

INTEGRATION OF OPTIMAL CLEANING SCHEDULING AND CONTROL OF HEAT EXCHANGER NETWORKS UNDERGOING FOULING: MODEL AND FORMULATION

Federico Lozano Santamaria & Sandro Macchietto.*

Department of Chemical Engineering, Imperial College London, South Kensington Campus,
London SW7 2AZ, UK

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* Author of correspondence

E-mail address: f.lozano-santamaria16@imperial.ac.uk (F. Lozano Santamaria)

Abstract

The performance and operability of heat exchanger networks (HEN) is strongly affected by fouling, the deposition of unwanted material, which reduces the heat transfer rate, and increases the pressure drop, the operational cost and the environmental impact of the process. Periodical cleaning and control of flow rate distribution in the HEN are used to mitigate the effects of fouling and restore the performance of the units. The optimal cleaning scheduling has been formulated as a MILP or MINLP problem and solved using various approaches. The optimal control has been formulated as a NLP and used to define the flow rate distribution of the network. Both problems share the same objective, the minimization of the total cost of the operation. In principle, the simultaneous solution of the optimal control problem and the optimal cleaning scheduling problem should provide greater savings than the independent or sequential solution of the two problems, as the interactions of the two mitigation alternatives are considered. However, these two problems have been typically considered separately due to modelling and solution challenges. Also, it is not quite clear what additional benefit a simultaneous solution may bring. The challenges for solving the integrated problem are the large scale of the associated optimization problem and the different time scales involved in each operational layer. Here, a general and efficient formulation is proposed using a continuous time discretization scheme for the integrated problem of scheduling and control of HEN subject to fouling. A dynamic model of heat exchangers is proposed that is sufficiently detailed to represent the physics of interest with novel modifications to address simultaneously their control and scheduling in a network. The problem is formulated as a MINLP and solved using deterministic optimization algorithms. The flexibility of the model and variations of the formulation are demonstrated with two small case studies. The formulation complexity vs. scale and advantages are analyzed. The results show that considering the two problems

simultaneously has a very strong synergistic effect, with over 20% decrease in operational cost achieved in comparison with using either fouling mitigation alternative individually.

Nomenclature

| Subscripts | Description |
|------------|--------------------------------------------------|
| a | Ageing parameter |
| c | Coke |
| cl | Cleaning mode |
| $flow$ | Condition at the flow boundary (fluid – deposit) |
| f | Film |
| fg | Fluid – gel interface |
| g | Gel |
| gc | Gel – coke interface |
| i | Inner side of the tube |
| o | Outer side of the tube |
| op | Operating mode |
| p | Periods |
| s | Shell side |
| t | Tube side |

| Symbol | Units | Description |
|------------|------------------------------|-----------------------------------------------------------|
| α | [m ² K/W.day] | Deposition parameter |
| γ | [kg/m ² W.day.Pa] | Removal parameter |
| δ | [mm] | Deposit thickness |
| ΔP | [bar] | Pressure drop |
| λ | [W/m.K] | Thermal conductivity |
| η | [-] | Furnace efficiency |
| ρ | [kg/m ³] | Density |
| τ | [days] | Period duration |
| τ_w | [Pa] | Shear stress |
| A | [m ²] | Transfer area |
| CIT | [K] | Coil inlet temperature |
| COT | [K] | Coil outlet temperature |
| C_p | [kJ/kg.K] | Specific heat capacity |
| E | [J/mol.K] | Activation energy |
| f | [-] | Friction factor |
| G | [kg/m ² s] | Mass flux rate |
| h | [W/m ² .K] | Convective heat transfer coefficient |
| k^0 | [1/s] | Pre-exponential factor |
| L | [m] | Heat exchanger tube length |
| M | [-] | Big M parameter |
| m | [kg/s] | Mass flow rate |
| N_p | [-] | Number of passes |
| N^{max} | [-] | Maximum number of cleanings per unit |
| NTU | [-] | Number of transfer units |
| P | [-] | Efficiency of heat transfer with respect to the tube side |
| Pr | [-] | Prandtl number |
| P_{kg} | [\$/kg] | Profit per kg |

| | | |
|------------|-----------------------|-----------------------------------------------|
| P_{fuel} | [\$/MW] | Price of fuel |
| P_{CO2} | [\$/ton] | Price of CO2 emission |
| Q | [W] | Heat transfer rate |
| Q_f | [MW] | Furnace duty |
| R | [mm] | Radius |
| R_c | [-] | Heat capacity ratio |
| R_f | [m ² K/W] | Fouling thermal resistance |
| Re | [-] | Reynolds number |
| t | [day] | Time |
| T | [K] | Temperature |
| T_t | [days] | Starting time of period t |
| U | [W/m ² .K] | Overall heat transfer coefficient |
| x_i | [-] | Mass fraction of component i in the deposit |
| y | [-] | Binary variable to switch operation tasks. |

1. Introduction

Fouling is the deposition of unwanted material over the surface of process equipment, which reduces the performance of heat transfer operations. It is a phenomena not yet fully understood, but it is known that it can be caused by the presence of impurities in the process streams, the crystallization of salts, biological reactions, deposition of suspended particles, thermal decomposition of certain components, and corrosion ^{1,2}. The causes of fouling vary among different processes. Some are process specific such as the biological fouling caused by the thermal degradation of proteins in milk pasteurization processes ³, and the crystallization of salts in water treatment applications ⁴. In other areas such as refining applications fouling can be caused by more than one mechanism at the same time ². Its consequences on the operation of chemical processes are of major concern.

In heat exchanger units, fouling reduces both thermal and hydraulic performance. The deposited material generates an additional thermal resistance that reduces the heat transfer rate and the potential to recover high amounts of energy in heat exchangers ⁵. Additionally, the deposit reduces the hydraulic radius which increases the pressure drop, and in extreme cases it causes a complete

blockage of the unit ⁵. These factors increase the operational cost, the risk of operation during cleanings, and the environmental impact.

The consequences of fouling are of major concern in refinery operations where large heat exchanger networks (HEN) are used in the energy integration of the process ⁶. This is most evident in the preheat train (PHT) of the crude distillation unit (CDU), which processes all the crude oil that comes into the refinery at extreme conditions, such as high temperature, varying range of composition, and high amounts of contaminants ². In this case the extra thermal resistance in the heat exchangers reduces the coil inlet temperature (CIT) to the furnace, to compensate for which more fuel is burned, increasing the amount of carbon emissions and the operational cost. If no mitigating action is performed in the HEN the operational cost of refining operations can increase by several million dollars per year ^{7,8}. Therefore, alternatives for fouling mitigation are needed and of major importance.

Some fouling mitigation alternatives are: cleaning in place (chemical cleaning), mechanical cleaning, the use of antifoulant agents, and changing the operation conditions (e.g. controlling the flow rate distribution) ^{1,2}. The cleaning options have been proven to be an effective way to recover the thermal and hydraulic efficiency ⁹, however it is not easy to decide which heat exchanger to clean and when such that the operational cost is minimum. These decisions are often made using heuristic criteria ², but quantitative, model-based mathematical programming approaches (with MILP and MINLP formulations) have also been used. Even with highly simplified models, the large size of the problems and its combinatorial nature make it hard to solve. Furthermore, in the case of MINLP formulations only a local minimum can be guaranteed. Solution approaches have been proposed such as simulated annealing ¹⁰ or greedy algorithms ¹¹ that produce a rapid solution, but give no guarantee this solution is optimal, and have problems with constraints.

Operationally, a practical alternative for fouling mitigation is to manipulate the flow rate distribution in the network over time, through use of by-passes of individual units and control of flow split between parallel branches in the HEN. Optimising such flow distribution profiles has also been formulated as a mathematical programming problem with the objective to minimize the operational cost ¹².

These are two mitigation alternatives. The first one is to tackle the problem as an optimal scheduling problem in which the main decision variables are binary variables associated with the operating states of the units (cleaning or operating), and the timing and sequencing of the task. The optimal cleaning scheduling problem is combinatorial in nature, and is typically addressed using steady-state (or pseudo-steady state) models. The second one deals with the optimization of the HEN flow rate distribution over time. This is a dynamic, optimal control problem which needs to deal with differential-algebraic equations. Most of the literature on fouling mitigation of HEN addresses the two alternatives individually, and most of it only focuses on the scheduling problem. ^{1,13,14}. On the other hand, some works tackle the second problem only from a dynamic optimization perspective ignoring the cleaning scheduling ^{12,15}.

Some attempts have been done to integrate scheduling and control for fouling mitigation in heat exchanger networks, but there are still gaps in formulation and solution. The two problems have very different time scales ranging from hours (for control) to years (for scheduling), and the choice of time representation and time discretization scheme is key for obtaining a simultaneous solution that is accurate for both problems ¹⁶. The problem formulation is also important because very detailed and accurate models (e.g. a distributed model that captures the composition and thickness of the deposit in the axial and radial domain of each exchanger ¹⁷) could be used in the control layer, but make the scheduling problem computationally prohibitive to solve, so they have to be

simplified to the point that satisfies the compromise between accurate representation of the physical phenomena and computational complexity for a large scale optimization problems ¹⁸. Finally, if such drastic simplifications of the models are required, that they fail to adequately capture the physics of deposition and its effects on thermo-hydraulic (and economic) performance, then the solution of the problem is not practical and pointless. Therefore, an efficient approach to the problem must consider realistic fouling models and include representation of both dynamics and scheduling aspects. Solution approaches based on deterministic optimization are preferred because they allow considering a detailed and complete integration of the scheduling and control problem for fouling mitigation in heat exchanger networks.

The problems of optimal control and optimal cleaning scheduling for heat exchangers fouling mitigation have been considered in previous works. For example, Ishiyama et. al ¹⁹ incorporate the desalter temperature control in the definition of the cleaning scheduling of HEN, addressing both problems at the same time. However, this approach presents limitations such as: 1) the solution approach is based on a heuristic algorithm and a merit function that defines the exchanger with the highest “fouling mitigation score”; 2) simple linear fouling models that may not be realistic, 3) the control of the desalter temperature has a small effect in terms of energy recovery, and 4) the flow rate control of the crude oil through the network is not considered. Another example is the work of Liu et. al ²⁰ where an integration of a HEN synthesis and cleaning scheduling is defined using MILP models. The flow rate in the network is defined in the synthesis stage based on the connectivity among exchangers, and fouling and possible cleanings are also considered at this stage. This approach used simplified fouling models that may not be realistic, and the original nonlinear problem is linearized to find a solution.

The integration of process operations across hierarchical layers has been acknowledged to improve the profit and/or operability of the process and it has been done successfully in some cases^{21,22}. The economic incentive provided by the integration of the scheduling and control layers of operation has increased the amount of research in this area, especially on alternative ways of formulating the problem and efficient solution strategies that can cope with the multiple time scales of the problem^{16,23}. For HEN, the extent of the additional benefits that integration of cleaning scheduling and flow distribution control may bring is not quite clear, and establishing this is another goal of this paper.

This paper presents an efficient and general formulation for solving the optimal cleaning scheduling problem and the optimal control problem of HEN under fouling. A model and formulation are presented which are versatile, in the sense that some variables can be fixed to deal with only one or both of the scheduling or control problems, or include just some aspects of both (e.g. to determine only the timing of the task in the scheduling problem while the assignment and sequence of task is fixed). The rest of the paper is structured as follows: Section 2 introduces the modelling aspects of each heat exchanger considering fouling and ageing, as well as the modelling of the network with bypasses and other flow distribution elements. Two time discretization schemes and their advantages and disadvantages for the integration of control and scheduling are presented and compared in Section 3. The general formulation of the optimal cleaning scheduling and optimal control of HEN under fouling is described in Section 4. A complexity analysis of the proposed formulation is presented and discussed in section 5. The case studies proposed are introduced in Section 6 and their results in Section 7. The case studies are divided to highlight a comparison of discretization schemes, partial scheduling as a NLP problem for HEN, and the

benefits of the integration of scheduling and control. Finally, Section 8 presents the conclusions and perspectives of this work.

