

# Heat Exchanger Network Cleaning Scheduling: From Optimal Control to Mixed-Integer Decision Making

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## Abstract

An approach for optimising the cleaning schedule in heat exchanger networks (HENs) subject to fouling is presented. This work focuses on HEN applications in crude oil preheat trains located in refineries. Previous approaches have focused on using mixed-integer nonlinear programming (MINLP) methods involving binary decision variables describing when and which unit to clean in a multi-period formulation. This work is based on the discovery that the HEN cleaning scheduling problem is in actuality a multistage optimal control problem (OCP), and further that cleaning actions are the controls which appear linearly in the system equations. The key feature is that these problems exhibit bang-bang behaviour, obviating the need for combinatorial optimisation methods. Several case studies are considered; ranging from a single unit up to 25 units. Results show that the feasible path approach adopted is stable and efficient in comparison to classical methods which sometimes suffer from failure in convergence.

*Keywords:* Optimal control problem; Bang-bang control; Fouling; Optimisation; Scheduling; Heat exchanger networks

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## 1. Introduction

Fouling of heat transfer surfaces is a long-established problem and has been described as “the major unresolved problem in heat transfer” (Taborek et al., 1972). It is one of the most significant issues affecting heat exchanger operation and thus has been depicted as “a nearly universal problem in heat exchanger equipment and design” (Watkinson, 1988). Heat exchanger fouling accounts for 0.25% of gross national product (GNP) in highly industrialised countries (Pugh et al., 2001).

This major industry-wide problem is caused by the deterioration in heat transfer resulting from fouling and leads to the loss of efficiency in heat exchangers which must be offset. This

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32 is achieved through process turndown, increased utility consumption with affiliated surge  
33 in greenhouse gas emissions until operation requirements such as temperature and pump-  
34 around targets are met, or in extreme cases plant shutdown. The reduction of production  
35 rates and increased energy consumption lead to economic losses which are more significant  
36 in larger networks of heat exchangers that require long continuous operational times between  
37 shutdowns, particularly crude distillation unit preheat trains (PHT) on oil refineries (Smaïli  
38 et al., 2001).

39 Based on 1995 figures, the costs associated specifically with crude oil fouling in PHT  
40 worldwide were estimated to be of the order of 4.5 billion USD (Pugh et al., 2001). Foul-  
41 ing mitigation techniques include addition of antifoulant chemicals, using more robust heat  
42 transfer equipment, and regular cleaning of fouled units. Cleaning of heat exchangers has  
43 a negative impact on operating costs due to the unit being taken offline, however with the  
44 development of optimisation strategies such as those proposed by Casado (1990), Smaïli et al.  
45 (1999),Georgiadis and Papageorgiou (2000), Lavaja and Bagajewicz (2004), Ishiyama et al.  
46 (2009b), Gonçalves et al. (2014), among others, these costs can be minimised resulting in  
47 overall gains due to improved heat transfer of the network over time.

48 The cleaning scheduling problem is a discrete decision making problem where a decision  
49 must be made as to whether cleaning should be performed, and which unit is to be cleaned.  
50 It consists of continuous as well as binary decision variables and hence it has combinatorial  
51 complexity that is handled traditionally by Branch and Bound (B&B) methods of one form  
52 or another. Due to its combinatorial nature and the existence of nonlinear models, mathem-  
53 atical programming (MP) techniques have been used to solve this mixed integer nonlinear  
54 programming (MINLP) problem based on time discretisation (Smaïli et al., 2001). Addi-  
55 tionally this problem has been solved by formulating certain models from a MINLP model  
56 to a mixed integer linear programming (MILP) model (Georgiadis and Papageorgiou, 2000).  
57 Stochastic optimisation frameworks using distinctive modifications of simulated annealing al-  
58 gorithms have been implemented (Smaïli et al., 2002a) as well as heuristic schemes composed

59 of a set of movements according to a greedy rationale (Gonçalves et al., 2014).

60 This problem has been addressed in the literature through extending the formulation  
61 of the general cleaning scheduling problem in a multitude of ways. Rodriguez and Smith  
62 (2007) combined the conventional cleaning scheduling problem with optimisation of operating  
63 conditions such as wall temperature and flow velocity in a comprehensive mitigation strategy  
64 while Ishiyama et al. (2010) considered the addition of the problem of controlling the desalter  
65 inlet temperature by using hot stream bypassing within a PHT fouling mitigation strategy  
66 based on heat exchanger cleaning.

67 Certain formulations include constraints set by pump-around operation (Smaïli et al.,  
68 2002a) and pressure drop (Smaïli et al., 2001), while both thermal and hydraulic impacts of  
69 fouling were considered by Ishiyama et al. (2009b) where variable throughput and control  
70 valve operation are implemented on the cleaning scheduling problem.

71 A cleaning operation will ideally remove all fouling deposits from a heat transfer surface.  
72 In practice the effectiveness of a cleaning operation depends on the nature of the deposit and  
73 the method of cleaning. Ishiyama et al. (2011) presented a framework for incorporating this  
74 complexity into the scheduling problem. The replacement of the single layer fouling model  
75 with a dual layer consisting of a soft exterior deposit (gel) and a harder interior layer (coke)  
76 was investigated by Pogiatzis et al. (2012). They considered the case where two cleaning  
77 methods were available: (a) cleaning-in-place methods and (b) off-line mechanical cleaning.  
78 An extra decision variable is added to the scheduling model, capturing the choice of cleaning  
79 method. The current paper addresses a single layer fouling model where the fouling kinetics  
80 exhibit linear and asymptotic behaviour.

