MODEL VALIDATION FOR THE OPTIMIZATION OF REFINERY PREHEAT TRAINS UNDER FOULING

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ABSTRACT

Fouling in refinery (and other) applications is a major issue affecting process efficiency and profitability. Many models are available that aim to quantify its effects on individual exchangers and whole networks, and the benefits of fouling mitigation techniques. A key question is how much model detail is required versus intended use, predictive accuracy, data requirement, and computational feasibility. This paper compares two dynamic thermo-hydraulic models for heat exchanger networks under fouling: a high fidelity model (A) suitable for simulations, and a simpler, model (B) suitable for optimisation. It identifies conditions and applications where the two models are broadly equivalent, presents a parameter estimation scheme to match them, and a validation methodology. A detailed comparison between the models is made for 37 exchangers in 8 networks. Results show that the simpler model (with parameters suitably fitted as indicated) can approximate well the high fidelity model for relatively long periods. The simpler model B is then successfully used to simultaneously optimize cleaning schedule and flow distribution of a pre heat train. This solution is validated against model A, with a difference in predicted operational cost of 1.4% over 1 year. Results indicate that the simpler model and fitting procedure approximate closely the high fidelity model over relatively long periods, and can be confidently used in a nonlinear model predictive control (NMPC) strategy.

INTRODUCTION

Fouling in the preheat train of crude distillation units (CDU) reduces the thermal and hydraulic performance of the process, and increases operational cost and environmental impact. Choosing the right mitigation technique is challenging due to many possible alternatives, complex trade-offs, and difficulty in quantifying future performance and benefits [1]. Suitable models, able to predict and quantify the effects of fouling in the preheat train, are therefore essential.

Operational mitigation techniques (cleaning the units and control of flow distribution in the network) improve operations without major design intervention and large capital investment. Mathematically, this requires solving dynamic optimization problems with integer variables, to minimize the total operating cost of the network over a specified horizon [1], [2]. Computationally, these are very demanding problems. Clearly, the effectiveness of a solution depends on the accuracy of the underlying models, many of which have been proposed. Some use linearised heat exchanger models [3], [4], others consider simple fouling models (e.g. linear fouling, constant fouling) [5]-[7]. Details of exchanger geometry, fluid and deposit thermo-physical properties, and interactions between units in the network are often ignored or highly approximated. Such simplifications make the optimization problem computationally easier to solve, but compromise the quality of the results. With more detailed thermo-hydraulic models, the optimization is compromised, having to rely on heuristic or stochastic methods with poor ability to deal with constraints and no guarantee of convergence to an optimum point (e.g. [8]).

A key question is how much model detail is required for an intended use, in terms of predictive accuracy, data requirement and computational feasibility. Intended uses may be exchanger and exchanger network design and, in operations, monitoring of fouling extent, diagnosis of abnormal events such as inorganics breakthrough, flow rate control, and planning and scheduling of cleanings. So far, most of these have been addressed using distinct models, ranging from very simple, R_f-based to CFD models (for a good discussion, see [9]). A trade-off is clearly necessary between tractable models suitable for optimization, and more accurate models which are too large and complex for this.

In this paper, the intended model use is the optimization of flow control and cleaning schedules, which have been shown to be highly synergistic [10]. Two thermo-hydraulic heat exchanger models are compared: Model A, a high fidelity, 2D-

distributed (axially and radially) dynamic model, and model B, a much simpler 1D, radially distributed but axially lumped dynamic model. The aim is to determine whether, to which extent and under which conditions model B can approximate model A in predicting the effects of fouling. An application of approximate but tractable models is online optimization within a nonlinear model predictive control strategy for fouling mitigation.

In the following, first some details of the two models (A and B) are given, with a comparison of their key features. Then, a scheme is presented for fitting the simpler model B to the high fidelity model A, which is taken as reference. The errors achieved in the estimation step, and in a subsequent prediction step using the simpler model are analyzed for 37 exchangers in 8 networks. Finally, a network optimization is carried out with model B and the results checked against the high fidelity model, showing that a very good approximation is achieved. Key conclusions are summarized in the last section.

