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PARAMETER ESTIMATION OF FOULING MODELS IN CRUDE PREHEAT TRAINS

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ABSTRACT

Several fouling mitigation techniques depend on the capacity of predicting fouling rates. Therefore, the identification of accurate fouling rate models is an important task. Crude fouling rates are usually evaluated through empirical or semi-empirical models. In both alternatives, there are parameters which must be determined through laboratory or process data. In this context, the proposed paper presents an analysis of the parameter estimation problem involving fouling rate models. A proposed procedure for addressing this problem is described through the development of a computational routine called HEATMODEL. An important aspect of this study is focused on the obstacles associated to the search for the optimal set of parameters of the Ebert and Panchal models and its variants. This optimization problem may present some particularities which complicate the utilization of traditional algorithms (e.g. multiple local optima). In the proposed paper, the performance of a conventional optimization algorithm (Simplex) is compared with a more modern numerical technique (a hybrid Genetic Algorithm) using real data from a Brazilian refinery. The results indicated that, due to the complexity of the parameter estimation problem, the Simplex method may be trapped in poor local optima, thus indicating the importance of the utilization of global optimization techniques for this problem.

INTRODUCTION

Considerable research efforts have been made to diminish the impact of fouling in industrial plants. However, due to the complexity of this phenomenon, there are still many unsolved problems in this area. In this context, the fouling problem in crude oil distillation is associated with considerable economical and environmental penalties.

Before entering the distillation column, the crude stream must be heated from ambient temperature to about 380 ºC. In order to reduce energy consumption, the hot product streams and pumparounds from the distillation column are used to preheat the crude oil stream in a series of heat exchangers, called the crude preheat train. The final heating step is done in a fired heater which consumes fuel.

However, during the refinery operation, there is an accumulation of deposits over the thermal surface of the heat exchangers. As a consequence, there is a reduction of the thermal effectiveness of the crude preheat train which imposes an increase of energy consumption and carbon emissions in the fired heater. Additionally, the fouling layer also increases the head loss along the preheat train. In more severe cases, due to limitations of the pumping system, it may be necessary to reduce the throughput.

In crude preheat trains, fouling is caused by different mechanisms, depending on if the heat exchanger is located upstream or downstream of the desalter (equipment designed to remove water and dissolved salts in the crude oil): (i) upstream the desalter: fouling is linked to the presence of particulate matter and salts and (ii) downstream the desalter: chemical reaction fouling becomes important, associated to the presence of asphaltenes.

Fouling rate models can be an important resource for fouling management. The prediction of the fouling rate can provide a forecast of the fouling impact, thus allowing a better planning of how to deal with the problem. An example of a mitigation action which can be explored based on the prediction of fouling rates consists in the optimization of the heat exchanger cleaning schedule (Smaïli et al., 2001).

Basically, fouling rates are modeled in the literature through two main approaches: (1) Empirical models, e.g. linear or asymptotic models; and (2) Semi-empirical models, e.g. Ebert and Panchal model.

The literature presents several examples of the application of Ebert and Panchal model and its variants for the analysis of crude oil fouling. In these cases, it is necessary to determine the values of the model parameters based on data from laboratory experiments or process instrumentation (Bories and Patureaux, 2003; Polley et al., 2007; Rafeen et al., 2007; Joshi et al., 2007). However, the discussion of the details of the parameter estimation problem has not been fully addressed in these papers.

In this scenario, the current paper presents a computational routine called HEATMODEL, developed for the parameter estimation of fouling rate models. The application of this routine is illustrated using real process data from a Brazilian refinery.

EBERT PANCHAL MODEL and ITS VARIANTS

The Ebert and Panchal model (Ebert and Panchal, 1995) is based on the fouling threshold concept, where the fouling rate can be predicted using an expression considering a (positive) deposition term and a (negative) suppression term:

$$\frac{dR_f}{dt} = \alpha \mathrm{Re}^{\beta} \exp\left(-\frac{E_a}{RT_f}\right) - \gamma \tau_w \qquad (1)$$

It is important to mention that this model and its variants were developed for the analysis of chemical reaction fouling in tube-side flow.