81 Current solution methods for the cleaning scheduling problem still present limitations.  
82 Due to the complexity of networks and the nonlinearity in the models, MINLP approaches  
83 sometimes suffer from failure in convergence (Georgiadis and Papageorgiou, 2000; Smaïli  
84 et al., 2001) whereas MILP techniques may be computationally expensive (Lavaja and Baga-  
85 jewicz, 2004) and involve the introduction of approximations to models. For example, Geor-

giadis and Papageorgiou (2000) used the arithmetic temperature difference instead of the logarithmic mean temperature difference, which is not suitable for large networks that feature extensive feedback of hot (and/or cold) streams (Smaïli et al., 2001).

Stochastic optimisation methods may not be capable of handling problems involving many variables of similar effect (Fouskakis and Draper, 2002). Furthermore, these approaches can be very dependent on parameter tuning (Gonçalves et al., 2014). Solutions found by heuristic schemes such as greedy algorithms are not guaranteed to be optimal. For the scheduling problem, such simple strategies consider cleaning actions only in the current period and may be inefficient (Smaïli et al., 2001). Therefore, there is a need to develop robust, reliable and inexpensive methods to solve the scheduling cleaning problem.

In this paper we show for the first time that the heat exchanger network (HEN) cleaning scheduling problems are in actuality mixed-integer optimal control problems (MIOCPs) which exhibit a nearly bang-bang solution. This paper is arranged as follows: section 2 describes the formulation as a multi-period optimal control problem (OCP), including the proof of linearity of the control resulting in this bang-bang optimal solution behaviour. The formulation considered for the general HEN cleaning scheduling problem is presented in section 3. Implementation and solutions to a number of case studies for crude oil PHT obtained using a commercial optimisation software are presented in sections 4 and 5, including comparison of solutions to those produced through MP techniques.

## 2. HEN Scheduling Optimisation as Multi-period Optimal Control

This section will demonstrate that the HEN cleaning scheduling problem is in actuality a MIOCP. In this problem the controls, *i.e.* cleaning decisions occur linearly in the system, thus resulting in a bang-bang solution. Hence, integrality of the solution can be obtained by solving only the relaxed MIOCP as a standard nonlinear programming (NLP). Furthermore, proof of linearity in the control is shown in this section.

The basic formulation for an OCP is expressed in equations (1a) to (1d) where the per-

112 formance index is minimised by selection of controls  $u(t)$  subject to differential and algebraic  
 113 equations involving differential and algebraic state variables  $x(t)$  and  $y(t)$ , respectively. Equa-  
 114 tions (1b) to (1c) describe an index-1 differential algebraic equation (DAE) system given the  
 115 initial condition  $x_0$ , and a fixed final time  $t_F$ . It is noted that the problem considered involves  
 116 binary control variables,  $u(t)$ , thus constituting a MIOCP.

$$\min_{u(\cdot)} O = \phi[x(t_F)] + \int_0^{t_F} L[x(t), y(t), u(t), t] dt \quad (1a)$$

117 subject to

$$\dot{x}(t) = f[x(t), y(t), u(t), t], \quad x(t_0) = x_0, \quad (1b)$$

$$g(x(t), y(t), u(t), t) = 0, \quad (1c)$$

$$u(t) \in \mathcal{U}, \quad \mathcal{U} \in \{0,1\} \quad \forall t \in [0, t_F] \quad (1d)$$

118 The OCP solution is obtained through discretisation of time into periods, where the  
 119 control profiles are allowed to be discontinuous at a finite number of points,  $t_p$ , termed  
 120 junctions. Period lengths have not been specified. Vassiliadis (1993) gives a general form of  
 121 junction conditions between stages (*i.e.* periods)  $p$  and  $p + 1$ . This is shown in equation 2  
 122 for the sake of clarity.

$$J_p(\dot{x}_{p+1}(t_p^+), x_{p+1}(t_p^+), y_{p+1}(t_p^+), u_{p+1}(t_p^+), \dot{x}_p(t_p^-), x_p(t_p^-), y_p(t_p^-), u_p(t_p^-), t_p) = 0 \quad \forall p = 1, 2, \dots, NP-1 \quad (2)$$

123 The basic formulation of a multi-period OCP over time periods,  $p = 1, \dots, NP$ ,  $t \in$   
 124  $[t_{p-1}, t_p]$  with  $t_{NP} = t_F$  is shown in equations (3a) to (3g).

$$\min_{u^{(\cdot)}} O = \sum_{p=1}^{NP} [\phi^{(p)} x(t_p), y^{(p)}(t_p), u^{(p)}, t^{(p)}] + \int_{t_{p-1}}^{t_p} L^{(p)} [x^{(p)}(t), y^{(p)}(t), u^{(p)}, t] dt \quad (3a)$$

125 subject to

$$\dot{x}^{(p)}(t) = f^{(p)}(x^{(p)}(t), y^{(p)}(t), u^{(p)}, t) \quad (3b)$$

$$0 = g^{(p)}(x^{(p)}(t), y^{(p)}(t), u^{(p)}, t) \quad (3c)$$

$$t_{p-1} \leq t \leq t_p, \quad p = 1, 2, \dots, NP \quad (3d)$$

$$x^{(1)}(t_0) = I^{(1)}(u^{(1)}) \quad (3e)$$

$$x^{(p)}(t_{p-1}) = I^{(p)}(x^{(p-1)}(t_{p-1}), y^{(p-1)}(t_{p-1}), u^{(p)}) \quad \forall p = 2, 3, \dots, NP \quad (3f)$$

$$u(t) \in \mathcal{U}, \quad \mathcal{U} \in \{0,1\} \quad (3g)$$

126 For the HEN cleaning problem the controls  $u^{(p)}t$  are considered to be piecewise constant  
 127 so as to reflect the on/off nature of having a unit cleaning or not. The stage switching times  
 128  $t_p$  are fixed in this initial derivation. The collective vector of controls over all stages is:

$$\mathbf{u} = ((u^{(1)})^T, (u^{(2)})^T, \dots, (u^{(NP)})^T)^T \quad (4)$$

129 At the junctions, conditions are set where differential state variables are allowed to be  
 130 reinitialised based on the control variable value:

$$x^p(t_{p-1}) = u^p(t) \cdot x^{p-1}(t_{p-1}) \quad \forall p = 2, \dots, NP \quad (5)$$

