process systems are represented by nonlinear models, and fouling modelling on a crude oil preheat train is no exception. Energy balances, thermal effectiveness and fouling rate models present a nonlinear nature, and these are contained within the operational constraints for the Data Reconciliation problem. Consequently, the approach for this methodology implements a nonlinear constrained optimisation problem for solving the minimisation of measurement error. A general formulation for this optimisation problem is defined in Eq(4).

$$\begin{aligned} &minimise\ (y-x)^T \psi^{-1}(y-x) \\ &subject\,to\ f(x)=0 \\ &\qquad g(x)\geq 0 \\ &\qquad x^L \leq x \leq x^U \end{aligned} \tag{4}$$

Where ψ is the measurement error covariance matrix, f and g are equality and inequality constraints respectively, and x^L and x^U are lower and upper bounds for each state variable, respectively. For this methodology, the optimisation problem shown in Eq(4) is solved using a Sequential Quadratic Programming solver (SQP). This solver presents several advantages when applying it into a Data Reconciliation problem. The first advantage is that the objective function in Eq(4) is quadratic with respect to the measurement error, therefore the use of an SQP solver shows itself as a convenient option for calculating an optimal solution. The second advantage is that the solver can easily handle inequality constraints and lower and upper bounds can be set on the optimisation variables (Romagnoli and Sanchez, 1999).

Gross Error Detection

Most common examples of gross errors are bias in measurements and leaks in operational equipment. For this work, only biased measurements are considered, where either single or multiple gross errors can be identified. Location and magnitudes for faulty measurements are calculated by including the effect of gross error into the optimisation problem defined in Eq(4). The solution of the Data Reconciliation and Gross error Detection problem is obtained by using the combinatorial approach proposed by Sánchez et al. (1999), where the identification and reconciliation problem are solved simultaneously. The general formulation for this problem is defined on Eq(5), where B_m is a matrix indicating the location of single or multiple gross errors.

$$\begin{aligned} &minimise\ (y-x-B_m g_\varepsilon)^T \psi^{-1}(y-x-B_m g_\varepsilon) \\ &subject\,to\ f(x)=0 \\ &\qquad g(x)\geq 0 \\ &\qquad x^L \leq x \leq x^U \\ &\qquad g_\varepsilon^L \leq g_\varepsilon \leq g_\varepsilon^U \end{aligned} \tag{5}$$

Presence of gross error is determined by statistical tests, based on the assumption that the measured data follows a chi-square probability distribution when no gross error is found (Narasimhan and Jordache, 1999). This test is also known as Global Test (GT) and sets the basis for the application of the above-mentioned approach. The optimisation problem is also solved by using SQP algorithm and reconciled values along with location and magnitudes of gross errors are obtained simultaneously.

2.3 Parametric fitting

The proposed fitting approach is designed to take into account three important challenges when regressing fouling model parameters (Costa et al., 2013). The first challenge is the drastic difference among each parameter magnitude, which can harm the accuracy of the optimal results. The second challenge is the presence of local optima. Different sets of fouling model parameters can be found during the optimisation solving, hence it is necessary to develop a strategy for finding a global optimal solution. The last challenge is the high level of dependency the solution may exhibit with respect to its initial guess.

These specific issues are addressed by implementing a hybrid optimisation strategy, combining the use of normalised optimisation variables, Genetic Algorithm (GA) for obtaining an initial estimation, and a deterministic gradient-based solver for fine-tuning the optimal solution.

The objective functions is defined by Eq(6). In this equation, it is of interest to minimise the relative square error for fitted and simulated fouling resistance, R_f^{fit} and R_f^{sim}, subject to lower and upper bounds. The entire set of data is divided in two parts; the first part used for fitting and second one used for predicting outlet network conditions and fouling behaviour for each heat exchanger.

$$\begin{aligned} &minimise\left(\frac{R_f^{fit}-R_f^{sim}}{R_f^{msr}}\right)^2 \\ &subject\,to\;\; R_f^{fit,L} \le R_f^{fit} \le R_f^{fit,U} \end{aligned} \tag{6}$$