The analysis of the impact of the surface temperature and fluid flow velocity indicates the existence of an boundary between a fouling region and a no-fouling region, i.e., a threshold that determine a “fouling envelope”, as shown in Fig. 1.

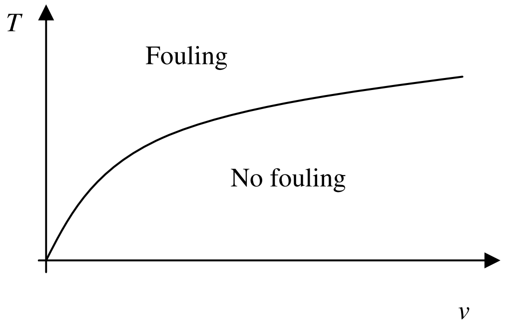

Fig. 1 Threshold model

After the proposition of this model, several authors have presented similar variants with minor modifications.

A modified version of the Ebert and Panchal model was proposed by Panchal et al. (1999):

$$\frac{dR_f}{dt} = \alpha \mathrm{Re}^{-0.66} \mathrm{Pr}^{-0.33} \exp\left(-\frac{E_a}{RT_f}\right) - \gamma \tau_w \qquad (2)$$

where the Prandtl number was inserted in the deposition term.

Polley et al. (2002) proposed that the suppression term would be better represented by a power of the Reynolds number instead of the wall shear stress, and the Reynolds number exponent in the deposition term should be -0.8. Additionally, the film temperature was substituted by the tube wall temperature:

$$\frac{dR_f}{dt} = \alpha \mathrm{Re}^{-0.8} \mathrm{Pr}^{-0.33} \exp\left(-\frac{E_a}{RT_w}\right) - \gamma \mathrm{Re}^{0.8} \qquad (3)$$

A more recent semi-empirical model was proposed by Nasr and Givi (2006):

$$\frac{dR_f}{dt} = \alpha \mathrm{Re}^{\beta} \exp\left(-\frac{E_a}{RT_f}\right) - \gamma \mathrm{Re}^{0.4} \qquad (4)$$

Model parameters

In all models presented, there is a set of parameters which must be determined through laboratory or process data. The values of these parameters depend on the type of the crude analyzed. Therefore, the results from a certain crude cannot be extended to another one. Additionally, the results obtained in laboratory experiments may not be adequate to represent the behavior of industrial units, as discussed by Asomaning et al. (2000).

The values of the model parameters in the corresponding papers where they were proposed are shown in Table 1.

Table 1. Models Parameter Values

Parameter	α (m^2K/J)	β	E_a (kJ/mol)	γ^1 ($m^2K/J \cdot Pa$)
Original Ebert-Panchal	8.39	-0.88	68	$4.03 \cdot 10^{-11}$
modified Ebert-Panchal	13.97	-	48	$4.03 \cdot 10^{-8}$
Polley *et al.*	277.8	-	48	$4.17 \cdot 10^{-13}$
Nars and Givi	0.011	-1.547	22.618	$2.67 \cdot 10^{-14}$

[1] For the models of Polley et al. and Nars and Givi the units of γ are (m^2K/J)

Due to the semi-empirical nature of the models, the determination of the values of the parameters involves the solution of an optimization problem of parameter estimation.

However, the particularities of the fouling rate models bring some relevant obstacles: (1) The values of the model parameters have a very different magnitude; (2) The problem has multiple local optima; and (3) The parameter estimation results are very dependent on the initial guess.

These features suggest that the utilization of modern optimization techniques can be fundamental for the identification of proper values for the model parameters.

HEATMODEL ROUTINE

The HEATMODEL routine developed in the present work can determine the values of fouling rate model parameters using a time series of fouling data. The routine HEATMODEL contains a library of empirical and semi-empirical models. The focus of this paper is addressed to semi-empirical models.