131 Proof that the control in the relaxed multistage MIOCP for cleaning scheduling is linearly  
 132 related to the process variables is provided as follows:

133 This multistage adjoint system is a linear time-varying coefficient semi-explicit index-1  
 134 DAE system. The performance index in equation (3a) is modified such that the Euler-  
 135 Lagrange multipliers are introduced:

$$\begin{aligned} \bar{O} = & \sum_{p=2}^{NP} \left\{ \right. \\ & \phi^{(p)}(x^{(p)}(t_p), y^{(p)}(t_p), u^{(p)}, t^{(p)}) \\ & + (\lambda^{(p)}(t_{p-1}))^T \cdot (I^{(p)}(x^{(p-1)}(t_{p-1}), y^{(p-1)}(t_{p-1}), u^{(p)}) - x^{(p)}(t_{p-1})) \\ & + \int_{t_{p-1}}^{t_p} L^{(p)}(x^{(p)}(t), y^{(p)}(t), u^{(p)}, t) dt \\ & + \int_{t_{p-1}}^{t_p} (\lambda^{(p)}(t))^T \cdot (f^{(p)}(x^{(p)}(t), y^{(p)}(t), u^{(p)}, t) - \dot{x}^{(p)}(t)) dt \\ & + \int_{t_{p-1}}^{t_p} (\mu^{(p)}(t))^T \cdot (g^{(p)}(x^{(p)}(t), y^{(p)}(t), u^{(p)}, t)) dt \\ & \left. \right\} \\ & + \phi^{(1)}(x^{(1)}(t_1), y^{(1)}(t_1), u^{(1)}, t^{(1)}) \\ & + (\lambda^{(1)}(t_0))^T \cdot (I^{(1)}(u^{(1)}) - x^{(1)}(t_0)) \\ & + \int_{t_0}^{t_1} L^{(1)}(x^{(1)}(t), y^{(1)}(t), u^{(1)}, t) dt \\ & + \int_{t_0}^{t_1} (\lambda^{(1)}(t))^T \cdot (f^{(1)}(x^{(1)}(t), y^{(1)}(t), u^{(1)}, t) - \dot{x}^{(1)}(t)) dt \\ & + \int_{t_0}^{t_1} (\mu^{(1)}(t))^T \cdot (g^{(1)}(x^{(1)}(t), y^{(1)}(t), u^{(1)}, t)) dt \end{aligned} \quad (6)$$

136 Variations on the parameter set of stage  $p'$ , of the form  $\delta u^{(p')}$  are considered, which result  
 137 in variations in the state values at all times as shown in equation (7). Clearly, the state vector

138 of stage  $p$ , where  $p < p'$ , will not be influenced. This results in  $\delta x^{(p)}(t) \triangleq 0$  and  $\delta y^{(p)}(t) \triangleq 0$ .

$$\begin{aligned}
\delta \bar{O} = & \sum_{p=2}^{NP} \left\{ \right. \\
& \left[ \frac{\partial \phi^{(p)}}{\partial x^{(p)}(t_p)} \delta x^{(p)}(t_p) + \frac{\partial \phi^{(p)}}{\partial y^{(p)}(t_p)} \delta y^{(p)}(t_p) + \frac{\partial \phi^{(p)}}{\partial u^{(k)}} \delta u^{(p)} \right] \\
& + (\lambda^{(p)}(t_{p-1}))^T \cdot \\
& \left( \frac{\partial I^{(p)}}{\partial x^{(p-1)}(t_{p-1})} \delta x^{(p-1)}(t_{p-1}) + \frac{\partial I^{(p)}}{\partial y^{(p-1)}(t_{p-1})} \delta y^{(p-1)}(t_{p-1}) + \frac{\partial I^{(p)}}{\partial u^{(p)}} \delta u^{(p)} - \delta x^{(p)}(t_{p-1}) \right) \\
& + \int_{t_{p-1}}^{t_p} \frac{\partial L^{(p)}}{\partial x^{(p)}(t)} \delta x^{(p)}(t) + \frac{\partial L^{(p)}}{\partial y^{(p)}(t)} \delta y^{(p)}(t) + \frac{\partial L^{(p)}}{\partial u^{(p)}} \delta u^{(p)} dt \\
& + \int_{t_{p-1}}^{t_p} (\lambda^{(p)}(t))^T \cdot \left( \frac{\partial f^{(p)}}{\partial x^{(p)}(t)} \delta x^{(p)}(t) + \frac{\partial f^{(p)}}{\partial y^{(p)}(t)} \delta y^{(p)}(t) + \frac{\partial f^{(p)}}{\partial u^{(p)}} \delta u^{(p)} - \delta \dot{x}^{(p)}(t) \right) dt \\
& + \int_{t_{p-1}}^{t_p} (\mu^{(p)}(t))^T \cdot \left( \frac{\partial g^{(p)}}{\partial x^{(p)}(t)} \delta x^{(p)}(t) + \frac{\partial g^{(p)}}{\partial y^{(p)}(t)} \delta y^{(p)}(t) + \frac{\partial g^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right) dt \\
& \left. \right\} \\
& + \left[ \frac{\partial \phi^{(1)}}{\partial x^{(1)}(t_1)} \delta x^{(1)}(t_1) + \frac{\partial \phi^{(1)}}{\partial y^{(1)}(t_1)} \delta y^{(1)}(t_1) + \frac{\partial \phi^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right] \\
& + (\lambda^{(1)}(t_0))^T \cdot \left( \frac{\partial I^{(1)}}{\partial u^{(1)}} \delta u^{(1)} - \delta x^{(1)}(t_0) \right) \\
& + \int_{t_0}^{t_1} \frac{\partial L^{(1)}}{\partial x^{(1)}(t)} \delta x^{(1)}(t) + \frac{\partial L^{(1)}}{\partial y^{(1)}(t)} \delta y^{(1)}(t) + \frac{\partial L^{(1)}}{\partial u^{(1)}} \delta u^{(1)} dt \\
& + \int_{t_0}^{t_1} (\lambda^{(1)}(t))^T \cdot \left( \frac{\partial f^{(1)}}{\partial x^{(1)}(t)} \delta x^{(1)}(t) + \frac{\partial f^{(1)}}{\partial y^{(1)}(t)} \delta y^{(1)}(t) + \frac{\partial f^{(1)}}{\partial u^{(1)}} \delta u^{(1)} - \delta \dot{x}^{(1)}(t) \right) dt \\
& + \int_{t_0}^{t_1} (\mu^{(1)}(t))^T \cdot \left( \frac{\partial g^{(1)}}{\partial x^{(1)}(t)} \delta x^{(1)}(t) + \frac{\partial g^{(1)}}{\partial y^{(1)}(t)} \delta y^{(1)}(t) + \frac{\partial g^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right) dt \tag{7}
\end{aligned}$$