HEAT EXCHANGER, NETWORK AND FOULING RATE MODELS

Although the following approach is general, only tube and shell heat exchangers are considered here, due to their large presence in the oil industry.

A preheat train model must include individual exchangers and how they are connected in a network. A heat exchanger network is defined as a multigraph that describes the nodes, the connections between them, and the direction of flow among the nodes for different streams. Nodes are classified as sources (So), sinks (Si), flow splitters (Sp), flow mixers (Mx), and exchangers (HEX). Each stream defines a unique graph which connects some nodes. Only in the exchanger nodes two streams interact via heat transfer. Fig 1 shows a network example defining all the nodes, and a furnace. The latter performance is modelled simply, by defining the coil inlet temperature (CIT), the coil outlet temperature (COT), throughput, and furnace duty. A network is defined by the following sets:

- Nodes = $HEX \cup Sp \cup Mx \cup So \cup Si$. Set of all the nodes in the network.
- Stream types = $\{1, 2, ..., n_{st}\}$. Set of all the fluids in the network.
- Arcs = {(i, j, k) |∃(i, j, k) ∈ Nodes × Nodes × Stream types}. Set of arcs that defines the connection between nodes for a given fluid.
- $Time = \{1, 2, ..., n_T\}$. Set of discrete points in time.

Each element in the set *Stream types* is a fluid in the network (e.g. crude oil, naphtha). The set *Arc* represents a connection between two nodes including the fluid that connects them. Finally, the set *Time* is not a physical entity, but is included because dynamic processes may be defined differently in different solution algorithms. The source nodes define the inlet flow rates and inlet temperature of a specific stream at every time. Each heat exchanger node is defined by the corresponding heat and mass transfer, fouling and deposit models (depending on model type). Here, network configuration and exchangers design are fixed.



Fig 1. Heat exchanger network representation

Given all inputs to the network (inlet streams temperature, flowrate and enthalpy), stream physical properties models (e.g. for density, heat capacity), and exchanger geometries, the aim is to predict the performance (in term of outlet streams temperature, duty and pressure drop in each node and for the network overall) under varying operating conditions, including fouling.

The models for an individual heat exchanger and fouling are discussed in more detail in the following, but the network model is invariant for any changes in the fouling or exchanger models.

Fouling rate model

Crude oil fouling is a complex process in which many fouling mechanisms take place [11]. A semiempirical approach has traditionally been favored [12] because these models are easy to implement and understand, and are claimed to capture the main effects of operating variables on the fouling rate. Most semi-empirical models in the literature state that the fouling rate is a function of two competing phenomena: a deposition rate, and a removal (or suppression) rate. Under certain conditions these balance out, defining a fouling threshold level. Fouling rate is also traditionally (and incorrectly, see [13]) equated with fouling resistance. For example, the Ebert-Panchal (EP) model, in the form of Eq. 1, has been widely used in crude oil applications [12], [14]. It defines fouling rate as a function of the Prandtl and Reynold number (reflecting the effects of fluid properties and operating conditions of the exchanger), and an Arrhenius term (reflecting the chemical reaction nature of crude oil fouling) [15], [16]. The removal (suppression) term is proportional to the shear rate, hence velocity in the tubes.

$$\frac{dR_f}{dt} = \alpha R e^{-0.66} P r^{-0.33} \exp\left(-\frac{E_f}{RT_f}\right) - \gamma \tau \quad (1)$$

By assuming constant thermal conductivity and uniform composition of the deposit, its thickness (hence the hydraulic performance of an exchanger) can be calculated. The EP model has three tuning parameters: the deposition constant, α , the removal constant, γ , and the activation energy, E_f , which must be determined from plant or experimental data. Assuming that the same set of parameters apply to many exchangers in the same network simplifies the parameter estimation problem by reducing the number of variables [5], [17]. However, there is no reason to assume this. Allowing different fouling parameter for each exchanger in the network can improve the overall prediction capabilities of the model, although it means solving a parameter estimation problem with more variables.