The HEATMODEL routine was developed to be a plugin of the software Fouling^{TR}, created in the Petrobras R&D Center (CENPES) for fouling analysis in crude preheat trains (Liporace and Oliveira, 2007). This system was developed for monitoring the thermal effectiveness of heat exchangers in crude preheat trains on a real time basis. Fouling^{TR} acquires real time operational data (flow rates, pressures and temperatures) from crude preheat trains through the PI System (databank for process information provided by OSIsoft) and uses a rigorous steady-state process simulator develop by Petrobras, called Petrox. The heat exchanger evaluations are done by Xist, a computational routine provided by the Heat Transfer Research Institute (HTRI). This integration of such systems provides Fouling^{TR} with the ability to simulate the behavior of a crude preheat train with rigorous numerical methods, employing the most modern correlations of heat transfer as well as crude composition. Today, this software is installed for monitoring the thermal performance of crude preheat trains in four Brazilian refineries.

Mathematical Problem

The parameter estimation problem is solved by the resolution of the following optimization problem:

$$\min \quad \sum_i \left(R_{f,i}^{calc} - R_{f,i}^{meas} \right)^2 \tag{5}$$

where the superscripts *calc* and *meas* indicate the fouling resistances calculated by the model and the fouling resistances determined through process data, respectively. The index *i* represents each individual point of the time series data provided by Fouling^{TR}.

The values of the fouling resistances evaluated through the model are determined by an integration of the fouling rate (forward Euler method):

$$R_{f,i+1}^{calc} = R_{f,i}^{calc} + \left(\frac{dR_f}{dt} \right)_i \Delta t \tag{6}$$

The integration of the fouling rate and the resolution of the optimization problem are solved using computational codes developed in *Scilab* (open source software similar to *Matlab*).

In order to avoid numerical problems related to the large differences between parameter values, a normalization procedure was applied, according to the following equations:

$$\alpha' = \frac{\alpha}{a} \tag{7}$$

$$\beta' = \frac{\beta}{b} \tag{8}$$

$$E_a' = \frac{E_a}{e} \tag{9}$$

$$\gamma' = \frac{\gamma}{c} \tag{10}$$

where { α, β, E_a, γ } are the values of the original parameters, { α', β', E_a', γ' } are the values of the normalized parameters, and { a, b, e, c } are the values of the model parameters in the original papers (see Table 1).

Therefore, the resultant expressions of the models become:

$$\frac{dR_f}{dt} = (a\alpha')\mathrm{Re}^{-b|\beta'|} \exp\left(-\frac{eE_a'}{RT_f} \right) - c|\gamma'|\tau_w \tag{11}$$

$$\frac{dR_f}{dt} = (a\alpha')\mathrm{Re}^{-0.66}\,\mathrm{Pr}^{-0.33} \exp\left(-\frac{eE_a'}{RT_f} \right) - c|\gamma'|\tau_w \tag{12}$$

$$\frac{dR_f}{dt} = (a\alpha')\mathrm{Re}^{-0.8}\,\mathrm{Pr}^{-0.33} \exp\left(-\frac{eE_a'}{RT_w} \right) - c|\gamma'|Re^{0.8} \tag{13}$$

$$\frac{dR_f}{dt} = (a\alpha')\mathrm{Re}^{-b|\beta'|} \exp\left(-\frac{eE_a'}{RT_f} \right) - c|\gamma'|Re^{0.4} \tag{14}$$

Additionally, it is important to observe that the parameters β' and γ' were inserted with an absolute value function in order to avoid unrealistic results.

Fouling Rate Evaluation

The fouling rate varies along the heat exchanger due to the temperature profile of the thermal surface. Although other methods could be used, in this work the evaluation of the fouling rate was based on an arithmetic mean of the values determined by the model at each heat exchanger end:

$$\frac{dR_f}{dt} = \frac{1}{2}\left[\left(\frac{dR_f}{dt} \right)_1 + \left(\frac{dR_f}{dt} \right)_2 \right] \tag{15}$$

where the indices 1 and 2 correspond to the heat exchanger terminal conditions. In this context, the wall temperature is calculated imposing countercurrent flow.

The film coefficients necessary for the evaluation of the wall temperature were determined through a correction of the values given by Xist (from HTRI):

$$h = h_{base} \left({}^{m}\!/_{m_{base}} \right)^n \tag{16}$$

where h is the film coefficient, m is the mass flow rate and the n exponent is 0.8 for tube side flow and 0.66 for shell side flow, considering turbulent regime. The subscript *base* means a base case scenario.