139 Integration by parts for the last term in the integrals involving  $\delta \dot{x}^{(p)}$  is used to obtain  
140 equation (8):



$$\begin{aligned}
\delta\bar{O} = & \sum_{p=2}^{NP} \left\{ \right. \\
& \left[ \frac{\partial\phi^{(p)}}{\partial x^{(p)}(t_p)} \delta x^{(p)}(t_p) + \frac{\partial\phi^{(p)}}{\partial y^{(p)}(t_p)} \delta y^{(p)}(t_k) + \frac{\partial\phi^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right] \\
& + (\lambda^{(p)}(t_{p-1}))^T \cdot \\
& \left( \frac{\partial I^{(p)}}{\partial x^{(p-1)}(t_{p-1})} \delta x^{(p-1)}(t_{p-1}) + \frac{\partial I^{(p)}}{\partial y^{(p-1)}(t_{p-1})} \delta y^{(p-1)}(t_{p-1}) + \frac{\partial I^{(p)}}{\partial u^{(p)}} \delta u^{(p)} - \delta x^{(p)}(t_{p-1}) \right) \\
& + \int_{t_{p-1}}^{t_p} \frac{\partial L^{(p)}}{\partial x^{(p)}(t)} \delta x^{(p)}(t) + \frac{\partial L^{(p)}}{\partial y^{(p)}(t)} \delta y^{(p)}(t) + \frac{\partial L^{(p)}}{\partial u^{(p)}} \delta u^{(p)} dt \\
& + \int_{t_{p-1}}^{t_p} (\lambda^{(p)}(t))^T \cdot \left( \frac{\partial f^{(p)}}{\partial x^{(p)}(t)} \delta x^{(p)}(t) + \frac{\partial f^{(p)}}{\partial y^{(p)}(t)} \delta y^{(p)}(t) + \frac{\partial f^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right) dt \\
& + \int_{t_{p-1}}^{t_p} (\dot{\lambda}^{(p)}(t))^T \delta x^{(p)}(t) dt \\
& + (\lambda^{(p)}(t_{p-1}))^T \cdot \delta x^{(p)}(t_{p-1}) - (\lambda^{(p)}(t_p))^T \cdot \delta x^{(p)}(t_p) \\
& + \int_{t_{p-1}}^{t_p} (\mu^{(p)}(t))^T \cdot \left( \frac{\partial g^{(p)}}{\partial x^{(p)}(t)} \delta x^{(p)}(t) + \frac{\partial g^{(p)}}{\partial y^{(p)}(t)} \delta y^{(p)}(t) + \frac{\partial g^{(p)}}{\partial u^{(p)}} \delta u^{(p)} \right) dt \\
& \left. \right\} \\
& + \left[ \frac{\partial\phi^{(1)}}{\partial x^{(1)}(t_1)} \delta x^{(1)}(t_1) + \frac{\partial\phi^{(1)}}{\partial y^{(1)}(t_1)} \delta y^{(1)}(t_1) + \frac{\partial\phi^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right] \\
& + (\lambda^{(1)}(t_0))^T \cdot \left( \frac{\partial I^{(1)}}{\partial u^{(1)}} \delta u^{(1)} - \delta x^{(1)}(t_0) \right) \\
& + \int_{t_0}^{t_1} \frac{\partial L^{(1)}}{\partial x^{(1)}(t)} \delta x^{(1)}(t) + \frac{\partial L^{(1)}}{\partial y^{(1)}(t)} \delta y^{(1)}(t) + \frac{\partial L^{(1)}}{\partial u^{(1)}} \delta u^{(1)} dt \\
& + \int_{t_0}^{t_1} (\lambda^{(1)}(t))^T \cdot \left( \frac{\partial f^{(1)}}{\partial x^{(1)}(t)} \delta x^{(1)}(t) + \frac{\partial f^{(1)}}{\partial y^{(1)}(t)} \delta y^{(1)}(t) + \frac{\partial f^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right) dt \\
& + \int_{t_0}^{t_1} (\dot{\lambda}^{(1)}(t))^T \delta x^{(1)}(t) dt \\
& + (\lambda^{(1)}(t_0))^T \cdot \delta x^{(1)}(t_0) - (\lambda^{(1)}(t_1))^T \cdot \delta x^{(1)}(t_1) \\
& + \int_{t_0}^{t_1} (\mu^{(1)}(t))^T \cdot \left( \frac{\partial g^{(1)}}{\partial x^{(1)}(t)} \delta x^{(1)}(t) + \frac{\partial g^{(1)}}{\partial y^{(1)}(t)} \delta y^{(1)}(t) + \frac{\partial g^{(1)}}{\partial u^{(1)}} \delta u^{(1)} \right) dt \tag{8}
\end{aligned}$$