2. Heat Exchanger and HEN model under fouling and ageing

Fouling is a local phenomenon, but it is computationally expensive to use a fully distributed 2D or 3D model to describe each heat exchanger in a large network. This would lead to an optimization problem with thousands of partial differential-algebraic equations (PDAE) which is difficult to solve because of its large scale and nonlinear terms. On the other hand, lumped parameters models are defined by algebraic equations and are relatively easy to solve, however they miss essential information about the performance degradation due to fouling. A reasonable compromise is to use axially lumped but radially distributed models that reflect the deposition and growth of deposits over time, together with its key properties (ageing and therefore, thermal conductivity, and depth). In the following, it is assumed that a heat exchanger is a shell and tube exchanger characterized as an E type with multiple passes in the shell, with the P-NTU model defined by Eq. (1) – (6)²⁴. The main assumptions of this model are as follows:

- Adiabatic operation with respect to the surroundings.
- No heat transfer effects in the axial direction.
- Radial effects on heat transfer and deposit growth.
- Constant physical properties.
- Counter-current flow.
- Average thermo-physical properties and heat transfer coefficients, calculated between the inlet and outlet conditions.
- Pseudo steady state. The heat transfer rate is a rapid process in comparison with the fouling rate.

$$NTU = \frac{UA}{C_{P_t} m_t} \quad (1)$$

$$R_c = \frac{C_{P_t} m_t}{C_{P_s} m_s} \quad (2)$$

$$P = 2 \left[1 + R_c + (1 + R_c^2)^{\frac{1}{2}} \frac{1 + \exp\left(-NTU(1 + R_c^2)^{\frac{1}{2}}\right)}{1 - \exp\left(-NTU(1 + R_c^2)^{\frac{1}{2}}\right)} \right]^{-1} \quad (3)$$

$$Q = P(m_t C_{P_t})(T_s^{in} - T_t^{in}) \quad (4)$$

$$T_t^{out} = T_t^{in} + P(T_s^{in} - T_t^{in}) \quad (5)$$

$$T_s^{out} = T_s^{in} - PR_c(T_s^{in} - T_t^{in}) \quad (6)$$

Fouling causes an increase in the thermal resistance and a decrease in the flow diameter, and both effects have to be included in the model. Also, when the deposit is exposed to high temperature for long time additional chemical reactions take place changing its composition and properties. This is known as ageing (or coking) and not taking this into account may lead to wrong performance prediction and interpretation of fouling data^{2,25}. Figure 1 shows a scheme of the heat transfer resistances in various (simplified) layers from the shell side to the tube side of the heat exchanger and the temperature on the boundaries. Although this model is a lumped parameter model in the axial direction of the exchanger, it considers radial variation of the temperature among different layer. Using a pseudo steady state approach the radial temperature profile can be solved explicitly to calculate the temperature at the boundaries between different layers. The effects of the radial distribution of the temperature in the heat transfer rate are captured in the thermal resistances that define the overall heat transfer coefficient (U).

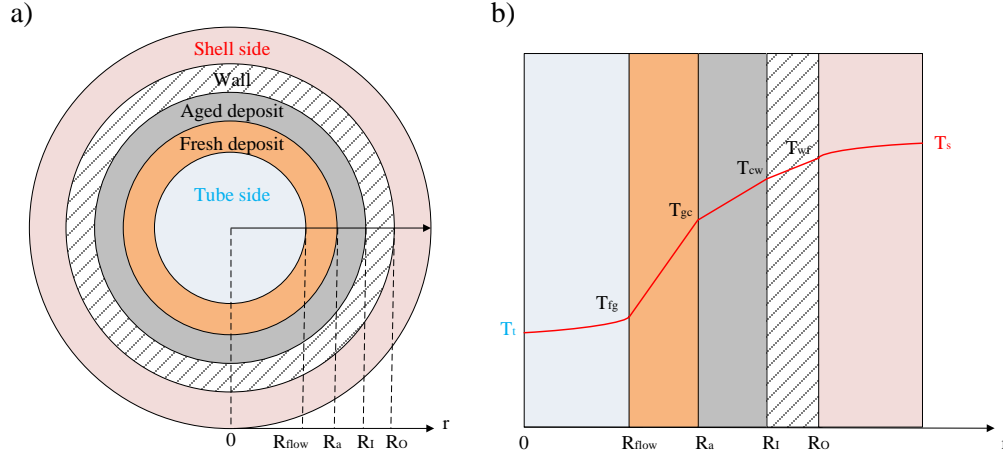


Figure 1. Multiple layer representation for the heat transfer between the shell side fluid and the tube side fluid.

Note that the fouling deposition happens at the boundary between the fluid and the fresh deposit, thus it is usually modelled as a function of the boundary layer temperature, which can be estimated using the temperature at the fluid-deposit interface (T_{fg}). On the other hand, the ageing reaction occurs inside the deposit material. Although this varies continuously along the deposit depth depending on its temperature^{5,17}, an approximate, two-layer representation is assumed here, whereby ageing only occurs at the interface between the fresh deposit (gel) and the aged deposit (coke)²⁵. Under this simplified radially distributed approach, the ageing rate is a function of the temperature at the gel-coke interface (T_{gc}). The temperatures at the interfaces can be estimated using the heat transfer coefficients, Eq. (7) for fluid-deposit temperature, Eq. (8) for film temperature, and Eq. (9) for gel-coke temperature. These expressions for the temperature at the boundary of the different domains are obtained by solving the steady state heat transfer problem in radial coordinates.

$$T_{fg} = T_t + \frac{U}{h_t} \frac{R_o}{R_{flow}} (T_s - T_t) \quad (7)$$

$$T_f = T_t + 0.55(T_{fg} - T_t) \quad (8)$$

$$T_{gc} = T_{fg} + \frac{U}{\lambda_g/R_o} \text{Ln} \left[\frac{R_I - \delta_c}{R_{flow}} \right] (T_s - T_t) \quad (9)$$

The Ebert-Panchal model (Eq. (10)) is used to describe the fouling deposition rate (here, in terms of rate of change in the thermal fouling resistance) and a first order kinetic expression to describe the ageing rate (Eq. (11)), in terms of a ‘youth’ variable, x_g , which for this binary gel-coke model is equivalent to the gel mass fraction of the deposit.

$$\frac{dR_f}{dt} = \alpha Pr^{-0.33} Re^{-0.66} \exp\left(-\frac{E_f}{RT_f}\right) - \gamma \tau_w, \quad R_f(t=0) = 0 \quad (10)$$

$$\frac{dx_g}{dt} = -k_a^0 \exp\left(-\frac{E_a}{RT_{gc}}\right) x_g, \quad x_g(t=0) = 1 \quad (11)$$

In reality, both rate equations are function of local variables that vary along the heat exchanger (e.g. heat transfer coefficient, Reynolds number, film temperature). To avoid an axial distributed model and achieve an axially- lumped parameter model, each rate is calculated at an average temperature between the inlet and outlet conditions. The fouling rate equation defines the total thermal fouling resistance, which is the summation of the resistance of the fresh and aged deposit. A mass balance on the deposit defines the gel mass fraction and relates it to the deposit thickness (Eq. (12)). The thickness of each deposit layer can be directly related to its thermal resistance following the classic definition of the overall heat transfer coefficient. Eq. (14) defines the thickness of the fresh deposit considering that the deposit can reach a significant thickness in comparison with the tube diameter, that is, avoiding the usual thin layer assumption. Eq. (13) defines the thickness of the aged deposit. The total thickness of the deposit (δ_T) is the summation of the thickness of the two layers, assuming that they do not mix.

The model presented here is a simplified instance of a more general approach that is based on the deposition rate and reaction rate of all the components that contribute to fouling. Under this general modelling framework, a mass balance for each component in the deposit defines the deposit composition and therefore the thermal resistance of the deposit. It is necessary to know the effective thermal conductivity of the deposit to calculate the thermal resistance, and there are many different mixing rules such as parallel layers or series layers^{26,27}. In this case, because of the no mixing assumption of the layer, a model of resistance in series is used.

$$x_g = \frac{[2R_I - (\delta_T + \delta_c)]\delta_g\rho_g}{[2R_I - (\delta_T + \delta_c)]\delta_g\rho_g + [2R_I - \delta_c]\delta_c\rho_c} \quad (12)$$

$$R_{f,c} = \frac{R_O}{\lambda_c} \ln \left[\frac{R_I}{R_I - \delta_c} \right] \quad (13)$$

$$R_{f,g} = \frac{R_O}{\lambda_g} \ln \left[\frac{R_I - \delta_c}{R_I - \delta_c - \delta_g} \right] \quad (14)$$

Hydraulic effects cannot be omitted from the model especially if the deposit thickness is significant in comparison with the tube diameter. The pressure drop is given by Eq. (15) where d_{flow} is the diameter available for the fluid flow and f is the friction factor defined, for example, by the White-Colebrook equation or any of its approximations.

$$\Delta P = \frac{G_t^2}{2\rho_t} \left[\frac{1.5}{N_p} + \frac{fL}{2R_{flow}} + 4 \right] N_p \quad (15)$$

In summary, this approximate heat exchanger model under fouling and ageing is composed by 2 differential equations (fouling rate and ageing rate), 2 differential variables (R_f and x_g), 13 algebraic equations, and 13 algebraic variables. It is an index 1 DAE and the subsystem of algebraic equations need to be solved at each time instance of the numerical integration. This model may be incorporated directly into an optimization formulation. There are two main alternatives to handle the differential equations. The first one is a sequential method in which a

partial discretization method is applied. Only the manipulated variables (mass flow rates) are discretized in intervals and are defined by a step-wise function or linear step-wise function. Using this approach, the DAE system has to be solved at each iteration of the optimization algorithm²⁸. The second alternative is a simultaneous method in which all the manipulated and state variables are discretized, for example using finite differences or orthogonal collocation, and solved together. This transforms the dynamic optimization problem into a NLP that can be solved with standard optimization solvers²⁸. For large scale problems, like the one addressed here, the full discretization approach is preferred because the DAE system is solved only once to give the optimal point, avoiding intermediate solutions of the system that may be hard to solve, or even infeasible²⁸.

3. Time discretization strategies

The discretization of the differential equations and how they are handled not only affects the control part of the problem, but also the scheduling constraints. The discretization of the time horizon allows defining the sequence of events and the changes in operation modes, and plays an important role in the complexity of finding a solution. The three main complicating components that increase the size and complexity of the problem are the number of units (e.g. heat exchangers), the number of tasks (e.g. cleanings), and the length of the time horizon²⁹. Although the size of the problem increases linearly with each of these components, the complexity of finding a solution tends to increase exponentially because of the combinatorial nature of the possible choices²⁹.

A scheduling problem aims to define three decisions: the assignment of tasks to units, the sequence of tasks, and the timing of each task. In the fouling mitigation problem of heat exchanger networks the units are individual heat exchangers, the tasks are the operation modes for each unit (for example “operating” and “cleaning”) and the scheduling decisions are: what operation mode to select for each unit (operating or cleaning), the sequence of cleanings in each unit, and the time

when each cleaning starts. The discretization approach used must be able to model all of those decisions simultaneously.

Two main approaches of time discretization have been used for solving scheduling problem, a discrete time representation and a continuous time representation ³⁰. The application of both approaches to the case of a heat exchanger network is described next.

3.1. Discrete time discretization approach

The prediction horizon is divided into a known number of periods of uniform predefined length τ , which produces a uniform time grid. The length of the periods must be capable of capturing all the time depending events relevant to the scheduling problem, usually defined as the greatest common factor of the characteristic times of the problem ³⁰. Figure 2 (a) shows a schematic representation of this approach, where the marks indicate the beginning and end of the periods. Only at these predefined points changes of the process can occur (e.g. a change of the operational mode of a unit). The start of the first interval is the beginning of the operation, and the end of the last interval is the final time of the scheduling horizon.

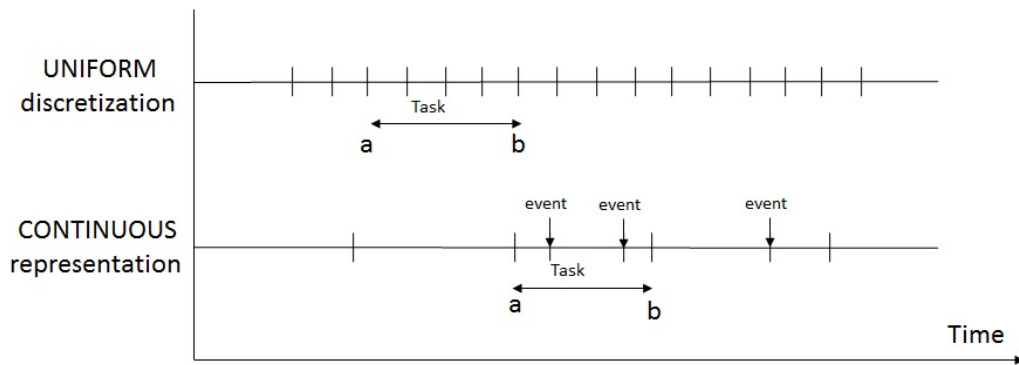


Figure 2. Time domain discretization for scheduling problems (adapted from ³¹). Points a and b delimit the duration of a task.