Optimization Algorithms

The HEATMODEL routine contains three different optimization methods which can be selected by the user: the Simplex method, the BFGS method and a Genetic Algorithm. The Simplex method and the BFGS are traditional deterministic methods (Edgard and Himmelblau,

1989) and the GA is a more modern stochastic method (Goldberg, 1989).

Genetic algorithms (GAs) are search methods based on natural selection and population genetics. In this class of methods, the search for solution is carried out through the generation of successive sets of points in the problem domain. Each point is an individual in a population represented by a string ("chromosome") of characters ("genes"). The transition between two generations is done by application of the genetic operators. These operators try to emulate the processes of selection, crossover and mutation that happen in the environment.

This method presents some important characteristics which make it an interesting alternative for the current parameter estimation problem: (1) GAs only use information of the value of the objective function, i.e., there are no derivative evaluations; and (2) GAs calculate a set of points at each step (called a population of individuals), allowing a global exploration of the search space, thus there is no request for good initial estimates and the chance of the method to be trapped in a poor local optimum is reduced (GAs are considered global optimization algorithms).

Aiming to increase the algorithm performance, the GA employed in the HEATMODEL involves a hybrid version. In this alternative, after the end of the GA run, the computational routine employs the best individual identified as a starting point to a Simplex run. This mixed alternative seeks to conjugate the advantages of both algorithms.

NUMERICAL RESULTS

In order to illustrate the performance of the proposed procedure, its application is presented in real time series data from a Brazilian refinery.

The Brazilian refinery focused on this paper processes 360,000 bpd of a Brazilian crude from Campos basis (API 19.6 and high asphaltenes content, 2.9% w/w) on two crude distillation units. The time series data of the crude preheat train used in this paper comes from the biggest one (200,000 bpd throughput). This train is composed of five branches of heat exchangers, three upstream the desalter and two downstream the desalter. This paper presents the results obtained for one of the heat exchangers downstream the desalter.

In order to provide a better assessment of the performance of the models, the time series data was divided into two parts. The first part ranges from April/2005 until December/2006 (before a unit shutdown) and it is employed for the determination of the model parameters. The second part ranges from December/2008 until August/2009 (after another unit shutdown) and it is used for assessing the prediction capacity of the model with the parameters determined in the first part. The extensions of both series are presented in Table 2.

Table 2. Time series analyzed.

Extension	Estimation	Prediction
Duration (days)	604	245
Number of points	378	77

Problem Data

The physical properties of the crude stream and the design data of the investigated heat exchanger are depicted in Table 3 and Table 4.

Table 3. Physical Properties of the Crude Stream.

Property	Value
Specific mass	819 kg/m^3
Thermal capacity	2378 J/kgK
Dynamic viscosity	$1.27 \cdot 10^{-3}$ Pa·s
Thermal conductivity	0.10 W/mK

Table 4. Heat Exchanger Data.

Variable	Value
Number of tube passes	2
Total number of tubes	1 520
Tube side flow	Crude
Tube outer diameter	19.05 mm
Tube inner diameter	14.85 mm

Performance of the Algorithms

The comparison of the performance of the deterministic and stochastic methods was conducted through the application of the Simplex and the GA methods. The initial guess of the Simplex method was the values of the parameters published in the literature, i.e., a vector of ones, considering the normalized parameters. Due to the stochastic nature of the GA, the performance analysis in this case was based on a sample of 3 different runs. The measurement of the performance of each algorithm was indicated by the average relative error in the parameter estimation period.

Simplex method. The performance of the Simplex method for each fouling rate model is presented in Table 5.

Table 5. Simplex Method Performance.

Model	Average relative error (%)
Ebert and Panchal	53.7
Ebert and Panchal mod	7.31
Polley et al.	35.8
Nasr and Givi	7.07

As it will be shown later, the different models can provide a similar accuracy. Therefore, the large errors obtained for the Ebert and Panchal and Polley et al. methods are resultant of poor parameter estimation results.

The set of results displayed in Table 5 indicates that the parameter values published in the literature served as an adequate initial estimate for only two models. The task of providing a satisfactory set of parameters for the other models would impose to the user a tedious series of algorithm runs with different initial estimates.