141 For a stationary point, infinitesimal variations in the right hand side should yield no  
142 change to the performance index, *i.e.*  $\delta\bar{O} = 0$ , and hence related terms must be chosen so

143 that they always guarantee this. This leads to the following set of Euler-Lagrange equations  
 144 and the Pontryagin et al. (1962) maximum (minimum) principle.  
 145 To cancel the  $\delta x^{(1)}(t)$  and  $\delta x^{(1)}(t_1)$  terms, the differential equations and final time stage  
 146 conditions as shown in equations (9a) to (10) must hold, respectively:

$$\dot{\lambda}^{(1)}(t) = - \left[ \frac{\partial f^{(1)}}{\partial x^{(1)}(t)} \right]^T \lambda^{(1)}(t) - \left[ \frac{\partial g^{(1)}}{\partial x^{(1)}(t)} \right]^T \mu^{(1)}(t) - \left[ \frac{\partial L^{(1)}}{\partial x^{(1)}(t)} \right]^T \quad (9a)$$

$$t_0 \leq t \leq t_1 \quad (9b)$$

$$\lambda^{(1)}(t_1) = \left[ \frac{\partial \phi^{(1)}}{\partial x^{(1)}(t_1)} \right]^T \quad (10)$$

147 Algebraic equations and final stage conditions (11a) to (11b) must hold in order to cancel  
 148 the  $\delta y^{(1)}(t)$  and  $\delta y^{(1)}(t_1)$  terms;

$$\left[ \frac{\partial f^{(1)}}{\partial y^{(1)}(t)} \right]^T \lambda^{(1)}(t) + \left[ \frac{\partial g^{(1)}}{\partial y^{(1)}(t)} \right]^T \mu^{(1)}(t) + \left[ \frac{\partial L^{(1)}}{\partial y^{(1)}(t)} \right]^T = 0 \quad (11a)$$

$$t_0 \leq t \leq t_1 \quad (11b)$$

$$\left[ \frac{\partial \phi^{(1)}}{\partial y^{(1)}(t_1)} \right]^T + \left[ \frac{\partial I^{(2)}}{\partial y^{(1)}(t_1)} \right]^T \cdot \lambda^{(2)}(t_1) = 0 \quad (12)$$

149 The  $\delta x^{(p)}(t)$  and  $\delta x^{(p)}(t_p)$  terms are cancelled through the condition that the following dif-  
 150 ferential equations and final time stage conditions are held;

$$\dot{\lambda}^{(p)}(t) = - \left[ \frac{\partial f^{(p)}}{\partial x^{(p)}(t)} \right]^T \lambda^{(p)}(t) - \left[ \frac{\partial L^{(p)}}{\partial x^{(p)}(t)} \right]^T \quad (13a)$$

$$t_{p-1} \leq t \leq t_p \quad \forall p = 2, 3, \dots NP \quad (13b)$$

$$\lambda^{(p)}(t_p) = \left[ \frac{\partial \phi^{(p)}}{\partial x^{(p)}(t_p)} \right]^T + \left[ \frac{\partial I^{(p+1)}}{\partial x^{(p)}(t_p)} \right]^T \cdot \lambda^{(p+1)}(t_p) \quad \forall p = 2, 3, \dots, NP - 1$$

152 To cancel  $\delta y^{(p)}(t)$  and  $\delta y^{(p)}(t_p)$  terms, the following algebraic equations must hold:

$$\left[ \frac{\partial f^{(p)}}{\partial y^{(p)}(t)} \right]^T \lambda^{(p)}(t) + \left[ \frac{\partial g^{(p)}}{\partial y^{(p)}(t)} \right]^T \mu^{(p)}(t) + \left[ \frac{\partial L^{(p)}}{\partial y^{(p)}(t)} \right]^T = 0$$

$$t_{p-1} \leq t \leq t_p \quad \forall p = 2, 3, \dots, NP$$

$$\left[ \frac{\partial \phi^{(p)}}{\partial y^{(p)}(t_p)} \right]^T + \left[ \frac{\partial I^{(p+1)}}{\partial y^{(p)}(t_p)} \right]^T \cdot \lambda^{(p+1)}(t_p) = 0 \quad \forall p = 2, 3, \dots, NP - 1$$

153 The terms  $\delta u^{(1)}$  and  $\delta u^{(p)}$  are cancelled on the condition that equations (15a) to (16b) hold.

154 These are equivalent to the Hamiltonian gradient condition:

$$\left[ \frac{\partial \phi^{(1)}}{\partial u^{(1)}}(t_1) \right]^T + \left[ \frac{\partial I^{(1)}}{\partial u^{(1)}} \right]^T \cdot \lambda^{(1)}(t_0) \tag{15a}$$

$$+ \int_{t_0}^{t_1} \left\{ \left[ \frac{\partial L^{(1)}}{\partial u^{(1)}}(t) \right]^T + \left[ \frac{\partial f^{(1)}}{\partial u^{(1)}}(t) \right]^T \cdot \lambda^{(1)}(t) + \left[ \frac{\partial g^{(1)}}{\partial u^{(1)}}(t) \right]^T \cdot \mu^{(1)}(t) \right\} dt = 0$$