Here, we use the Ebert-Panchal model to represent deposition rate locally (model A) or, in the form of (Eq. 1), overall fouling resistance (model B).

Heat exchanger model

Given as inputs: the flow rates of the tube and shell side, the temperature of the hot and cold streams, the physical properties of the fluids, and the geometry specification of the exchangers, a heat exchanger model (coupled with a fouling model) must be able to predict: i) the outlet stream temperature of the fluids on the tube and shell side; ii) the heat transferred from the hot stream to the cold stream and iii) the pressure drops on the tube and/or the shell side.

Here we focus on two models: (A) a high fidelity, 2D dynamic model, and (B) a much simpler 1D dynamic model. Both models use the same input information described above and are able to predict the main operating variables of the exchanger. The key difference is in the level of detail with which they account for the geometry of the exchanger. This has significant implications on model complexity, ease of solution, and prediction capabilities.

Model A: this 2D distributed dynamic model [18], [19] includes a detailed description of the energy balances and hydraulic effects. These are defined by a set of algebraic and partial differential equations along both the axial and radial directions (hence, 2D distributed), for shell and tube exchangers. Differential equations are discretized and solved using a state of the art numerical integrator. Details are found in [18], [19].

This model considers four domains (tube side per pass, shell side, tube wall, and deposit), linked by boundary and continuity conditions. A tube side domain is associated to each pass of the exchanger, with a single tube representing the whole bundle. On the shell side domain, the heat flux from all passes is included in the differential energy balance. In the wall and deposit domains the energy balance is solved in the radial direction. The deposit domain has a moving boundary layer (handled using a Lagrangean transformation [18], [19]), as the thickness of the deposit changes with time and with the axial position in the exchanger. Each point in the deposit (radially and axially) is characterized by its own thermal conductivity, which changes over time reflecting operation history. This high fidelity model has demonstrated excellent ability to predict plant many measurements and performance in applications, for single exchangers and large networks. It has been validated against refinery data [18], [20], [21], and used for monitoring, diagnostic and retrofit of industrial networks [9], [22], [23]. performed Simulations are in reasonable computational time, however its large size hinders its application to optimisation.

Model B: this simpler radially-distributed but axially-lumped parameter exchanger model (hence, 1D-distributed) considers the overall effect of the exchanger inputs on the outputs, without much detail for the heat transfer inside the unit. It is based on the P-NTU model [24] and the definition of the P efficiency (the actual heat transfer in the exchanger with respect to the maximum possible heat transfer), which is related to the number of transfer units and the exchanger geometry. The time evolution of the system is given by the fouling/agein model, and at every time a steady state algebraic model for the exchangers determines the outlet streams temperature and pressure.

Model B considers the deposit thickness (hence pressure drop) based on the fouling resistance, accounting for curvature effects on heat transfer in the radial direction (Eq. 2). Notably, Eq. 2 overcomes the usual thin layer assumption of similar models (e.g. [25]).

$$\delta = \frac{d_i}{2} \left[1 - \exp\left(-\frac{\lambda_d R_f}{d_o/2}\right) \right]$$
(2)

Although models (A) and (B) have similar inputs and can predict the same outputs for each exchanger, their level of detail and mathematical complexity are significantly different, and their applicability may also be different. Table 1 shows a qualitative comparison of the two models in terms of number of equations after discretization. For both models, the time domain is discretized using orthogonal collocation in finite elements [26]. Model A uses finite differences in others domains.