For a heat exchanger network under fouling with only mechanical cleanings, the greatest common factor of the characteristic times is the duration of the cleanings tasks, which here is fixed a priori and are all the same length. The length of each discrete period is chosen as the length of a mechanical cleaning, so that the number of periods is minimum and a cleaning task takes place only in one period. If desired, a finer grid may be used to have a more accurate representation of the process dynamics, or for cleaning tasks of different duration, each requiring multiples of the discrete period.

Here, only two possible operating modes or tasks are envisaged for each heat exchanger: “cleaning” and “operation”. The following sets are introduced:

$HEX = \{1, 2, \dots, n_{HEX}\}$ the set of heat exchanger units, and

$Periods = \{0, 1, 2, \dots, N_p\}$, the set of discrete points in the time horizon.

The binary variable $y_{t,i}$ represents the starting of a cleaning task at period t in heat exchanger i . The constraint in Eq. (16)³⁰, where α_i is the fixed duration of the mechanical cleaning in the heat exchanger i , states that if a cleaning starts in unit i at time t no other cleanings can start in the same unit until it finishes. To simplify, it is assumed that the duration of all cleanings is constant and does not change depending on the fouling degree nor on the type of heat exchanger.

$$\sum_{t'=t}^{t+\alpha_i-1} y_{t',i} - 1 \leq M(1 - y_{t,i}), \quad \forall i \in HEX, t \in Periods \quad (16)$$

The differential equations, Eq. (10) and (11), are discretized using a backward difference scheme which is compatible with the discrete time representation of the scheduling problem. In this case, the differential equations and the initial values of the corresponding variables are transformed into a set of algebraic equations of the form of Eq. (17), where τ is the duration of each period, x is a

differential variable with initial value x^0 at time $t = 0$, and F is the right-hand side expression of the differential equation.

$$\begin{aligned} x_t &= x^0, & \forall t \in Periods | t = 0 \\ \frac{x_t - x_{t-1}}{\tau} &= F_{t-1}, & \forall t \in Periods \setminus \{0\} \end{aligned} \tag{17}$$

The discrete time representation presents some main shortcomings that has made it unattractive for solving large-scale problems. The fact that changes on the operation can only occur at predefined time points of the time grid leads to inaccurate solutions, and in order to gain back some accuracy a fine grid has to be used which increases the size and the number of binary variables of the problem³². The inaccuracy of the solution is caused by the approximation of the continuous time domain with a fixed grid, so that by definition this approach produces suboptimal solutions, and if the grid is too coarse the problem may even be infeasible³⁰. For example, using this representation a cleaning task can only start at a time which is a multiple of the period length, while an optimal solution of the problem might require that the cleaning starts at an intermediate time.

3.2. Continuous time discretization approach

In the continuous time discretization, the timing, sequencing, and duration of events are represented by continuous variables, and binary variables are used to represent important state changes of the system³⁰. This approach gives more flexibility and more accuracy than the discrete time representation because events can take place at any point of the continuous time domain³⁰. The continuous time representation of scheduling problems is usually preferred over the discrete time representation due to its capability of modelling the exact duration and starting time of the tasks, and the reduction in the number of discrete variables³². However, the modelling of certain

time depending events is not as easy as in the discrete time approach, the number of nonlinear variables is higher, and the relaxation of the problem is not as tight ³².

Under the same conditions of the discrete time approach the following sets are introduced:

$HEX = \{1,2, \dots, n_{HEX}\}$ set of heat exchanger units,

$Periods = \{1,2, \dots, N_p\}$ set of periods or events in the time horizon, and

$Points = \{0,1,2, \dots, N_t\}$ set of internal points within each period.

The time set is a tuple composed by two elements, the period and the internal points. Figure 3 presents a schematic representation of the time horizon in which each period has a fixed number of internal discretization points and any discretization scheme (e.g. backward finite differences, orthogonal collocation) can be applied inside the periods. Note that changes in operation (e.g. cleanings) can only take place when switching between periods and the same operation mode is maintained for all the internal points of that period. The internal points of a period help to increase the accuracy of the integration as the length of the period is variable, but bounded.

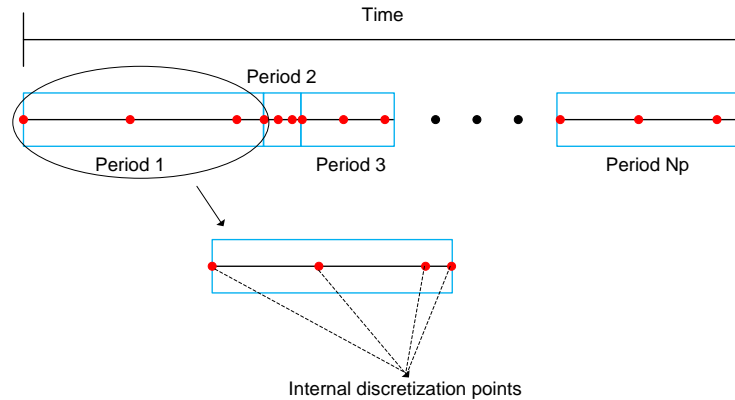


Figure 3. Representation of the time horizon using a continuous time discretization scheme

To model the allocation of cleaning tasks to heat exchangers, the time horizon is divided into a global, pre-defined and fixed number of periods of variable length (Figure 2 (b)), and the following variables are introduced: T_p , the continuous starting time of period p , $y_{p,i}$, a binary variable that

indicates whether or not a cleaning task is performed for heat exchanger i at period p , and w_p , a binary variable that indicates whether any heat exchanger is being cleaned during period p . Also, included in the formulation ³⁰ are timing constraints that indicate the monotonically increasing behavior of the starting times, Eq.(23), the duration of the tasks, Eq. (19), the assignment of total number of cleanings, Eq. (20), and the disjunction between a fixed duration for cleaning periods and free duration for operational periods, Eq. (21).

$$0 = T_1 < T_2 < \dots < T_p < t_f, \quad \forall p \in \text{Periods} \quad (18)$$

$$\tau_p = T_p - T_{p-1}, \quad \forall p \in \text{Periods} \setminus \{N_p\} \quad (19)$$

$$\tau_p = t_f - T_p, \quad \forall p \in \text{Periods} | p = N_p$$

$$w_p \leq \sum_{i \in \text{HEX}} y_{t,i} \leq w_p N_T^{\max}, \quad \forall p \in \text{Periods} \quad (20)$$

$$\tau_{cl} w_p + \tau_{op}^{\min} (1 - w_p) \leq \tau_p \leq \tau_{cl} w_p + \tau_{op}^{\max} (1 - w_p), \quad \forall p \in \text{Periods} \quad (21)$$

In this representation of the time horizon the differential equations can be discretized using a backwards finite difference scheme, but continuity constraints have to be imposed at the boundary of the periods. Eq. (22) illustrates how the differential equations are treated using this time discretization approach, where τ_p is the duration of period p , x is a differential variable and F is the right-hand side expression of the differential equation. Note that on the right-hand side of the difference equations the bilinear term $\tau_p F_{p,l-1}$ appears introducing more nonlinearities than in the discrete time approach formulation. These bilinear terms increase the complexity of the problem leading to possible infeasibilities and local optimal solutions. In addition, when the length of the periods tends to zero the optimization problem becomes badly conditioned as it does not satisfy any constraint qualification conditions ²⁸.

$$x_{p,l} = x^0, \quad \forall p \in \text{Periods} | p = 1, l \in \text{Points} | l = 0 \quad (22)$$

$$x_{p,l} = x_{p-1,l'}, \quad \forall p \in Periods \setminus \{1\}, l \in Points | l = 0, l' \in Points | l' = N_t$$

$$x_{p,l} - x_{p,l-1} = h\tau_p F_{p,l-1}, \quad \forall p \in Periods, l \in Points \setminus \{0\}$$

4. Optimal cleaning scheduling and optimal control problem formulation

The heat exchanger network model has to capture what happens when a unit is taken out of service for cleaning. The mass flow rates directed to a unit that undergoes a cleaning have to be bypassed or diverted to other units in the network for its duration. This is done by introducing a flow splitter upstream and a mixer downstream of the heat exchanger for both its inlet streams, on the tube side (subscript t –also used elsewhere for time, but obvious from context) and shell side (subscript s) and corresponding auxiliary bypass streams. Figure 4 depicts the representation of a single heat exchanger including the bypass streams on each side. During a cleaning the respective mass flow rates are diverted from the splitters to the mixers without passing through the heat exchanger. Note that in this paper we only consider mechanical cleanings that restore completely the thermal and hydraulic efficiency of the heat exchanger, but other types of cleaning tasks can be included in the optimization problem with a small modification of this model.

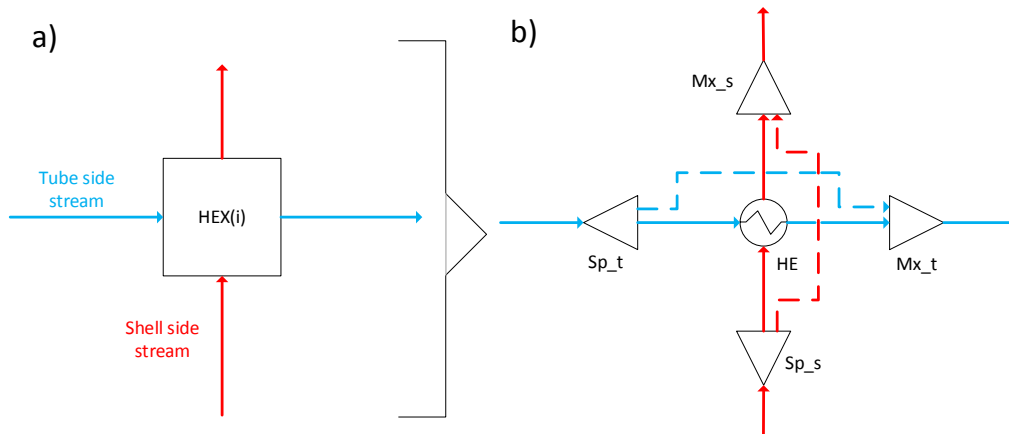


Figure 4. Representation of a heat exchanger as a block (a) and expanded with auxiliary splitters/mixers and streams (b).

This ‘block’ representation of heat exchanger facilitates the problem formulation and the modelling of cleaning and bypasses for optimization purposes. However, it does not mean that the auxiliary units (splitters and mixers and bypasses) are actually installed in a real refinery. In practice the diversion of the flow rates can be done differently for each heat exchanger, so that no capital cost investment is required for additional units to operate the system.

Additional degrees of freedom in a heat exchanger network, may come from flow splitters that divert the flow between parallel branches. In certain HEN configurations, this split fraction may be manipulated through suitable control valves, for example, fixed a priori and kept constant for the entire time horizon, or controlled along some suitable time profile. Alternatively, if the flow split is not controlled, it will be defined at any time by the hydraulic characteristics of the network, so that the pressure drop in the two branches is the same. As discussed, considering the split fraction as a time-varying decision variable (and introducing the corresponding constraints in the optimization) the process profit can increase.

In the optimal cleaning scheduling problem, the main decision variables are the starting time of cleanings tasks, and the sequence of cleanings of the units in the network, which require the introduction of binary variables. In the optimal control problem for the operation of a network, the key decision variables are the mass flow rates as a function of time, which are continuous variables. The formulation below allows both problems to be solved simultaneously.

4.1. Sets

Table 1 introduces the sets to formulate the optimal cleaning and optimal control problem for a general heat exchanger network.

Table 1. Problem formulation: sets and index

$HEX = \{1, 2, \dots, n_{HEX}\}$. Set of heat exchanger units

$Sp = \{1, 2, \dots, n_{Sp}\}$. Set of splitters in the network

$Mx = \{1, 2, \dots, n_{Mx}\}$. Set of mixers in the network
 $So = \{1, 2, \dots, n_{So}\}$. Set of source nodes
 $Si = \{1, 2, \dots, n_{Si}\}$. Set of sink nodes
 $Nodes = HEX \cup Sp \cup Mx \cup So \cup Si$. Set of all the nodes in the network
 $Fluids = \{1, 2, \dots, n_F\}$. Set of fluids in the network
 $Arcs = \{(i, j, k) | \exists (i, j, k) \wedge (i, j, k) \in Nodes \times Nodes \times Fluids\}$.
 Connections between exchangers for a specific fluid
 $Time = \{1, 2, \dots, n_t\}$. Set of points in the time domain
 $Mx = \{1, 2, \dots, n_{Mx}\}$. Set of mixers in the network
 $So = \{1, 2, \dots, n_{So}\}$. Set of source nodes

The heat exchanger network is modelled as a directed multigraph, with five types of nodes: heat exchangers (*HEX*), splitters (*Sp*), mixers (*Mx*), sources (*So*), and sinks (*Si*), each defined by a different set. Their union defines the set of nodes. The mixers and splitters are used to control the mass flow rates through the network. The source nodes are the inlets to the network and their mass flow rate and temperature (in this paper) are pre-specified. The sink nodes are the outlets of the network.