The fouling model is applied to each side of each heat exchanger depends on their relative location within the network. For this work, two different fouling models are used. A constant fouling rate is set to be on the cold end of the network on both sides of each heat exchanger, whilst a chemical reaction rate model is applied to the tube side of each exchangers at the hot end of the preheat train. A widely accepted model for this mechanism is the one proposed by Polley et al. (2007). This model present three parameters that need to be determined and it is defined in Eq(7).

$$\frac{dR_f}{dt} = \alpha\, Re^{-0.8}\; Pr^{-0.33}\; exp\left(\frac{-E_A}{R_g T_W}\right) - \gamma\, Re^{0.8} \tag{7}$$

Where α, E_A and γ are the fouling model parameters. Re and Pr represent Reynold and Prandtl numbers respectively, R_g is the gas constant and T_W is the wall surface temperature calculated at bulk temperature. This set of three parameters, along with the constant fouling rate value for the cold end of the preheat train represent the set of parameters that needs to be fitted for determining a specific crude oil fouling model. Upper and lower bounds are applied onto the set of fouling model parameters and the constant fouling rate value for the fitted fouling resistance in Eq(7).

3. Case study

The presented case study is depicted in Figure 1. This HEN is based on the work proposed by Akpomiemie and Smith (2015). The network consists on seven process-to-process heat exchangers, one furnace as hot utility, four water coolers as cold utilities, one cold stream and five hot streams. The simulation time is one year, during which a constant fouling rate of 5.50e-04 $m^2K\ kW^{-1}h^{-1}$ is set on exchangers E1 to E4 on both sides of the heat exchangers, and also on the shell side of exchangers E5 to E7. Chemical reaction fouling based on Eq(7) is set on the tube side of exchangers E5 to E7. Base values for these fouling model parameters can be found in Table 1.

Input data are set to be flow rates and inlet temperatures of all six streams connected to the network (one cold stream and 5 hot streams). Random noise and a bias of 10 °C are added into the data set and the furnace inlet temperature, respectively. Standard deviations for each measurement instrument have been selected according to average accuracies for flow rate and temperature measurement instruments. For this work, standard deviations of 1.5 kg s^{-1} and 1 °C are set for flow rates and temperatures respectively. The proposed approach is applied for discussing the network in terms of redundancy, reconciled values and fitted fouling model parameters.

By applying the simulation scheme mentioned in Section 2.1, a unique solution for the network mass and energy balance is achieved for each time step. This means that in order to obtain a feasible set of reconciled values and accurate predictions, it is necessary to measure the inlet conditions (flow rates and temperatures) for each main stream. Any other stream inside the network can be estimated by exploiting the existing redundancy among equipment and streams, using the selected simulation approach.

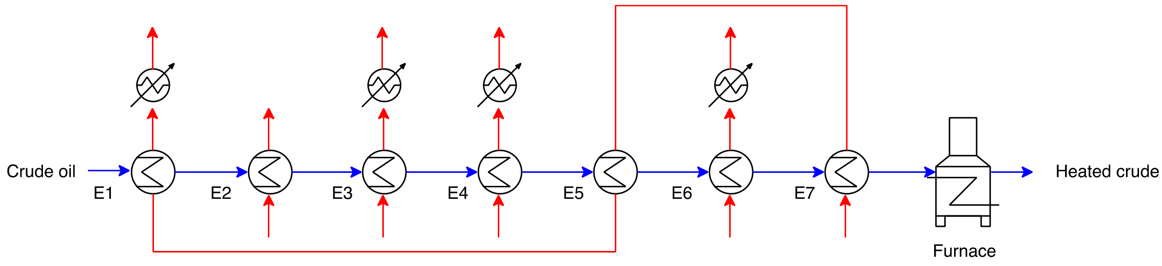

Figure 1: Heat Exchanger Network for case study

Data Reconciliation and Gross Error Detection results are shown in Table 2. The estimated location and average magnitude (over time) of the single gross error added into the data is correctly estimated, based on its average estimated value. Figure 2 illustrates parity plots for fouling resistances on each heat exchanger within the network. These results show good agreement between predictions and simulated data. The accuracy of the parametric fitting is directly related with the performance of the Data Reconciliation solution. Thus, if an accurate fitting is to be obtained, each measurement error needs to be successfully mitigated by the Data Reconciliation procedure. Fitted fouling model parameters for each heat exchanger are shown in Table 3.