The intended application here is the optimization of flow rate distribution and cleaning schedule over long horizons. For flow control, the decision variables (flowrates) are continuous. For the cleaning scheduling it is necessary to introduce binary decision variables (to clean or not) at each time of interest, for each exchanger. The number of binary variables increases rapidly with problem size. They are the hardest to tackle in an optimization problem, and should be reduced to a minimum. For the optimal cleaning scheduling formulation, they also introduce disjunctions (logical OR, e.g. a unit is either in operation or being cleaned). Their complexity is directly related to the size and

characteristics of the model. A large model means a more difficult optimization problem to solve (a comprehensive complexity analysis is given in [27]). From Table 1 the size of the high fidelity model A can be well over ten times that of model B. It has therefore a very large disadvantage with respect to model B.

Table 1. Model comparison and estimation of the number of equations	3.
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	Lumped parameter model		Distributed model	
	Algebraic (A) or differential (D) equation.	Estimated number of equations after discretization*.	Algebraic (A) or differential (D) equation.	Estimated number of equations after discretization*.
Mass balance	А	(2*N _{HEX})*N _T	А	(2*N _{HEX})*N _T
Energy balance	А	(2*N _{HEX})*N _T	D	(N _{HEX} *N _Z *N _P *(2*N _R +1))*N _T
Fouling model	D	$(N_{HEX})*N_T$	D	$(N_{HEX}*N_Z*N_P*N_R)*N_T$
Deposit thickness	А	(N _{HEX})*N _T	D	(N _{HEX} *N _Z *N _P)*N _T
Heat transfer	А	$(3*N_{\text{HEX}})*N_{\text{T}}$	А	$(2*N_{\text{HEX}}*N_Z*N_P)*N_T$
Pressure drop	А	$(N_{\text{HEX}})^*N_{\text{T}}$	D	(N _{HEX} *N _Z *N _P)*N _T
Total		(10*N _{HEX})*N _T		$N_{HEX}*(2+N_Z*N_P*(5+2*N_R))*N_T$

*N_{HEX}, number of heat exchangers in the networks (≥ 1).

 N_T , number of discretization points in time (≥ 2).

N_Z, number of discretization points in the axial direction (\geq 5).

 $N_{\text{R}},$ number of discretization points in the radial direction ($\geq 20).$

N_P, number of tube passes (≥ 1).

PARAMETER ESTIMATION AND MODEL VALIDATION

The prediction ability and accuracy of the models are compared for a collection of heat exchanger networks operating in different conditions. Model A is used as a reference benchmark as it was validated against many plant data, with reported error of \pm 2.0 K in outlet streams temperatures, and duty and tube side pressure drop within a 1.5% relative error [9], [18].



Fig 2. Model validation strategy.

The model validation process adopted, summarized in Fig 2, starts with the generation of operational data for each case study by running one or more scenarios with the high-fidelity model A. Model A had been previously fitted (i.e determining fouling parameters) and validated against real dynamic plant data collected from the refinery. Then simulated data for the same inputs are generated from model A (including soft-measured variables) and divided in two subsets: data in the estimation horizon (EH) are used for fitting parameters (α , E_f . and γ in the EP model, plus deposit roughness) in model B, in a network-wide estimation; those in the prediction horizon (PH) are used for validating the prediction of model B against those of model A. The length of the estimation horizon (EH) may be varied. Fig 3 shows that model B uses a full set of temperature and pressure "measurements" produced using model A. In practice, this would include some pressures made available through model A as softsensed variables. The fitting also considers the effect of complex interactions between units on the network.

$$\min J = \sum_{k \in \mathbb{N}} \sum_{i \in HEX} w_{Tt} (T_{t,i,k} - \widehat{T}_{t,i,k})^2 + w_{Ts} (T_{s,i,k} - \widehat{T}_{s,i,k})^2 + w_{\Delta P} (\Delta P_{i,k} - \widehat{\Delta P}_{i,k})^2 s. t.$$

Heat exchanger model

(3)

Fouling model Network connectivity Mass and energy balances Pressure drop Operational constraints