The arcs in the directed multigraph (connections between nodes), are defined in terms of the node of origin, node of destination, and type of stream. The type of stream refers to the fluid that flows through the arc. This is defined in the set *Fluids* that is also used to represent the physical properties of the streams. Examples of elements that belong to this set are: “crude oil”, “residue”, “steam”, “water”. Only in the heat exchanger nodes fluids in two separate arcs may interact (by exchanging enthalpy).

Note that the Time set is introduced in a general way, without mention of the specific discretization scheme used. The elements of this set may be considered as events in the time horizon without being related to a specific discretization scheme. However, the representation of this set (discrete or continuous) changes significantly the scheduling problem formulation. Moreover, some discretization schemes can be more efficient for certain problems than others, as discussed in Section 2.

4.2. Decision variables

The main decision variables of this problem are:

- $y(\text{Time}, \text{HEX})$. Binary variable, that takes the value of 1 when the heat exchanger (i) is undergoing a “cleaning” task at time (t), and 0 if it is “operating”.
- $m(\text{Time}, \text{Arcs})$. Continuous variable that defines the mass flow rate distribution in the network.

The y variables are associated with the scheduling problem and the m variables with the control problem. The size of the problem increases rapidly with the number of units and number of events in the time horizon. However, the solution difficulty is directly related to the number of binary variables, as discontinuities and discrete events are harder to handle than continuous ones. The common approach is to solve first a scheduling problem with constant flow rate distribution, and then for that given schedule apply a control strategy to further reduce the effects of fouling, if possible, while satisfying the relevant operational constraints. The simultaneous solution of these problems is not straightforward, and the complexity of the problem increases. The inclusion of the control elements increases the nonlinearity of the problem, and the possibility to have multiple optimal solutions and many infeasibilities during the exploration of feasible schedules.

4.3. Constraints

The network constraints are the mass and energy balances for all the nodes in the network except the energy balance for the heat exchangers, the only units where two different fluids interact. Mass balances and energy balances are defined using the set of *Arcs* according to Eq. (23) and Eq. (24) respectively. The treatment of the source nodes is different in the sense that, in principle, it would be possible to control both the inlet mass flow rate and the inlet temperature of those streams. However, this leads to nonlinearities, and discrepancies in the solution as the same operation may

be achieved by an infinite number of mass flow rates and temperature combinations. To avoid this the inlet temperature of the source nodes is fixed (Eq. (25)). This is in line with the usual operation of large heat exchanger networks, where source streams are typically recycle streams from a unit at the end of the process. The inlet mass flow rates are considered as decision variables.

$$\sum_{i \in Nodes | (i,j,k) \in Arcs} m_{t,i,j,k} - \sum_{i \in Nodes | (i,j,k) \in Arcs} m_{t,j,i,k} = 0, \quad (23)$$

$$\forall t \in Time, j \in \{Mx \cup Sp \cup HEX\}, k \in Fluids$$

$$\sum_{i \in Nodes | (i,j,k) \in Arcs} Cp_k T_{t,i,j,k} m_{t,i,j,k} - \sum_{i \in Nodes | (i,j,k) \in Arcs} Cp_k T_{t,j,i,k} m_{t,j,i,k} = 0, \quad (24)$$

$$\forall t \in Time, j \in \{Mx \cup Sp \cup HEX\}, k \in Fluids$$

$$T_{i,k}^0 - T_{t,i,j,k} = 0, \quad \forall t \in Time, i \in So, j \in Nodes, k \in Fluids | (i,j,k) \in Arcs \quad (25)$$

Scheduling constraints may be included to avoid schedules that are known a priori to be unrealistic, ineffective or infeasible for any practical reason (e.g. to avoid simultaneous cleaning of certain units, specifying that specific units cannot or should not be cleaned). This set of constraints includes specifying that immediately sequential cleanings of the same unit are disallowed (Eq. (26)), a maximum number of simultaneous cleanings, N_T^{max} (Eq. (27)), dictated, for example, by the capacity of off-line cleaning equipment or availability of maintenance cranes, a maximum number of cleanings for a unit during the horizon, N_U^{max} (Eq. (28)), and a minimum number of units to be operating at any one time for a section of the network, N_{op}^{min} (Eq. (29)).

$$y_{t+1,i} \leq 1 - y_{t,i}, \quad \forall t \in Time \setminus \{n_t\}, i \in HEX \quad (26)$$

$$\sum_{i \in HEX} y_{t,i} \leq N_T^{max}, \quad \forall t \in Time \quad (27)$$

$$\sum_{t \in Time} y_{t,i} \leq N_U^{max}, \quad \forall i \in HEX \quad (28)$$

$$\sum_{i \in \text{HEX}_{\text{sub}} \subseteq \text{HEX}} (1 - y_{t,i}) \geq N_{\text{Op}}^{\text{min}}, \quad \forall t \in \text{Time} \quad (29)$$

Additional constraints based on heuristics (e.g. local operating experience) may be similarly introduced to define a desired cleaning sequence and/or prune non-optimal solutions faster in the MINLP algorithm. For example, constraints of the type: “after cleaning a unit wait at least one month before cleaning the same unit again”, are easily introduced in similar way of Eq. (26). Operational constraints include equipment limits on the operation, such as maximum and minimum furnace duty, and maximum pressure drop constraints across the network. The coil inlet temperature has a lower bound to guarantee a feasible operation (Eq. (30)), the furnace duty has a firing limit that depends on the amount of fuel it is capable to burn and the construction materials (Eq. (31)). When the mass flow is split into two or more branches in an uncontrolled split, the pressure drop must be equal in each branch to prevent back flow (Eq. (32)). Although not shown here, all the variables defined in the optimization problem have a lower and an upper bound which are related to realistic or expected values and help the convergence of the algorithm. This also applies for pressure drop limits on the tube side of each heat exchanger (hydraulic limitation).

$$CIT_t = T_{t,i,j,k} \geq CIT^{\text{min}}, \quad \forall t \in \text{Time}, (i,j,k) \in \text{Arcs} | (i,j,k) = \text{"to furnace"} \quad (30)$$

$$Q_{f,t} = m_{t,i,j,k} C p_k (COT - T_{t,i,j,k}) \leq Q_f^{\text{max}}, \quad (31)$$

$$\forall t \in \text{Time}, (i,j,k) \in \text{Arcs} | (i,j,k) = \text{"to furnace"}$$

$$\sum_{i \in \text{Branch}_{1,b} \subseteq \text{HEX}} \Delta P_{t,i} = \sum_{i \in \text{Branch}_{2,b} \subseteq \text{HEX}} \Delta P_{t,i}, \quad \forall t \in \text{Time}, b \in \text{Branch pairs} \quad (32)$$

As indicated, two operating tasks are considered here for each exchanger: “operating” and “cleaning”. The changes of operational tasks are modelled using disjunctions and a big-M formulation. A switch from “operating” to “cleaning” for a unit has four effects: adding a cleaning cost, disabling the heat exchanger inlet flow rates, enabling the bypasses, and relaxing the heat

exchange constraints of the heat exchanger model. To enable/disable the inlet flow rates and bypass of the heat exchanger big-M type constraints are introduced, Eq. (33) and Eq. (34). The formulation can be easily modified by removing Eq. (33) and Eq. (34), if it is desired to maintain the bypass during the whole operation, or to have a bypass only on the tube side or only on the shell side. Slack variables are included in the NTU equation (Eq. (1)), the fouling rate model (Eq. (10)), and the ageing model (Eq. (11)), so that when a cleaning takes place these variables are fixed (as $NTU = 0, R_{f,g} = 0, x_g = 1$) and those constraints are not required to be satisfied. Eq. (35) shows the general form of the disjunctions for the slack variables, and Eq. (36) - Eq. (38) are constraints that fix or free the value of $NTU, R_{f,g}$ and x_g for a unit, depending on the task it is performing.

$$0 \leq m_{t,Sp_k,HE,k,i} \leq M(1 - y_{t,i}), \quad \forall t \in Time, i \in HEX, k \in \{\text{tube side, shell side}\} \quad (33)$$

$$0 \leq m_{t,Sp_k,Mx_k,k,i} \leq My_{t,i}, \quad \forall t \in Time, i \in HEX, k \in \{\text{tube side, shell side}\} \quad (34)$$

$$0 \leq s_{t,i,l} \leq My_{t,i}, \quad \forall t \in Time, i \in HEX, l \in \{NTU, R_{f,g}, x_g\} \quad (35)$$

$$0 \leq NTU_{t,i} \leq M(1 - y_{t,i}), \quad \forall t \in Time, i \in HEX \quad (36)$$

$$0 \leq R_{f,g,t,i} \leq M(1 - y_{t,i}), \quad \forall t \in Time, i \in HEX \quad (37)$$

$$y_{t,i} \leq x_{g,t,i} \leq 1, \quad \forall t \in Time, i \in HEX \quad (38)$$

4.4. Objective function

The objective function selected here for minimization is the operational cost associated with fouling, that is, the additional cost compared to the cost of the operating the HEN for the entire horizon under cleaned conditions. This objective function (Eq. (39)) originally proposed by Coletti, F and Macchietto, S ⁶, is composed by four terms: the loss of production cost, the furnace

extra fuel consumption cost, the extra carbon emission cost, and the cleaning cost. The loss of production cost reflects any turndown in throughput that may be required to meet either thermal (furnace capacity) or hydraulic (maximum pressure drop) limits. The pumping or power cost required to compensate the effects of fouling could be easily included in this formulation, but it has been reported ⁶ that it usually represents a small fraction (less than 1%) of the total operational cost, so it is neglected in this case.

$$\begin{aligned}
 F(m, y) = & P_{kg} \int_0^{t_f} (m_{production}^{clean} - m_{production,t}) dt + P_{fuel} \int_0^{t_f} \frac{(Q_f - Q_f^{clean})}{\eta} dt \\
 & + P_{CO_2} m_{CO_2} \int_0^{t_f} \frac{(Q_f - Q_f^{clean})}{\eta} dt + \sum_{i \in HEX} \sum_{t \in Time} P_{cl} y_{t,i}
 \end{aligned} \tag{39}$$

This objective function is minimised in all the problems address in this paper. It is valid for the optimal control problem and the optimal cleaning scheduling problem when they are analyzed on their own or simultaneously. Note that for the optimal control problem, there are no cleaning actions, and therefore the cleaning cost term is zero.

4.5. Formulation summary

The simultaneous optimal cleaning scheduling and optimal control problem formulation is summarized in Eq. (40). It is composed by: the heat exchanger model (Section 1), the time discretization scheme constraints (Section 2), network constraints, scheduling constraints, operational constraints, changes in operation (from “operating” to “cleaning”) constraints, and objective function. The formulation changes slightly depending on the discretization scheme used, but the set of constraints and objective function are the same. The only difference is how the time set is treated and the additional constraints associated with it. This however has a significant effect

on the number of binary variables and the nonlinearities of the problem, as discussed in the next section.

$$\begin{aligned}
& \min F(m, y), \quad Eq. (39) \\
& s. t. \text{ Heat exchanger model}(t,i) \text{ Eq. (1) – (6)}, \quad \forall t \in Time, i \in HEX \\
& \quad \text{Fouling and ageing model}(t,i) \text{ Eq. (7) – (14)}, \quad \forall t \in Time, i \in HEX \\
& \quad \text{Pressure drop model}(t,i) \text{ Eq. (15)}, \quad \forall t \in Time, i \in HEX \\
& \quad \text{Time discretization constraints}(t) \text{ Eq. Section 2}, \quad \forall t \in Time \\
& \quad \text{Network constraints}(t,j,k) \text{ Eq. (23) – (25)}, \\
& \quad \quad \forall t \in Time, j \in Nodes, k \in Fluids \\
& \quad \text{Scheduling constraints}(t,i) \text{ Eq. (26) – (29)}, \quad \forall t \in Time, i \in HEX \\
& \quad \text{Operational constraints}(t,i) \text{ Eq. (30) – (32)}, \quad \forall t \in Time, i \in HEX \\
& \quad \text{Disjunctions}(t,i) \text{ Eq. (33) – (38)}, \quad \forall t \in Time, i \in HEX
\end{aligned} \tag{40}$$

5. Problem size scale up

This section provides an initial analysis of how the problem size scales up with the number of units in a heat exchanger network for up to 20 exchangers, for the two discretization formulations presented. To enable a realistic comparison, some parameters are fixed: the maximum number of simultaneous cleanings is set to two, the maximum number of cleanings per unit per year is set to two, the time horizon is one year and the duration a mechanical cleaning task at 10 days. The scenarios considered to determine the total number of periods required in the model are summarized in Table 2.