GA method. Each individual in the GA corresponds to a set of model parameters. The crossover is given by an interpolation between two points (parents) in order to create two new individuals (offspring). The mutation corresponds to a random movement of the point in its neighborhood. The control parameters employed for the GA method and the algorithm performance are illustrated in Table 6 and Table 7. In Table 7, the models are identified by EB1 = Ebert and Panchal, EB2 = modified Ebert and Panchal, P = Polley et al., NG = Nasr and Givi

Table 6. Control Parameters of the GA

Control parameters	Value
Population size	60
No of generations	30
Crossover %	90
Mutation %	10

Table 7. GA performance in three runs

Run	Average relative error (%)			
	EB1	EB2	P	NG
1	7.08	7.10	7.35	7.08
2	7.12	7.10	7.37	7.09
3	7.06	7.10	7.36	7.09

According to Table 7, the parameter estimation procedure involving the GA method reached good results in all runs, thus indicating that this algorithm is better suited to this problem. It is also important to mention that, despite the similarity of the average relative error found in the different of runs; these results are related to a set of distinct individual local optima, stressing the complexity of the parameter estimation problem.

Accuracy of the Models

The comparison of the average relative error in the parameter estimation for each model (Table 7) showed that all methods presented a similar accuracy performance.

Parameter Estimation Results

The presentation of the parameter estimation results is illustrated using the modified Ebert and Panchal model (Run 1). The corresponding values of the parameters are shown in Table 8.

Table 8. Parameter Values of the modified Ebert and Panchal Model.

Model	Value
α	127.7 m^2K/J
E_a	76 kJ/mol
γ	$3.44 \cdot 10^{-15}$ $(m^2K)/(J \cdot Pa)$

The profiles of the fouling resistance evaluated by the FOULING^{TR} software and the corresponding values from the parameter estimation are shown in Figure 2. The histogram of the errors is shown in Figure 3

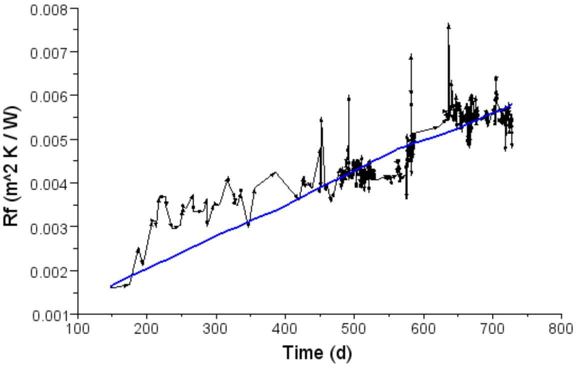

Fig. 2. Fouling resistance profile in the parameter estimation time series - Experimental data (thin line) and Model data (thick line).

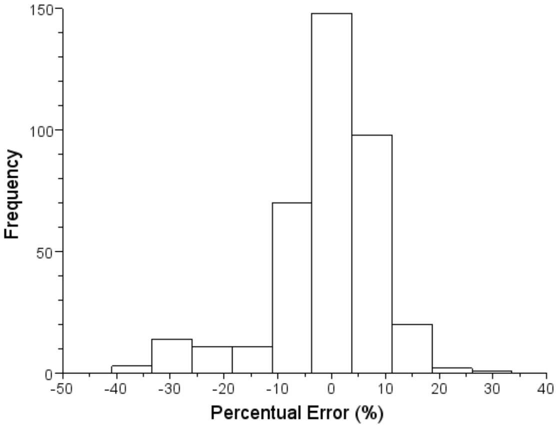

Fig. 3. Histogram of the errors in the parameter estimation.

The analysis of these graphics indicates a good match between the process data and the model using the parameters obtained in the proposed procedure.

Prediction Results

In order to provide a better assessment of the fouling rate model and its parameters, these results were employed in the analysis of the other time series. In this case, the parameters were not estimated again, since the objective of the analysis is to test the prediction capacity of the model with the parameter previously estimated.

The average relative error found was 8.9%, slightly larger than the value in the parameter estimation. The profiles of the fouling resistances and the histogram of the prediction errors are presented in Figure 4 and Figure 5.