The parameter estimation problem solved here (Eq. 3) minimises the square error of the difference in measurements (tube side outlet temperature, shell side outlet temperature, and tube side pressure drop) between models A and B. It determines optimally the fouling parameters and deposit roughness model B. The weights w define the relative importance of

each objective. The optimization problem is subject to all equations of the model, including network connectivity, pressure drop, operational constraints variables) (e.g. bounds on and heat exchanger/fouling models, which are nonlinear equations. The size of this NLP optimization problem depends on the size of the network and on the number of available data points (i.e. length of EH) and sampling frequency. This estimation procedure is therefore quite different from, much richer than, and with superior results to, those typically used for fitting fouling parameters. In

approaches that rely on the calculation of the fouling resistance (R_f) (boxes at the bottom of Fig. 3) the noise and error of the primary measurements are amplified [5], [28] and only temperature measurements are used. Alternative methods (dashed line in Fig.3) cannot exploit the full set of pressure drop information made available by the soft sensors in model A [9]. In addition, here is possible to assess the quality of model B estimates (and predictions) against the high fidelity model.



Fig 3. Model fitting and validation approached, from plant data to a representative model.

This methodology is applied to eight networks taken from the literature, all at the hot end of preheat trains [9], [21], [22], [27]. The networks range from small (2 exchangers) to relative large ones with 9 exchangers. The total of 37 heat exchangers cover a wide range of operating conditions and design specifications and provide a significant sample. In all the cases the overall operation time is set at 365 days. Initial conditions are case dependent and some exchangers present an initial fouling resistance. The inlet conditions in all the cases are assumed constant (no changes in the flow rate or inlet temperatures). All cases are solved for the following EH: 360 days, 270 days, 180 days, and 90 days (the PH is the balance to the end of the year). This allows checking the minimum information required to fit a model and prediction quality.

Hexxcell studio [29] is used to simulate the operation of the networks using distributed model A and generate the data for fitting model B. The results are exported to Python, and the parameter estimation problem is solved in Pyomo 5.2 [30] using the solver IPOPT, an interior point algorithm for NLP problems.

RESULTS AND DISCUSSION

The results are divided in two groups. The first one presents the results of the parameter estimation problem, and compares the two models for all exchangers studied. The second one optimizes the operation a specific case study with model B, and validates the solution obtained against model A.

Parameter estimation and model comparison

The average absolute error between models A and B is calculated for the primary measured variables: outlet tube side temperature, outlet shell side temperature, and tube side pressure drop. Fig 4 plots the errors for the estimation data set (EH error, for data within the model fitting horizon) and prediction data set (PH error, for data not included in the model fitting) for all 37 exchangers, for various estimation horizons, EH. The average estimation error between the two models is low $(\leq 1.5 \text{ K for the tube side temperature}, \leq 2.0 \text{ K for}$ the shell side temperature, and ≤ 0.15 bar for the pressure drop) and does not change significantly with the length of the estimation horizon. This indicates that the simpler model B is able to match well the high fidelity model A. The average prediction error is larger, particularly for short estimation horizons, however still quite acceptable. In isolated cases, an estimation horizon of 90 days leads to >5 K prediction errors in the shell side outlet temperature. Including too few data in the parameter estimation step may lead to wrong long term

predictions. In some case the large variation in prediction error is due to bad parameter estimates for the B model. In others, the estimation data are not sufficient to capture the network variability. Estimation horizons of ~180 days give good results.



Fig 4. Average error for a) tube side outlet temperature, b) shell side outlet temperature, and c) tube side pressure drop in the estimation horizon (EH) and in the prediction horizon (PH).

Fig 5 shows values of the estimated deposition constant parameter (α) in each exchanger vs the

estimation horizon. In some cases, as the estimation horizon decreases the value of α increases (e.g. exchangers no. 10-15 in Fig 5). Although they give a good fit within the estimation horizon, these large values overestimate the effect of fouling for longer operating times causing erroneous predictions. In model A the same fouling parameters were used for all the exchangers in a network, in the simpler model B different values are estimated for each exchanger. This additional degrees of freedom enables model B to make equally good predictions when enough data is used to fit the parameters of the simpler model.