Table 2. Scenarios to define problem size using the continuous time discretization

| Scenario | Max cleaning per unit | Simultaneous cleanings | Sequence of tasks |
|-------------|-----------------------|------------------------|----------------------------------|
| Worst-case | N^{max} | No | Operating > Cleaning > Operating |
| Normal-case | 1 | No | Operating > Cleaning > Operating |
| Best-case | 1 | Yes | Operating > Cleaning > Operating |

A maximum number of 20 heat exchangers is considered. This value is sufficiently large to cover most of the networks used as examples in academic literature and to have practical industrial

significance. For instance, the hot end section of preheat trains in refining operations (before the crude distillation units) usually has less than 20 heat exchangers.

Figure 5 illustrates a comparison of problem size for the discrete time and the continuous time formulations. The number of periods required to model the problem using a continuous time representation increases linearly with the number of units, while the number of integer variables increases quadratically. Moreover, there is a critical number of units after which the discrete time approach results in a smaller problem size (in terms of number of events, Figure 5 (a)) and fewer binary variables (Figure 5 (b)) than the continuous time approach. After this critical point, the number of event or changes in operation becomes so high that it would require many periods of varying length to model it accurately and then a fixed time grid is likely to be a better approach. Under these conditions the critical point to decide which discretization approach is more suitable for the problem is around 9 heat exchangers for the “worst-case” scenario. If less frequent changes in operation are expected (e.g. a smaller number of cleanings), the critical number of units becomes larger.

The number of periods presented in Case study *set 1 results* - is only an estimate valid for the conditions selected. Solution times will also depend on the number of internal discretization points chosen for the continuous time approach (five in this analysis), nonetheless it gives a realistic basis for choice of time discretization.

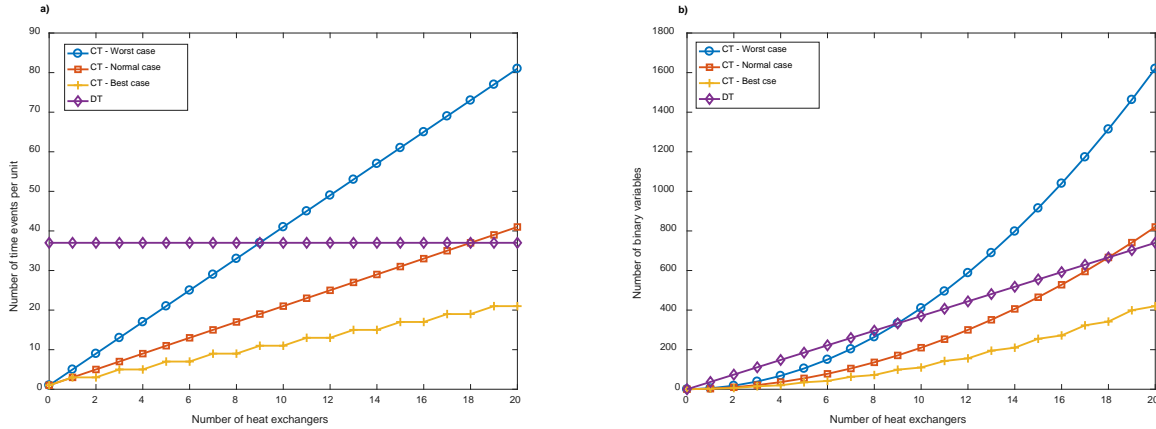


Figure 5. Problem size comparison and scale-up between the discrete time approach and the continuous time approach. a) Number of time events per unit, b) total number of integer variables. [CT: continuous time, DT: discrete time]

The difference in the number of binary variables generated by the two discretization approaches is significant. For example, a network of 5 heat exchangers requires 105 binary variables for the “worst-case” scenario with the continuous time discretization and 185 binary variables with the discrete time approach. This difference can lead to a very big difference in solution times, and an increase of the order magnitude of days is expected because of the combinatorial nature of the problem. On the other hand, after the critical point of 9 heat exchanger the behaviour changes. A network of 15 heat exchangers needs 915 binary variables in the continuous time representation and 555 in the discrete time representation. To model the large number of operation/cleaning changeovers expected, more periods have to be introduced in the formulation, and the average length of an operating period (2.2 days for 15 HEX) becomes lower than that of a cleaning period (10 days), meaning that it is not an efficient problem formulation.

Standard, general purpose MINLP solvers can typically only handle hundreds of variables, so based on this preliminary analysis, are expected to have problems dealing scheduling problems of networks with more than just a few (2-5) heat exchangers. . The solution of larger problems would

take days, considering the large number of combinations and that the NLP relaxed problem is not easy to solve. For realistically large networks, more efficient solution strategies that exploit the structure of the problem are a necessity to reach a solution in a practical time.

6. Case studies

To highlight the flexibility and performance of the models and the solution with the two time discretization approaches, this section presents three sets of case studies. The first set compares the two discretization approaches for the optimal cleaning scheduling and control of small HEN. The second set considers a larger network in which the cleaning schedule is partially defined and the continuous time formulation is used to define the optimal cleaning starting times or partial schedules. The third set involves a small HEN with parallel branches, which is used to highlight the important interactions between control and scheduling elements and demonstrate the synergies achievable.

The network configurations analyzed here were adapted from ^{6,33}, where results were validated against refinery data. Some important operational parameters are presented in Table 3. All heat exchangers are of shell and tube type and, for simplicity, with the same internal configuration. The shell diameter is 1.4m, the tubes length is 5.7m, the number of tubes is 880, the number of passes per shell is 4, and the internal diameter of the tubes is 19.05 mm. Again, for simplicity, the same fouling and ageing model parameters are adopted for all exchangers. It is assumed that each cleaning takes 10 days and recovers completely the thermo-hydraulic performance of the heat exchanger. Physical properties, operation conditions and cost parameters are also taken from previous works ^{6,33}. Crude oil goes through the tube side of all the heat exchangers, and recycle streams coming from the crude distillation unit or other downstream units are used on the shell side.

Table 3. Important operational data for case studies

| Parameter | Symbol | Value |
|------------------------------------------------|-------------|-------------------------------------------------|
| Tube side roughness – Fouled tube (worst case) | ϵ | 150 mm |
| Fouling deposition coefficient | α | 142.56 K.m ² /W.day |
| Fouling suppression coefficient | γ | 8.04x10 ⁻⁸ K.m ⁴ /N.W.day |
| Fouling activation energy | E_f | 28500 J/mol.K |
| Ageing pre-exponential factor | A_a | 8.64 day ⁻¹ |
| Ageing activation energy | E_a | 50000 J/mol.K |
| Max. mass flow rate on the tube side | m_t^{max} | 88 kg/s |
| Max. mass flow rate on the tube shell | m_s^{max} | 26 kg/s |
| Source temperature for tube side sub-network | T_t^0 | 483.15 K |
| Source temperature for shell side sub-network | T_s^0 | 603.15 K |
| Coil outlet temperature | COT | 640.00 K |
| Max. Furnace duty | Q_f^{max} | 50.0 MW |
| Price of product | P_{kg} | \$ 0.23/kg |
| Price of fuel | P_{fuel} | \$ 27/MW-h |
| Price of carbon emissions | P_{CO_2} | \$ 30/ton |
| Carbon emissions to fuel consumption ratio | m_{CO_2} | 0.011 ton/MW-h |
| Price of a cleaning task | P_{cl} | \$ 30000 |

6.1. Case study set 1 - Comparison of discretization approaches

Three case studies are considered here to compare the discretization approaches and the integration of control elements within the scheduling problem. The first case is a single heat exchanger (“1HE”) that serves to analyze the problem structure, complicating constraints, and sensitivity to parameters. The other two cases are small heat exchanger networks composed by two units, in one configuration in parallel (“2HE-P”), in the other configuration in series (“2HE-S”). In the parallel configuration the split fraction of the stream that goes to each heat exchanger is an additional decision variable, which links the effects of control elements with the scheduling problem. Figure 6 illustrates the flowsheet of the three cases, where for clarity the source and sink nodes are shown explicitly with their names.

a)

b)

c)

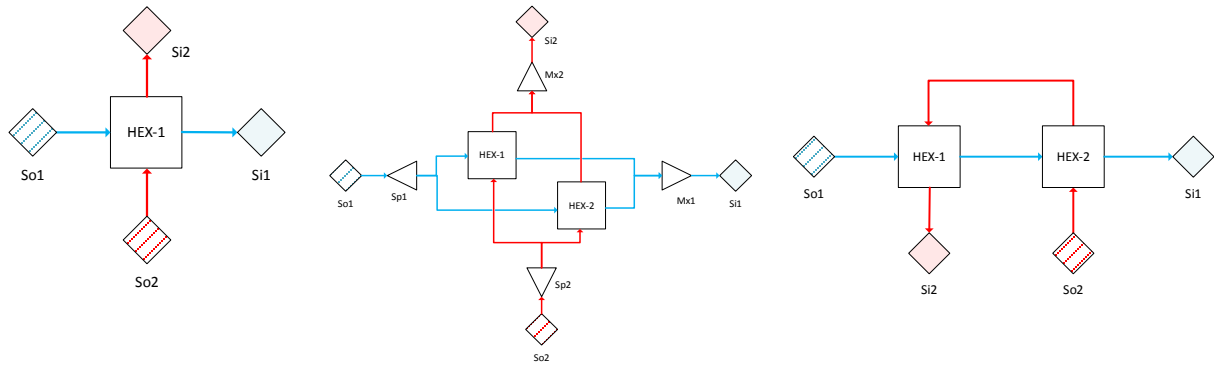


Figure 6. Flowsheet representation of case studies. a) Single heat exchanger ("1HE"), b) Parallel network configuration ("2HE-P"), c) Series network configuration ("2HE-S")

6.2. Case study set 2 - Partial scheduling using a continuous time formulation

The continuous time representation of the scheduling problem is used here. The purpose of this case study is to show how an analyst may interact with the problem definition to refine and improve cleaning sequences which include heuristics or practical considerations. This solution defines exactly the starting time of cleaning tasks when the cleaning sequence of units and cleaning constraints are known, based on other considerations. In other words, when the task assignment to units and the sequence of task are pre-defined, two of the three elements of the scheduling problem are fixed and the optimization problem is solved only to determine the optimal timing of the tasks. Figure 7(a) shows a small heat exchanger network considered in this set (all exchangers have the specifications described in Table 3) and Figure 7(b) shows a desired schedule defining the number of cleanings and relative cleaning sequence, in terms of periods. The starting time of the cleaning tasks is not specified, nor is the length of the operating periods. This kind of partial schedule could be the result of heuristic rules or practical considerations such as: “clean first those exchangers closer to the furnace because the level of fouling is usually higher”, “never clean HE-1 because of low fouling level”, “clean HE-2 immediately after cleaning HE-3”. Once the schedule is defined in these terms, the binary variables in the optimization problem are fixed because the periods of

cleaning and operation and their sequence are known. The continuous time formulation is then used to determine the optimal starting time of the cleaning tasks defined in Figure 7b. The optimization problem becomes a NLP in which the decision variables are the starting time of the changes in operation (which define the variable periods length) and the flow rate distribution in the network. The complexity of the optimization problem is reduced significantly.