Table 1: Fouling rate model parameters for HEN simulation

Parameter	Unit	Value
α	$m^2K\ kW^{-1}h^{-1}$	1.00e+06
E_A	$kJ\ mol^{-1}$	48.0
γ	$m^2K\ kW^{-1}h^{-1}$	1.50e-09

Table 2: Location and average estimation of gross error for data reconciliation

Bias magnitude (°C)	Average estimation (°C)
10.0	10.02

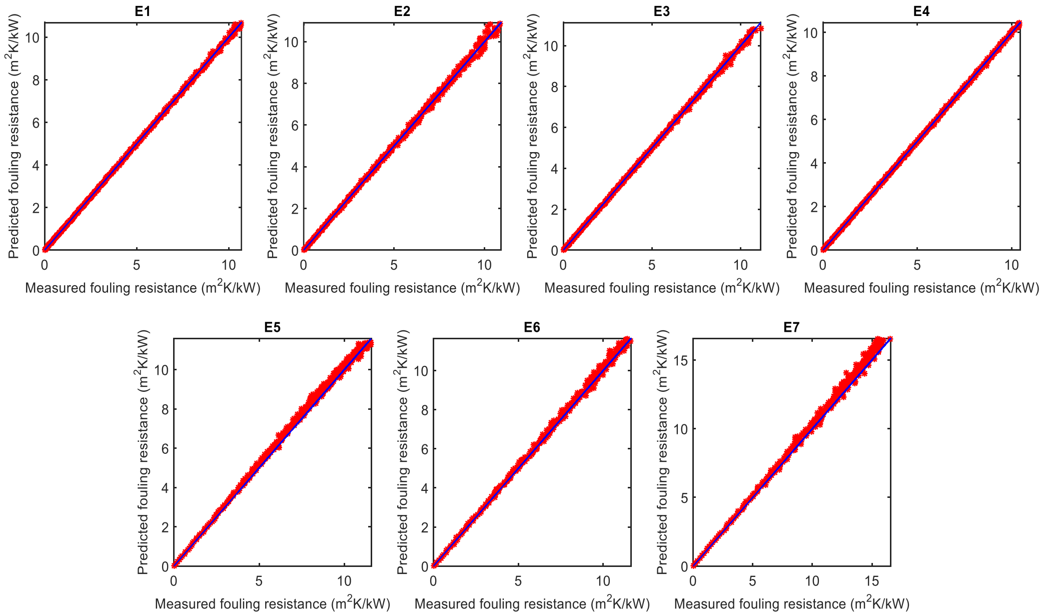

Figure 2: Parity plots for fitted fouling resistance on each network heat exchanger

Table 3: Fouling rate model fitted parameters

Heat Exchanger	α ($m^2K\ kW^{-1}h^{-1}$)	E_A ($kJ\ mol^{-1}$)	γ ($m^2K\ kW^{-1}h^{-1}$)	Constant rate ($m^2K\ kW^{-1}h^{-1}$)
E1	--	--	--	5.50e-04
E2	--	--	--	5.5e-04
E3	--	--	--	5.50e-04
E4	--	--	--	5.50e-04
E5	3.63e+05	43.31	8.61e-08	6.13e-04
E6	1.01e+06	47.96	8.33e-08	7.49e-04
E7	1.43e+06	49.53	8.24e-08	8.69e-04

4. Conclusions

Fouling significantly impacts the performance on any heat exchanger; especially on crude oil preheat trains. Determination of fouling models includes time-consuming experimental tests that in some cases do not represent entirely the dynamic nature of fouling deposition. This work attempts to obtain a specific set of fouling models for both sides of heat exchangers based on the information given by a specific set of operating data. A simulation approach is used so it can be integrated within a Data Reconciliation algorithm, which is further used for determining fouling models using a hybrid parametric fitting method.

Results show that the proposed methodology is able to predict fouling dynamics on a Heat Exchanger Network, using reconciled noisy data even when one (or more) measurement presents a systematic error. The faulty instrument is located in terms of the measurement containing such error, and its magnitude is correctly estimated. Fouling resistances are successfully predicted, presenting a high level of agreement with the simulated (or measured) data.

The integration of this three-part methodology can be applied using existing operational data, when the available instrumentation satisfies the input information requirement for achieving convergence on both, simulation and reconciliation of the Heat Exchanger Network.

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