Fig 5. Optimally determined deposition constant (α) for each exchanger of all the cases studied varying the estimation horizon.

Network optimization and validation

The heat exchanger network of Fig 6 (taken from [9]) is considered here. After fitting the parameters as described above, model B is used to simultaneously optimize its cleaning schedule and flow distribution, over 365 days. Here, the objective function is the minimization of the total operating cost (fuel cost + CO2 emission cost + cleaning cost). Details of formulation and solution strategy are in [10], [27]. The optimal cleaning schedule for this network consist on cleaning E01A/B and E04 four times. In three occasions those three shells are cleaned simultaneously (at 30 days, 200 days, and 290 days of operation). The other cleanings are at 110 days for E4 and 120 days for E01A/B. The optimal flow split through the parallel branches, bounded between 30% and 70% for feasible operation, changes during the year (Fig 7) to enhance energy recovery when the units performance changes due to fouling and/or the cleanings. The optimal operation is then run with model A and the trajectories from the two models are compared. Fig 8 shows the CIT prediction for this optimal operation for the simpler model B, and the corresponding profiles when the same operation is run with the high fidelity model A. Both models follow very similar trends. The average error in CIT prediction between the two over 1 year is 0.31 K.

Model B predicts an overall operation cost of \$ 13.7 M, while model A predicts \$ 13.4 M, a difference of only 1.4%. Therefore, the operational

decisions, including choice of cleanings and flow distribution, made with the model B are taken to be valid



Fig 6. Heat exchanger network structure used as an example in comparing the models (A) and (B).



Fig 7. Optimal split fraction for the case study.



Fig 8. Comparison of the CIT profile for the case study using the simple and high fidelity models.

CONCLUSION

Fouling mitigation in refinery applications is paramount to ensure a profitable, safe, and reliable operation. Accurate models are necessary to predict the network performance under fouling and reliable predictions to support fouling mitigation decisions. A detailed comparison of two dynamic heat exchanger models (a high fidelity, 2D distributed vs simpler 1D distributed) was presented, as well as a methodology to optimally estimate the parameters of the simpler model, without relying on indirect quantities such as the calculated fouling resistance. This parameter estimation approach considers all the interactions among the units in the network and exploits all measurements, including any softsensed pressure drop, and incorporates them into individual tuning parameters for each exchanger.

proposed estimation The parameter methodology was applied in 8 heat exchanger networks with a total of 37 exchangers. With an estimation horizon of appropriate length, the simpler model approximates the predicted performance of the network within a small error, relative to the high fidelity model. The much smaller size of the simpler model enables its use in advanced optimal fouling mitigation formulations, in particular for the demanding simultaneous optimal cleaning scheduling and flow distribution control problem, which was shown to be highly beneficial [10], [27]. This was confirmed here with a case study, where the combined optimal strategy generates significant savings. The optimal operation thus calculated (cleaning schedule and flow split control profiles over 1 year) was validated against the responses obtained with the full high fidelity model. The error between the models in the predicted operational cost is 1.4%. This confirms that the simpler model (with the proposed parameters fitting procedure) can approximate closely the more complex model over relatively long periods. It also indicates it can be confidently used within a nonlinear model predictive control (NMPC) strategy.

NOMENCLATURE

- d_i Tube inner diameter, mm
- d_o Tube outer diameter, m
- E_f Fouling activation energy, kJ/kmol
- Pr Prandtl number
- R Universal gas constant, J/molK
- Re Reynolds number
- R_f Fouling resistance, m²K/W.
- T_f Film temperature, K
- T_t Tube side outlet temperature, K
- T_s Shell side outlet temperature, K
- P Pressure, bar
- w Objective weight
- α Deposition constant, m²K/W day
- γ Removal constant, m⁴K/N W day
- δ Deposit thickness, m
- λ_d Deposit thermal conductivity, W/m K
- τ Shear stress, N/m²

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