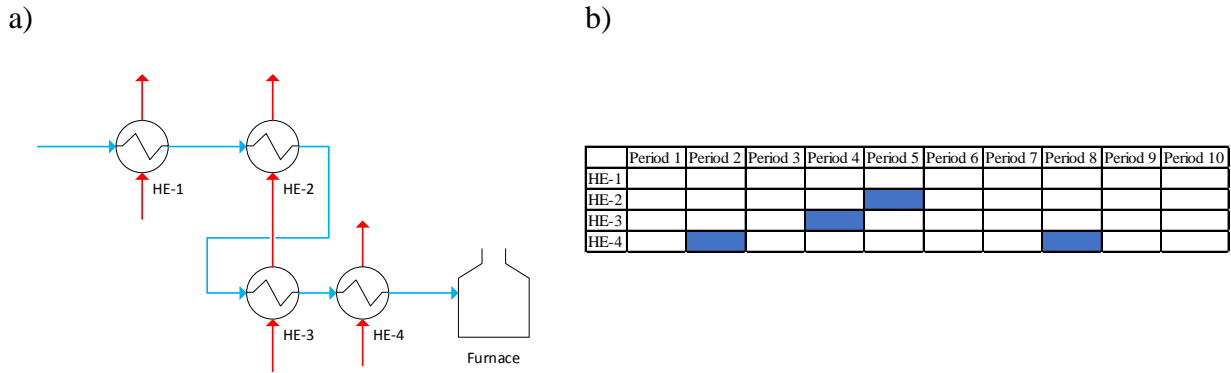


Figure 7. Example of predefined schedule definition and improvement using the continuous time representation. a) Network representation, b) Task assignment and sequence, defined in terms of periods of undefined length.

A variation of partial schedule for this case study is also considered. The same partial cleaning schedule is defined for HE-1, HE-2, and HE-3, however the number and sequence of cleanings for exchanger HE-4 are now unknown. HE-4 is the last exchanger in the network, and the one exposed to a higher temperature, and therefore with higher fouling rates, making it a critical unit. This variation of the partial scheduling problem consists in optimising the cleaning schedule for HE-4, and the timing of all tasks, given a partial schedule for the rest of the exchangers.

6.3. Case study set 3 - Integration of scheduling and control

This case study investigates the operation of the small network composed of two heat exchangers in a parallel configuration shown in Figure 6b. This configuration (with more exchangers in each branch) is commonly found in practice to supply large thermal requirements and to give more

flexibility to the operation ¹². Here the exchangers are identical, but it is assumed that at the initial time HE-1 has a fouling resistance of $0.005 \text{ m}^2\text{K}/\text{W}$ and HE-2 is clean. In this case the mass flow rate through each branch is a continuous decision variable which is determined simultaneously with the optimal cleaning schedule.

To analyze the interaction of scheduling and control and the benefits of a simultaneous solution of the two problems, four possible scenarios are considered: 1) a base case with no mitigation: no cleaning is performed and the flow split fraction between the parallel branches is fixed at 0.5 during the whole operation; 2) only control: no cleaning is performed but the split fraction is a free variable to be optimised; 3) only scheduling: the split fraction is fixed at 0.5 during the whole operation and the scheduling binary variables are optimised; 4) integrated control and scheduling: both the split fraction and the scheduling binary variables are optimally chosen.

If the split fraction between the branches is not controlled, its value must balance the pressure drop in each branch, such that the outlet pressure of both branches is equal and there is no backflow. This pressure drop constraint is included in the formulation and three additional scenarios are considered to assess the benefits of solving the two problems simultaneously in this more restricted case: only optimal control (5), only optimal cleaning scheduling (6), and integrated control and scheduling (7).

7. Results and discussion

All optimization problems are solved in GAMS using a branch and bound algorithm for the MINLP problem and a reduced gradient solver (CONOPT) for the relaxed NLP problems. At first the problem was formulated and solved in Pyomo, but due to license restriction the only NLP solver available was IPOPT and this led to a high number of infeasibilities and high computational time with the continuous time formulation. However, the Pyomo implementation is very useful

and efficient, especially when the binary variables are fixed in the continuous time approach. It makes the implementation attractive for decomposition alternatives in which NLP subproblems are solved frequently.

7.1. Case study set 1 results - Time discretization approaches

The no mitigation base case (NM) with no cleanings and no changes in flow rate distribution in the network was included so that the effectiveness of the mitigation techniques applied could be measured. Table 4 shows the problem size, the computational time, the objective function value at the optimum, and the potential savings achieved (relative to the base case) for each network using the discrete time (DT) and continuous time (CT) discretization, for the three problems considered (1HE, 2HE-P, 2HE-S). In terms of problem size, the number of binary variables with the continuous time representation is lower than that of the discrete time representation, which is advantageous since their combinatorial nature makes the problem more difficult to solve. The reduction is greater than 70% for all the case studied. The number of continuous variables is often greater in the continuous time representation than that in the discrete time representation, but it depends on the number of internal points chosen. All the continuous time cases are solved with the “worst-case” number of periods (see Section 5, problem scale up), 5 for 1HE case and 9 for 2HE cases, and five internal points for each period. While the complexity of solving the optimal scheduling problem using the discrete time representation arises from the high number of binary decision variables, the complexity of using the continuous time representation comes from the nonlinearities and non-convexities of the formulation. There is a compromise between these two factors and identifying which one is dominating depends on the size of the heat exchanger network.

Table 4. Comparison of performance and computational results between the discrete time discretization and the continuous time discretization approaches for all the case studied (1HE, 2HE-P, 2HE-S)

| Network Scenario* | 1HE | | | 2HE-P | | | 2HE-S | | |
|------------------------------------------|--------|--------|--------|--------|----------|---------|---------|----------|--------|
| | NM | DT | CT | NM | DT | CT | NM | DT | CT |
| No. Equality constraints | 1978 | 1978 | 1633 | 3993 | 3993 | 5692 | 3651 | 3651 | 5206 |
| No. Inequality constraints | 797 | 797 | 594 | 1632 | 1632 | 2213 | 1556 | 1556 | 2137 |
| No. Continuous variables | 2243 | 2243 | 1786 | 4637 | 4637 | 6616 | 4105 | 4105 | 5860 |
| No. Integer variables | 0 | 37 | 5 | 0 | 70 | 18 | 0 | 70 | 18 |
| CPU secs | | 272.77 | 7.58 | | 48742.08 | 1308.16 | | 38623.01 | 497.70 |
| Loss of production cost [10^3 \$] | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fuel extra cost [10^3 \$] | 502.88 | 361.50 | 352.81 | 987.84 | 622.69 | 609.77 | 1098.42 | 719.35 | 704.83 |
| CO2 extra cost [10^3 \$] | 5.88 | 4.23 | 4.13 | 11.52 | 7.29 | 7.13 | 12.85 | 8.42 | 8.25 |
| Cleaning cost [10^3 \$] | 0.00 | 60.00 | 60.00 | 0.00 | 120.00 | 120.00 | 0.00 | 120.00 | 120.00 |
| Value of objective function [10^3 \$] | 508.76 | 425.73 | 416.93 | 999.37 | 749.98 | 736.90 | 1111.27 | 847.77 | 833.07 |
| Savings in operational cost [10^3 \$] | 0.00 | 83.03 | 90.68 | 0.00 | 249.39 | 256.18 | 0.00 | 263.50 | 275.06 |
| Percentage savings [%] | 0.00% | 16.32% | 17.86% | 0.00% | 24.95% | 25.80% | 0.00% | 23.71% | 24.82% |

* NM: no mitigation (base case), DT: discrete time approach, CT: continuous time approach

Table 4 shows that the computational effort of solving the problem, measured as the CPU seconds required to reach a solution, is much lower with the continuous time discretization approach than with the discrete time approach. The solution time is reduced on average by 97% for the three cases studied, from an order of magnitude of hours for the discrete time formulation to an order of magnitude of seconds/minutes for the continuous time formulation. However, the continuous time formulation is very sensitive to the initialization of the problem and even for these small case studies the algorithm can terminate early at a local infeasible point. Also, feasibility and solution time are very sensitive to the number of points selected per period, and to the minimum

and maximum length of each period. Meanwhile, the discrete time approach is more robust because the fixed grid reduces the nonlinearities and the complicating bilinear terms.

The optimal solutions of the scheduling and control problem do not change significantly between the discrete time and continuous time discretization approaches. As shown in Table 4 the objective function value with both approaches is similar, the greatest part of the operational cost coming from the fuel cost and the cleaning cost. The loss of production cost is zero in all the case studied because the firing limit of the furnace and the hydraulic limit are never reached. Nevertheless, there is a consistent increase in the savings achieved when the continuous time approach is used in comparison with to those obtained with the discrete time approach. The variable length of the periods in the continuous time representation increases the accuracy with which the starting cleaning times are defined and thus the operational cost can be reduced more than when using fixed time points in the discrete time approach.

For the three cases studied, Figure 8 illustrates the furnace duty profile over the 1-year horizon with the optimal cleaning schedule, the comparison with the base case, and the comparison between the discretization approaches. The optimal schedules involve two cleanings for case 1HE, and four cleanings for cases 2HE-S and 2HE-P. When the problem is solved using the continuous time approach the cleaning tasks start earlier than with the discrete time approach. Table 5 summarizes the starting cleaning time for the cases studied showing that it is more efficient to clean the units at times that are not represented in the discrete time approach, as these optimal cleaning starting times fall in between two discrete points. The continuous time optimal savings are 1.2% greater than those of the discrete time, in average. Otherwise, from a practical point of view there is no big difference between the two approaches in terms of objective function, and only criteria based on the ease of the solution should be considered.

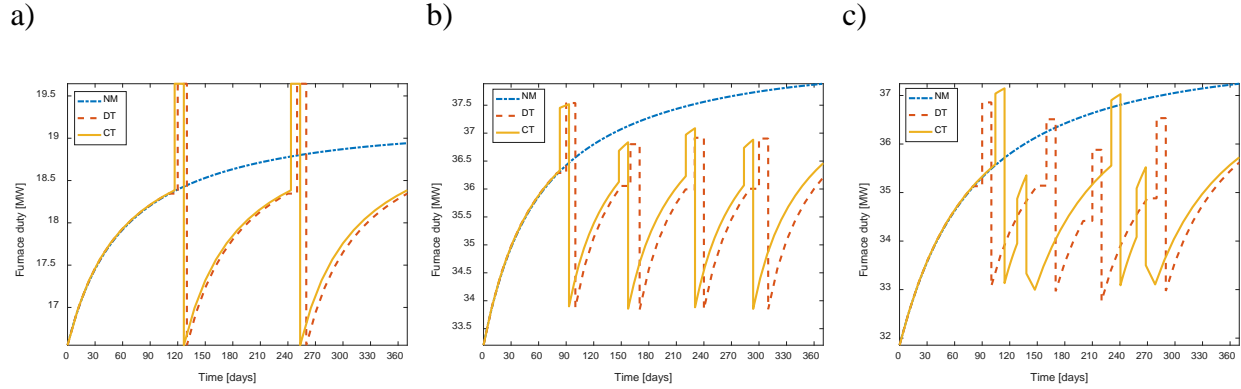


Figure 8. Furnace duty for the three cases studied and discretization approaches. NM: no mitigation, CT: continuous time, DT: discrete time. a) 1HE, b) 2HE-P, c) 2HE-S

Table 5. Optimal cleaning schedule for discrete time (DT) and continuous time (CT) approaches

| <i>Network</i> | <i>Unit</i> | <i>Cleanings starting time [days] - DT</i> | | <i>Cleanings starting time [days] - CT</i> | |
|----------------|-------------|--------------------------------------------|-------|--------------------------------------------|-------|
| <i>1HE</i> | HE-1 | 120.0 | 250.0 | 116.7 | 243.3 |
| | HE-1 | 160.0 | 300.0 | 147.4 | 283.6 |
| <i>2HE-P</i> | HE-2 | 90.0 | 230.0 | 83.1 | 220.3 |
| | HE-1 | 160.0 | 280.0 | 128.1 | 258.2 |
| <i>2HE-S</i> | HE-2 | 90.0 | 210.0 | 104.3 | 230.6 |

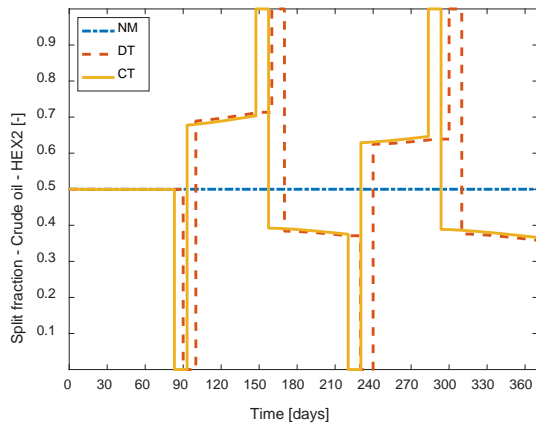
The higher savings with the continuous time approach are due to three main reasons: i) the better compromise between the cost of a cleaning and the future reduction of the furnace duty, the operating time between cleanings is usually longer ; ii) the more accurate definition of the starting time of cleaning actions produces a lower furnace duty in cases 2HE-P and 2HE-S. Figure 8 (b) shows that the furnace duty at the cleaning starting times for the continuous time approach is lower than that for the discrete time approach, which is translated in greater savings. iii) Finally, the correct sequencing and operational time between cleanings. For example, in the 2HE-S case (Figure 8 (c)) the time between the second and third cleaning with the discrete time approach is

lower than with the continuous time approach. This produces larger increases in furnace duty and the length of the operation periods does not allow reducing costs as much as in the continuous time approach.