$$t_0 \leq t \leq t_1 \tag{15b}$$

$$\left[ \frac{\partial \phi^{(p)}}{\partial u^{(p)}}(t_p) \right]^T + \left[ \frac{\partial I^{(p)}}{\partial u^{(p)}} \right]^T \cdot \lambda^{(p)}(t_{p-1}) \tag{16a}$$

$$+ \int_{t_{p-1}}^{t_p} \left\{ \left[ \frac{\partial L^{(p)}}{\partial u^{(p)}}(t) \right]^T + \left[ \frac{\partial f^{(p)}}{\partial u^{(p)}}(t) \right]^T \cdot \lambda^{(p)}(t) + \left[ \frac{\partial g^{(p)}}{\partial u^{(p)}}(t) \right]^T \cdot \mu^{(p)}(t) \right\} dt = 0$$

$$t_{p-1} \leq t \leq t_p \quad \forall p = 2, 3, \dots NP \quad (16b)$$

155 When the functions appearing in equations (15a) and (16a) are linearly related to the  
 156 control, the optimal control for the relaxed MIOCP will exhibit bang-bang behaviour (with  
 157 potential singular arcs). Bang-bang solutions occur when the optimal control action is at  
 158 either bound of the feasible region (Bryson and Ho, 1975). Controls that are not bang-  
 159 bang, where the control lies between the bounds, are called singular. In this case, singular  
 160 arcs exist. Pure bang-bang controls are demonstrated in minimum-time problems for linear  
 161 systems (Bellman et al., 1956) and bilinear systems (Mohler, 1973), optimal control of batch  
 162 reactors (Blakemore and Aris, 1962), optimal thermal control (Belghith et al., 1986), *etc.*  
 163 For nonlinear optimisation systems, this bang-bang principle does not always hold. Zandvliet  
 164 et al. (2007) investigated reservoir flooding problems, where the control is linear in relation  
 165 to the continuous variables, and showed that if the only constraints are upper and lower  
 166 bounds on the control, then due to their particular structure, these problems will sometimes  
 167 have bang-bang optimal solutions. This is advantageous since bang-bang solutions can be  
 168 implemented with simple on-off control valves.

169 Approaches for optimal control of nonlinear dynamical systems with binary controls (on/off)  
 170 were reviewed by Sager (2009). To satisfy requirements for bang-bang behaviour, the general  
 171 OCP is reformulated such that the binary controls are presented linearly in the system  
 172 dynamics. Solutions in this case may require use of heuristics *e.g.* rounding up or a sum  
 173 up rounding strategy, or algorithms such as Branch and Bound when singular arcs appear  
 174 (Sager, 2009).

175 For the scheduling cleaning problem, reformulation is not necessary as the controls involved  
 176 already have linear presentation in the system. More importantly, the formulation of this  
 177 problem as an OCP facilitates the solution of the relaxed nonlinear programming (NLP)  
 178 problem through the feasible path approach, obviating the need to discretise the system  
 179 equations. This otherwise leads to a very large scale optimisation problem with a strongly

180 nonlinear system of equality constraints. This approach avoids failures of convergence pro-  
181 duced by direct solutions of MINLPs resulting from discretisation, such as in previous work  
182 of Georgiadis and Papageorgiou (2000) and of Smaïli et al. (2001).

### 183 3. HEN Scheduling Optimisation Formulation

184 The effect of fouling on heat transfer performance is often quantified in lumped parameter  
185 models of process heat transfer via the fouling resistance,  $R_f$ .

$$\frac{1}{U} = \frac{1}{U_c} + R_f \quad (17)$$

187 Equation (17) expresses the overall heat transfer coefficient  $U$  in relation to the fouling  
188 resistance and  $U_c$ , its value when clean.

189 The impact of fouling resistance is more severe for heat exchangers with a high overall  
190 heat transfer coefficient. Both linear (equation (18)) and exponentially asymptotic fouling  
191 behaviour (equation (19)) are considered in this paper , which are quantified via

$$\dot{R}_f = a \quad (18)$$

$$R_f = R_f^\infty (1 - \exp(-t'/\tau)) \quad (19)$$

192 where  $a$  is the linear fouling constant for a particular heat exchanger,  $R_f^\infty$  is the asymptotic  
193 fouling resistance,  $\tau$  is the decay constant, and  $t'$  is the operating time elapsed since the last  
194 cleaning action.

195 The heat duty of a single-pass shell and tube heat exchanger operating in counter-current  
196 mode is given by equation (20), which is based on the log-mean temperature difference  
197 method.

$$Q = UA\Delta T_{lm} \quad (20)$$

199 Here  $A$  is the area and  $\Delta T_{lm}$  is the logarithmic mean temperature difference.

200 The heat duty,  $Q$ , is also linearly related to the stream inlet and outlet temperatures through  
 201 the energy balances outlined in equations (21) and (22):

$$Q = F_c C_c (T_c^{\text{out}} - T_c^{\text{in}}) \quad (21)$$

203

$$Q = F_h C_h (T_h^{\text{in}} - T_h^{\text{out}}) \quad (22)$$

204 where  $F_h$  and  $F_c$  are the mass flow-rates of the hot and cold streams respectively, and  $C_h$   
 205 and  $C_c$  are their specific heat capacities.