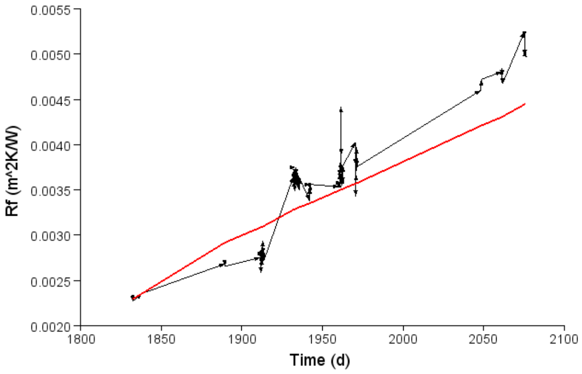

Fig. 4. Fouling resistance profile in the prediction time series - Experimental data (thin line) and Model data (thick line).

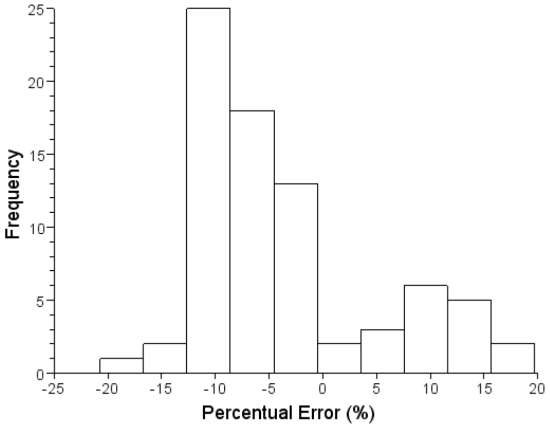

Fig. 5. Histogram of the prediction errors.

Fouling Envelope

The fouling model and its parameters can be employed to describe the fouling envelope according to the threshold concept, indicating the fouling and no-fouling regions.

The location of the operational points and the fouling envelope can be found in Figure 6, for the time series of the parameter estimation, and in Figure 7, for the time series of the prediction.

The fouling envelopes in Figure 6 and Figure 7 show that the operational points are deep inside the fouling region. Compared with other results published in the literature (Polley et al., 2002; Nasr and Givi, 2006; Rafeen et al., 2007; Polley et al., 2007), it can be observed that the no fouling region is limited by relatively low temperatures.

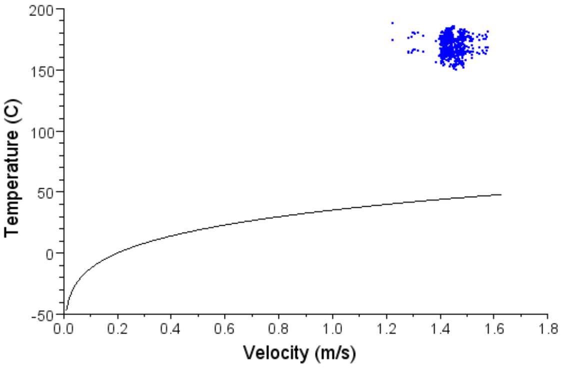

Fig. 6. Fouling envelope with the operational points of the parameter estimation time series - Ebert and Panchal Modified model.

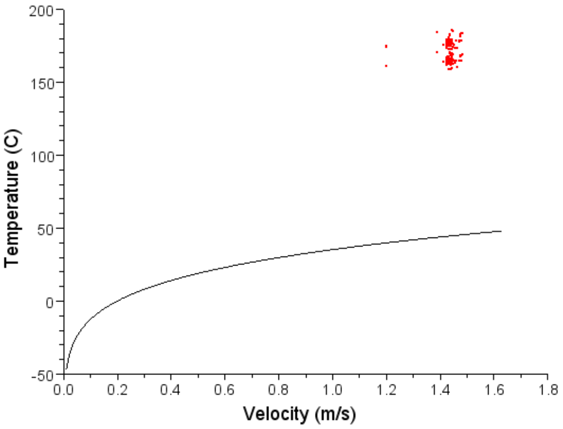

Fig. 7. Fouling envelope with the operational points of the prediction time series - Ebert and Panchal Modified model.