The 2HE-S case shown in Figure 8 (c) exhibits the greatest differences between the two discretization approaches. It is possible that the algorithm may have stopped at a local minimum or pruned local infeasible solutions due to the nonlinearities and nonconvexities of the problem. However, in both cases exchanger HE-2 is cleaned before HE-1. HE-2 is exposed to higher temperatures and so the level of fouling is greater and the deposit is older than in HE-1 at the time the first cleaning takes place. For example, with the discrete time approach, at day 90, when the first cleaning is performed, the fouling resistance and age of the deposit for HE-2 are 0.01322 m²/W.K and 0.986, and for HE-1 they are 0.01128 m²/W.K and 0.992.

The 2HE-P case is different from the other cases, in the sense that it includes flow split as an additional control element, and the split fraction of the cold stream and of the hot streams are optimized at the same time of the cleaning schedule. Figure 9 presents the optimal split fraction of the cold and hot streams. The split fraction changes with time: after a cleaning a high fraction of the inlet flow rate is sent to the clean heat exchanger, and because of this a higher heating flow rate is also required. Subsequently, such the flow rates are not held constant, but change with time so that the capacity of recovering energy of each heat exchanger is maximised. After a cleaning, the crude oil flow rate of the less fouled heat exchanger increases with time to satisfy the pressure drop constraint between the parallel branches, and the heating flow rate to the most fouled heat exchanger increases with time to increase the duty in that unit.

a)



b)

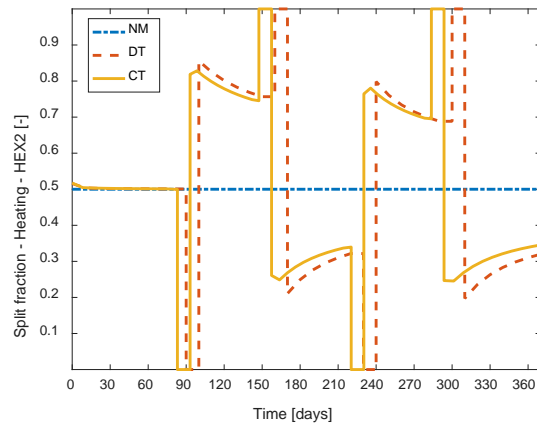


Figure 9. Flow rate distribution of the 2HE-P network. a) Split fraction of the cold stream with respect to HE2, b) Split fraction of hot stream with respect to HE2

7.2. Case study set 2 results – Partial scheduling

The continuous time formulation offers the additional capability of defining individual sub-elements of the scheduling problem. The assignment of task to units and the sequence of task for the network in Figure 7a was defined in Figure 7b. As discussed, the continuous time formulation leads to a NLP problem the solution of which defines the optimal cleaning starting times. The Gantt chart of Table 6 shows the sequence and assignment of cleaning actions, which were predefined by the analyst, and (inside the cells of the Gantt chart) the optimal starting times of each task, which are the solution of the optimization problem. Table 7 shows the optimal cleaning scheduling the variation of case study set 2 when the cleanings of HE-4 are unknown. Note that in comparison to the previous solution (Table 4) the starting times of the cleanings of HE-2 and HE-3 change and the number and timing of HE-4 cleanings is different (a single cleaning is now performed), highlighting the interaction between the cleaning sequence and the timing of the events. This shows that carrying out two cleanings for HE-4, as it was predefined for the first

scenario, is inefficient because the potential economic savings do not compensate for the cost of the additional cleaning.

Table 6. Gantt chart of the optimal cleaning starting time for case study 6.2 of fixed cleaning sequence (starting times round to whole days).

| | Period 1 | Period 2 | Period 3 | Period 4 | Period 5 | Period 6 | Period 7 | Period 8 | Period 9 | Period 10 |
|------|----------|----------|----------|----------|----------|----------|----------|----------|----------|-----------|
| HE-1 | | | | | | | | | | |
| HE-2 | | | | | 188 | | | | | |
| HE-3 | | | | 178 | | | | | | |
| HE-4 | | 125 | | | | | | 246 | | |

Table 7. Gantt chart of the optimal cleaning starting time for case study 6.2 of partial cleaning schedule (starting times round to whole days).

| | Period 1 | Period 2 | Period 3 | Period 4 | Period 5 | Period 6 | Period 7 | Period 8 | Period 9 | Period 10 |
|------|----------|----------|----------|----------|----------|----------|----------|----------|----------|-----------|
| HE-1 | | | | | | | | | | |
| HE-2 | | | | | 175 | | | | | |
| HE-3 | | | | 165 | | | | | | |
| HE-4 | | | | | | | | 205 | | |

Figure 10 shows the furnace duty for the no mitigation base case (NM), for the fixed cleaning sequence and for the partial optimal schedule. During most of the operation the furnace duty of both cleaning scheduling is much lower than in the base case, indicating that less fuel is required to maintain the coil outlet temperature of the furnace. When the cleaning schedule for HE-4 is optimized the number of cleanings is reduced by one, and still the energy consumption is lower than that of the base case.

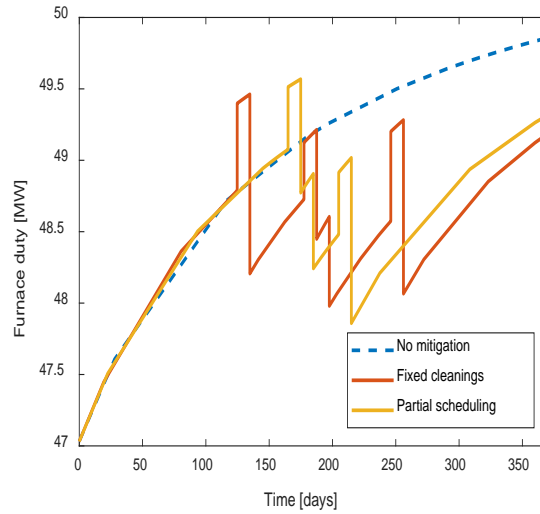


Figure 10. Furnace duty for case study 6.2

The continuous time formulation of the optimal cleaning scheduling problem is flexible and allows solving for the timing of events alone when the other elements of the schedule are defined, or to optimize partial cleaning schedules when some cleanings are fixed for certain exchangers. Optimizing just the timing of the cleanings generates a 3.3% savings which respect to the base case, and optimizing the timing of events and the cleaning schedule for HE-4 yields savings of 4.9%. This low savings may indicate that the predefined cleanings of HE-2 and HE-3 are inefficient or very costly in comparison with the future economic potential of a cleaned unit. The allocation and timing of task are equally important in the definition of the cleaning schedule, although they can be solved independently when the other is fixed, defining all the elements of the schedule simultaneous provides additional savings.

The NLP for the fixed cleanings scenario is solved in 1 min, which is significantly faster than solving the MINLP associated with all the elements of the scheduling problem. The MINLP that defines the complete cleaning scheduling problem for this network of four exchangers has 68 binary variables and it is estimated its solution would require more than 24 h of CPU time.

7.3. Case study set 3 results - Integration of scheduling and control

The case of two exchangers in parallel, 2HE-P, of Figure 5 is considered again for the 7 scenarios presented in section 6.3. Table 8 presents the optimal value of the objective function for each scenario as well as the components of the total cost. In Table 5 all starting times (continuous variables) were rounded to the nearest whole day. The loss of production cost is again zero for all the scenarios as none reaches an operational limit that forces to reduce the throughput. All the scenarios that have some mitigation action (flow control, cleaning scheduling, or both, scenarios 2 - 7) present a reduction of the total operational cost relative to the no mitigation base case (scenario 1), with fuel consumption representing the highest contribution (>90%). The cases when only flow rate distribution is optimised (scenarios 2 and 5) reduce the operational cost by sending a higher fraction of the flow to the heat exchange with less fouling, but this alternative alone produces savings of less than 1%.

Table 8. Comparison of operational cost and savings for the different scenarios of operation of the parallel HEN

| No* | Scenario | | | | | | |
|------------------------------------------|-------------------|---------|------------|------------|-----------------|-----------------|-----------------|
| | 1 BASE CASE | 2 | 3 | 4 | 5 | 6 | 7 |
| Cleaning scheduling | X | X | O | O | X | O | O |
| Flow rate control - shell side | Fixed | O | Fixed | O | O | Fixed | O |
| Flow rate control - tube side | Fixed | O | Fixed | O | Pressure driven | Pressure driven | Pressure driven |
| HE1 - Cleaning starting times [day] | N/A | N/A | (91, 225) | (67, 212) | N/A | (76, 216) | (74, 216) |
| HE2 - Cleaning starting times [day] | N/A | N/A | (128, 255) | (139, 282) | N/A | (137, 270) | (142, 282) |
| Loss of production cost [10^3 \$] | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fuel extra cost [10^3 \$] | 1068.40 | 1060.01 | 769.53 | 640.96 | 1063.97 | 732.21 | 681.73 |
| CO2 extra cost [10^3 \$] | 9.77 | 10.66 | 6.27 | 5.78 | 10.27 | 5.88 | 5.86 |
| Cleaning cost [10^3 \$] | 0.00 | 0.00 | 120.00 | 120.00 | 0.00 | 120.00 | 120.00 |
| Extra operational cost [10^3 \$] | 1078.17 | 1070.67 | 895.80 | 766.74 | 1074.24 | 858.09 | 807.59 |
| Savings in operational cost [10^3 \$] | 0.00 | 7.50 | 182.37 | 311.43 | 3.93 | 220.09 | 270.59 |
| Percentage increase in savings [%] | 0.00% | 0.70% | 16.91% | 28.89% | 0.36% | 20.41% | 25.10% |

* X: no cleaning actions. O: the variable is a free decision variable in the optimization formulation.

On the other hand, optimising the cleaning scheduling alone, with fixed, pre-selected flow split (scenarios 3 and 6) produces significant savings as it allows a full restoration of the thermo-hydraulic performance of the cleaned units. The cleaning tasks are scheduled at times such that the operation window between two consecutive cleanings is long enough to offset the extra cost (Figure 11). Exchanger HE-1 is always cleaned first because it starts operations with the defined initial fouling resistance (maybe as the result of a previous cleaning schedule or an inefficient/partial cleaning). The simultaneous solution of the optimal control problem and optimal scheduling problem (scenarios 4 and 7) shows that although optimising flow rate distribution alone

did not reduce significantly the operational cost of the process, it presents a strong interaction with the cleaning scheduling problem and when used together, a large additional benefit is achieved over optimal scheduling alone (29% savings over the base case vs. 17%). The increase of savings between scenarios 2, 6 (optimal control) and scenarios 3, 6 (simultaneous optimal control and scheduling) presented in Table 8 serves to illustrate the strong synergy between these two mitigation techniques and demonstrate why they should be considered together at the same decision level. Solving these two problems simultaneously further reduces operational cost by 5% to 12% with respect to optimal cleaning scheduling alone.

The trends in scenarios 5 – 7 (pressure driven flow split) are similar to those with controlled flow split. The solution of the optimal control problem produces small savings (<1%), the savings obtained from the optimal scheduling are significant (20.4%), but it is the integration of both decisions that provides the greatest savings (25.1%). However, these savings are smaller than those obtained when the tube side flow rate is controlled. The additional constraint introduced in the formulation to equalize the pressure of the branches at all time reduces the possibilities of improving the process operation. Although the pressure drop equalization defines the tube side flow rate, the shell side flow rate of each exchanger was still a variable in the optimization formulation corresponding to the control degree of freedom. However manipulating it presented small scope for improvement of the objective function.