206 The cleaning scheduling problem is a multi-period OCP where a decision must be made  
 207 regarding when, *i.e.* in which period(s), cleaning should occur, and which unit is to be  
 208 cleaned. The control action is discretised into time periods of equal length, where each  
 209 period is discretised further into a cleaning and operating sub-period. This is represented by  
 210 binary variable  $y_{np}$  which is used to describe the cleaning status of each exchanger in each  
 211 cleaning sub-period, where

$$y_{np} = \left\{ \begin{array}{ll} 0 & \text{if the } n\text{th heat exchanger is cleaned in period } p \\ 1 & \text{otherwise} \end{array} \right\} \forall n, p \quad (23)$$

212 Within an operating sub-period, this binary variable is fixed to 1 for all  $n$  *i.e.* all units are  
 213 online. The objective is to minimise the operating and cleaning costs due to fouling over  
 214 a specified horizon of time  $t_F$ . The objective function is given by equation (24). The form  
 215 of this objective function is generally common to all approaches. Local considerations may  
 216 give slightly different mathematical expressions. However, the differences lie in the solution  
 217 approach.

$$Obj = \int_0^{t_F} \frac{C_E Q_F(t)}{\eta_f} dt + \sum_{p=1}^{NP} \sum_{n=1}^{NE} C_c (1 - y_{np}) \quad (24)$$

219 The extra furnace energy consumption is described by the term  $Q_F(t)$  which is determined  
 220 based on the temperature of the crude oil entering the furnace, *i.e.* the crude inlet temper-  
 221 ature (CIT).  $C_E$  represents the cost of fuel,  $\eta_f$  is the furnace efficiency,  $NE$  is the number

222 of exchangers considered for cleaning,  $NP$  is the number of periods, and  $C_c$  is the cost per  
 223 cleaning action. For the purpose of attaining results that can be compared to published ones  
 224 from case studies in the open literature,  $C_c$  is taken to be independent of the exchanger size  
 225 and duty. In industrial practice this is not the case, as larger exchangers take more effort to  
 226 clean and will thus have a higher value of  $C_c$  and vice versa. The amount of time taken to  
 227 clean depends on the installation: if the exchanger must be isolated, removed and relocated  
 228 for cleaning, these operations can determine the cleaning time. Furthermore, different clean-  
 229 ing methods will have different durations, but this is not considered in this work. Through  
 230 incorporation of binary variable  $y_{np}$ , equations (18) and (19) can be rewritten as:

$$\dot{R}_f = y_{np}a \quad \forall n, p \quad (25)$$

$$R_f = R_f^\infty (1 - \exp(-t'/\tau)) \quad (26a)$$

$$\dot{t}' = y_{np} \quad \forall n, p \quad (26b)$$

231 The HEN optimisation is started from a clean condition, *i.e.* the initial fouling resistance  
 232 is 0 for the first period for all heat exchangers. In consecutive periods, the initial fouling  
 233 resistance is related to the fouling resistance at the end of the previous period by integration  
 234 in time and this value is allowed to be reset through a junction condition when cleaning  
 235 OCCURS.

236 The number of transfer units (NTU) effectiveness method is used to assess the performance  
 237 of each heat exchanger. This is achieved by rearranging equation (20) in terms of a rating  
 238 calculation. The units are modelled as simple countercurrent exchangers. The effectiveness  
 239 term denoted by  $\alpha$  and the ratio of capacity flow-rates  $P$  defined by equations (27) and (28)  
 240 are reproduced from Smaïli et al. (2001) :

$$\alpha = \frac{UA}{F_h C_h} \quad (27)$$

$$P = \frac{F_h C_h}{F_c C_c} \quad (28)$$

242 Through combination and rearrangement of equations (20), (21) and (22) the temperature  
 243 of the hot and cold streams leaving each exchanger can be calculated. The temperatures of  
 244 the cold and hot streams leaving an exchanger are determined by:

$$T_c^{\text{out}} = T_c^{\text{in}} + P (T_h^{\text{in}} - T_h^{\text{out}}) \quad (29)$$

246

$$T_h^{\text{out}} = y_{np} \left[ \frac{(1 - P)T_h^{\text{in}} \exp(-\alpha(1 - P)) + T_c^{\text{in}}(1 - \exp(-\alpha(1 - P)))}{1 - P \exp(-\alpha(1 - P))} \right] \quad (30)$$

$$+ (1 - y_{np})T_h^{\text{in}} \quad \forall n, p$$

247 The above equations are applicable to most preheat configurations which feature  $P < 1$ . If  
 248 the alternative case arises, these equations must be amended.

#### 249 4. Implementation

250 The implementation is performed in MATLAB<sup>®</sup> R2016b with its Optimisation Toolbox<sup>™</sup>  
 251 and Parallel Computing Toolbox<sup>™</sup> (The MathWorks Inc., 2016). It is noteworthy that this  
 252 methodology cannot be implemented in current commercial simulators directly. For example,  
 253 gPROMS<sup>™</sup> (Process Systems Enterprise, 2017), which is one of the most advanced commer-  
 254 cial simulators, does not facilitate multi-period optimal control problem solutions as it does  
 255 not allow for junction conditions.

256 The MATLAB<sup>®</sup> code works as a standard multi-period optimal control problem solver  
 257 using the feasible path approach (*i.e.* sequential approach) by linking together the Ordinary  
 258 Differential Equation (ODE) solver ode15s with the optimiser fmincon. The default set-  
 259 tings for ode15s are used, with absolute tolerance of  $10^{-6}$  and relative tolerance of  $10^{-3}$ . The  
 260 optimiser fmincon is used with the Sequential Quadratic Programming (SQP) algorithm op-  
 261 tion whilst keeping the remaining settings at their default values: constraint, optimality and  
 262 step tolerances of  $10^{-6}$  using a forward finite difference scheme for the estimation of gradi-



263 ents. Gradient evaluations conducted via finite differences are costly and require repeated  
264 simulations of the dynamic process model.

265 Additionally, since this problem is non-convex, multiple runs with different starting points  
266 are performed and the best solution is reported. A test was run using the Parallel Computing  
267 Toolbox<sup>TM</sup> to compare the computational time between parallelisation of the gradient evalu-  
268 ations versus parallelising a loop of multiple starting points. On a 4GHz Intel Core i7, 16 GB  
269 RAM iMac running on macOS Sierra the latter was faster than the former. Parallelisation  
270 of a loop of 50 runs is performed using a parfor loop. For cases where singularities appear in  
271 the control, a rounding up scheme is employed.