Employing a distinct model may imply differences in the fouling threshold curve. For example, Figure 8 presents the fouling envelope using the Polley et al. model (Run 1).

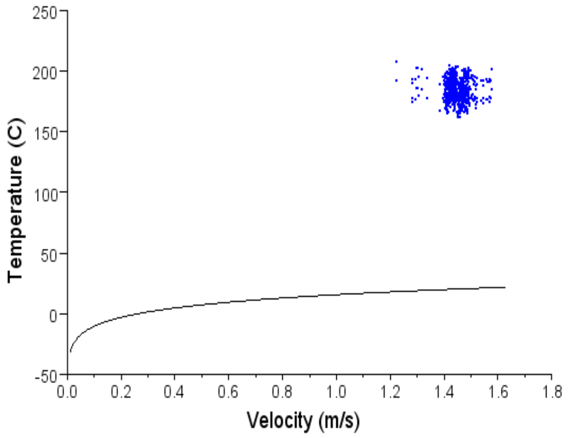

Fig. 8. Fouling envelope with the operational points of the parameter estimation time series - Polley et al. model – Run 1.

The different optima found in the parameter estimation for a same model may also imply differences in the fouling threshold curves. For example, Figure 9 contains the fouling envelopes for the three set of parameters of the modified Ebert and Panchal model (Runs 1, 2 and 3).

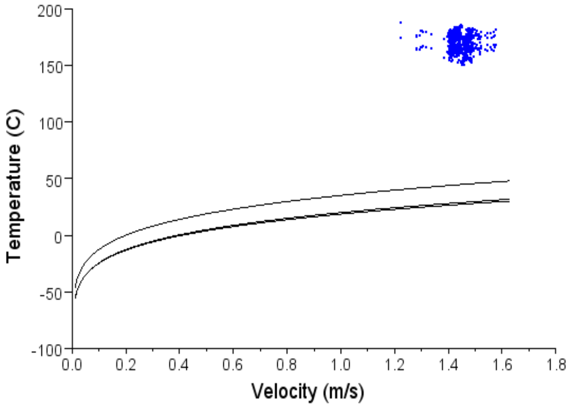

Fig. 9. Fouling envelope with the operational points of the parameter estimation time series - Polley et al. model – Run 2.

CONCLUSIONS

This paper discussed the utilization of a computational routine for the analysis of empirical and semi-empirical fouling rate models. These models can be employed to forecast the fouling impact, assuming an important role in several fouling mitigation techniques.

Focusing on semi-empirical models, the computational routine can determine the values of the parameters of different fouling models available in the literature: Ebert and Panchal, modified Ebert and Panchal, Polley et al. and Nasr and Givi.

The average relative error of the parameter estimation and prediction in the system analyzed were lower than 10%. Considering the uncertainties in the fouling resistance evaluations, the deviations observed were reasonable.

Further research will involve different aspects in the improvement of the routine, e.g., the analysis of the fouling rate spatial distribution along each heat exchanger, the utilization of a single set of parameters to analyze different heat exchangers simultaneously, and the application of the computational routine for an entire databank of fouling data collected by FOULING^{TR} in a set of different Brazilian refineries.

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NOMENCLATURE

Cp	heat capacity, J/kg K
D	tube inner diameter, m
E_a	activation energy, J/mol
k	thermal conductivity, W/m K
h	film coefficient, W/m^2 K
m	mass flowrate, kg/s
n	exponent of Eq. 16, dimensionless
Pr	Prandtl number, dimensionless
R	universal gas constant, J/K mol
Re	Reynolds number, $D\ v\ \rho/\mu$, dimensionless
R_f	fouling resistance, m^2 K/W
T	temperature, K
t	time, s
v	velocity, m/s
α	fouling model parameter, m^2 K/J
β	fouling model parameter, dimensionless
γ	fouling model parameter, m^2 K/J Pa or m^2 K/J
μ	dynamic viscosity, Pa s
ρ	specific mass, kg/m^3
τ_w	wall shear, Pa

Subscript

i	index of a individual point in a time series
1,2	heat exchanger end

Superscripts

calc	calculated by the model
meas	determinet through process data

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