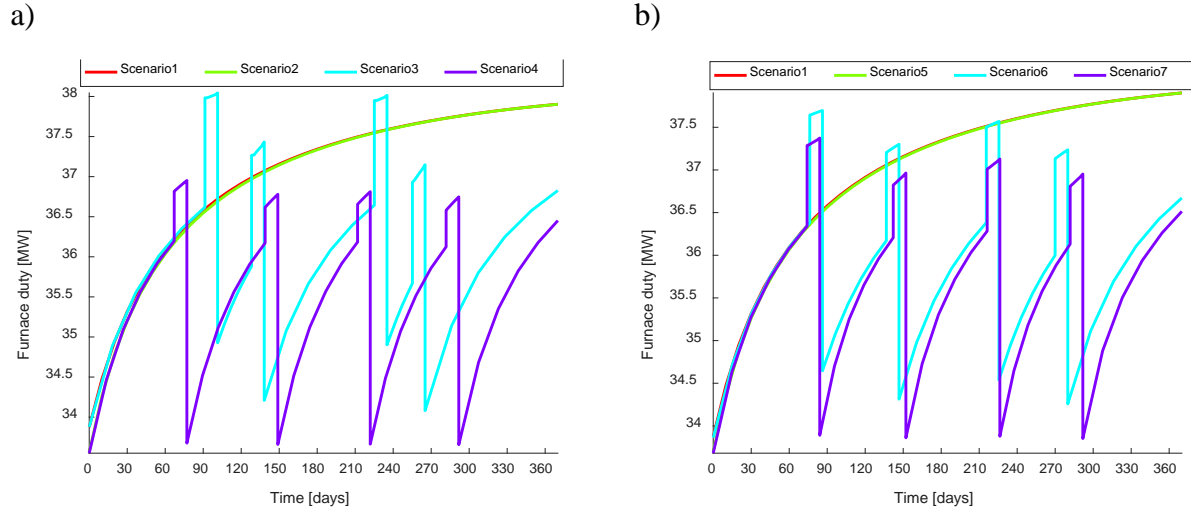


Figure 11. Furnace duty for scenarios of optimal control and optimal cleaning scheduling

scenarios. a) Free flow rates b) Pressure driven flows on tube side

Figure 11 shows the furnace heat duty for all the scenarios considered, when the flow rate is controlled (Fig 11 a), and when it is hydraulically determined (Fig 11 b). Figure 12 shows the split fraction of the cold stream and the hot stream when the flow rate is controlled (Fig 12 a, b), and when the pressure drop in the branches defines the mass flow rate (Fig 12 c, d). In the no mitigation base case the furnace duty increases monotonically with time. The optimal flow control scenarios, 2 and 5, present a similar behaviour to the base case and only a small difference is observed in the furnace duty that explains why the savings of this scenario are less than 1%. Although its effect is not significant, the split fraction of the cold and hot stream change significantly with time. Note that the optimal split fraction at the initial time is different than the design value of 0.5 because the initial fouling resistance of exchanger HE-1. When the mass flow rate is pressure driven the crude oil split fraction to HE-1 decreases with time, while the heating split fraction increases to satisfy the pressure drop and to keep up the duty in this exchanger. On the other hand, when the mass flow rate is controlled, both split fractions increase over time to increase the thermal duty in HE-1.

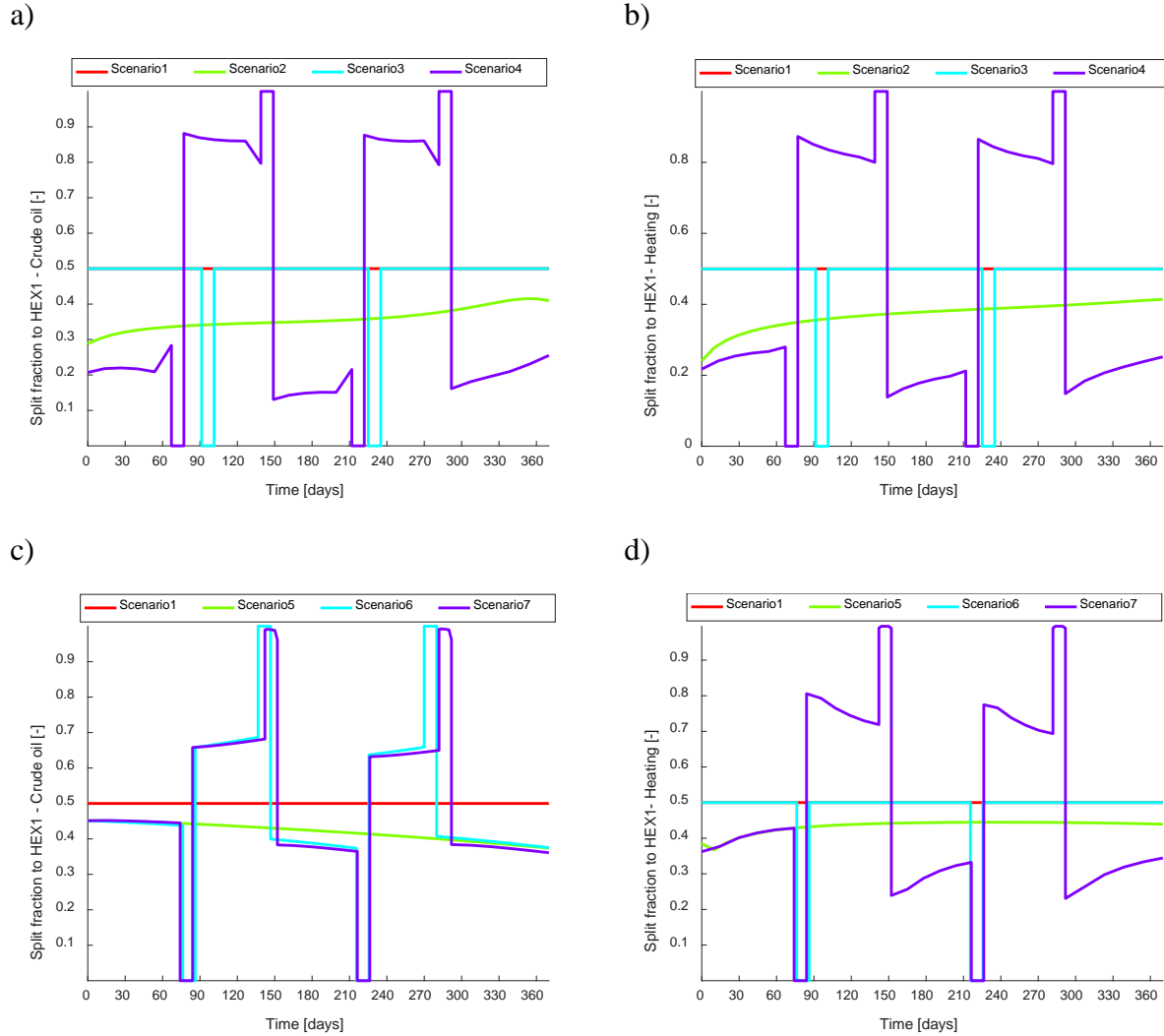


Figure 12. Branches split fraction of optimal control and optimal cleaning scheduling scenarios.

a, b) Free flow rates c, d) Pressure driven flows on tube side

In Figure 12 it can be observed that in all the cleaning scheduling scenarios both exchangers are cleaned twice. The cleanings are discrete actions that allow recovering the thermal and hydraulic performance of the exchanger and introduce discontinuities in the response variables. In the simultaneous solution of the optimal control and optimal scheduling all the cleaning tasks, except for the first one, start later than in the solution of the optimal cleaning scheduling problem alone.

The optimal control of the flow rate distribution allows increasing substantially the operation periods between cleanings, thus reducing the operational cost.

After a cleaning the flow rate distribution in the network changes significantly in order to improve the overall thermal recovery in the process. Regardless of whether the tube side flow is controlled or pressure driven, after a cleaning a higher fraction of the crude oil is sent to the cleaned heat exchanger where more energy can be recovered, and the fraction changes over time due to the increasing fouling resistance or to satisfy the pressure drop constraint. Note also that the split fraction of the heating fluid changes with time depending on which exchanger has a higher crude oil flow rate or which requires a higher heat transfer because of a higher fouling level.

For all scenarios, the optimal control problem formulation results in a NLP that can be solved efficiently in less than 2 min. On the other hand, the optimal scheduling problem and the integration of optimal control and scheduling are defined as a MINLP. Although the number of binary variables for the case studies discussed here is low (18 in the continuous time representation), their solution requires more than 10 hr of computational time with the standard general purpose solvers used, because of the many possible combinations and the not so tight formulation that produce a slow update of the lower bound. This computational difficulty makes it necessary to implement more efficient solution algorithms in order to address the optimal cleaning scheduling and control problem of larger heat exchanger networks of industrial importance.

To further investigate scale-up and computational issues, we analyzed two HEN, one with 3 exchangers and other with 4. For the one with 3 exchangers 13 periods are used to discretize the time horizon, and for the one with 4 exchanger 17 periods. These networks are variations of the one presented in Section 6.2 for the partial cleaning scheduling, either with exchangers HEX1 to

HEX 3 (3 units) or HEX1 to HEX4 (4 units). After over 96 h of computation no optimal solution was found using the same standard branch and bound algorithm used for solving the earlier optimal scheduling problems. The relative optimality gap at this point was 236% for the HEN with 3 exchangers, and 278% for the HEN with 4 exchangers. This clearly indicates that the solution of even these small networks is already challenging due to the large number of combinations that define a feasible solution.

Although the computational time with three and four exchangers is clearly too high, the continuous time problem formulation is still more efficient than the discrete time one. The number of binary variables per exchanger is reduced almost in half, to 13 and 17 against 37. With the computational time increasing exponentially with respect to the number of binary variables of the problem, it is therefore expected that developments in solution algorithms should focus on using the continuous time formulation rather than the discrete time one.

8. Conclusions and perspectives

Fouling is a recurrent problem in many heat exchanger networks that reduces their thermal and hydraulic efficiency. Control and cleaning mitigation strategies to counter its effects and recover performance (of individual units and of the network as a whole) provide ample scope for optimization. The new representation presented here, of fouling and ageing phenomena in conjunction with the additional devices introduced for splitting, mixing and bypassing hot and cold streams, combines a reasonably detailed dynamic thermo-hydraulic heat exchange model with the ability to take exchangers in and out of operation for cleaning, within an optimization framework. The representation is sufficiently flexible to be used for the simultaneous solution of the optimal cleaning scheduling and optimal control problem of a heat exchanger network, the individual sub-problems, and various combinations of them, including partial scheduling with predefined task

sequences, or partial optimization of the cleaning tasks. This new approach represents the heat exchanger model using a DAE index 1 system, in which the differential equations are the fouling resistance of the deposit and the age of the deposit (mass fraction of gel). The usual thin layer assumption is eliminated and the age of the deposit is represented as a kinetic expression which is function of the layer concentration. Although this is an axially-lumped model that captures local effects in terms of space averages, models of this type have been used before³⁴. A full validation remains to be done.

The flexibility of the representation, illustrated by means of small heat exchanger networks, show that: i) the optimal cleaning scheduling and the optimal control problem can be handled simultaneously. ii) all problems can be solved using two time discretizations: a discrete time approach and a continuous time approach. The discrete time approach uses a fixed grid representation leading to a higher number of binary variable than the continuous time approach in which the length of periods is variable. The small case studies show that the continuous time representation leads to a faster solution than the discrete time alternative. Although the objective function values are similar, the total operational cost of the heat exchanger network is consistently lower with the continuous time discretization because of the more flexible definition of starting times of the cleaning tasks. Finally, the results of a small heat exchanger network with parallel units show that it is highly beneficial to consider scheduling and control simultaneously.

While the generality and flexibility of the formulation and simultaneous solution were presented here with small networks for illustrative purpose, there is clearly the need to apply them to larger networks. To this purpose, the scale-up analysis presented in section 5 indicates that, based on problem size alone, it should be feasible to tackle networks with up to 10-15 exchanger units if suitably tailored solution algorithms are used. . The number of complicating variables and

constraints increases linearly with the number of units with the discrete time approach and quadratically with the continuous time approach, thus there is a critical number of units when the former approach becomes more favorable. However, the continuous time approach leads to formulations with more nonlinearities and nonconvexities. Moreover, the size and complexity of the problem will increase if more types of cleanings (e.g. chemical cleaning, partial cleaning) are introduced. The problem formulation presented here is very flexible and can be easily extended to take into account combinations of different cleaning types.

In terms of solution, all solvers used here were standard, off the shelf ones. The results presented indicate their potential to address other than small scale problems is presently limited. More efficient solution approaches should be considered for solving large scale problems, to take advantage of the very large scope for economic improvement offered by a simultaneous solution of control and scheduling of HEN under fouling. The use of specifically tailored decomposition techniques, cuts and constraints will be presented elsewhere. Finally, it will be necessary to validate all results against more rigorous (validated) models or plant data.

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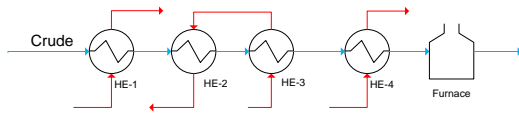
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