## 272 5. Case Studies

273 Computation experiments for the scheduling of cleaning actions for HENs located in  
274 crude oil distillation unit PHTs undergoing fouling are considered here. We present case  
275 studies appearing in the work of Lavaja and Bagajewicz (2004): a single heat exchanger  
276 unit; 4 units in series, a network of 10 units; and the more complex network of 25 units  
277 presented by Smaïli et al. (2002a). These are shown in figures 1 to 3. Stream data for each  
278 model are presented in tables 1 to 3 and 5. For the 10 unit HEN case study presented in  
279 the Lavaja and Bagajewicz (2004) formulation and the 25 unit HEN case study presented  
280 in the Smaïli et al. (2002a) formulation, the selection and operational constraints imposed  
281 through consideration of performance targets or acceptable operating practice are shown in  
282 tables 4 and 6, respectively. These constraints are based only on exchanger cleaning actions.  
283 However, in practice temperature bounds on the performance of exchangers are required to  
284 be applied, for example in the case of desalter temperature control considered by Ishiyama  
285 et al. (2010). For the purpose of achieving results that can be compared to published ones  
286 from case studies in the open literature, only the constraints shown in tables 4 and 6 are  
287 imposed on the corresponding case studies.

288 The number of periods considered is  $NP = 24$  for the single unit and  $NP = 18$  for the

289 10 unit HEN case studies while this is  $NP = \{12, 18\}$  for the 4 unit heat exchanger case  
290 study. A longer duration is considered for the 25 unit HEN, with  $NP = 36$ . Both linear and  
291 asymptotic fouling models are considered in the single unit and 10 unit HEN cases whilst  
292 only linear fouling is modelled in the 4 units and 25 unit HEN case studies. This is done for  
293 comparison purposes.

294 The extra energy cost required due to fouling  $C_E$  in the objective function displayed in  
295 equation (24) is £0.34/kW day for the 25 unit HEN case. There is no mention of the furnace  
296 fuel cost in the work of Lavaja and Bagajewicz, so a cost of £2.93/MM Btu is used here based  
297 on the value reported by Smaïli et al. (2002b). The work of Smaïli et al. is the source of  
298 data for Lavaja and Bagajewicz’s models where they compared the solutions from their MILP  
299 approach with those obtained by Smaïli et al. using the OA/ER algorithm. Although Lavaja  
300 and Bagajewicz stated that they accounted for the decay in the heat transfer coefficient in  
301 each sub-period, expressed by  $\eta_c$ , there is no mention of the value of this parameter in their  
302 work. Hence, we considered the value of parameter  $\eta_c$  to be 1 in our model. This decay  
303 parameter is also fixed at the value of 1 in the 25 unit HEN case study along with the  
304 furnace efficiency  $\eta_f$ . Smaïli et al. (2002b) did not consider these parameters in their model.  
305 The cleaning cost incurred for cleaning operations,  $C_c$ , is £5000 per cleaning action in the 25  
306 unit HEN case and £4000 for all other cases. For the former case, the duration of the cleaning  
307 and operating sub-periods are equal with  $\Delta t^{cl} = \Delta t^{op} = 15$  days. If the cleaning time did  
308 depend on the size of the exchanger, these durations would have to be unit dependent.

309 The scheduling problem was reformulated into a MILP problem by Lavaja and Bagajewicz  
310 (2004) whereas Smaïli et al. (2002a) solved the MINLP problem directly using two methods:  
311 a Backtracking Threshold Accepting (BTA) algorithm and the Outer Approximation (OA)  
312 method.

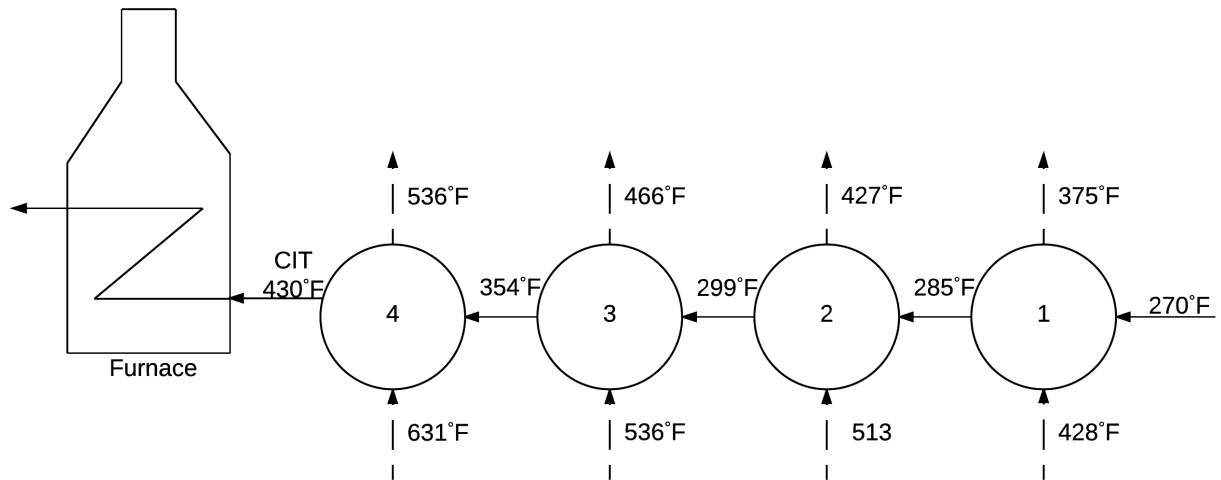


Figure 1: Four heat exchanger case. Temperature values are given for initial, clean condition. Adapted from Lavaja and Bagajewicz, 2004.

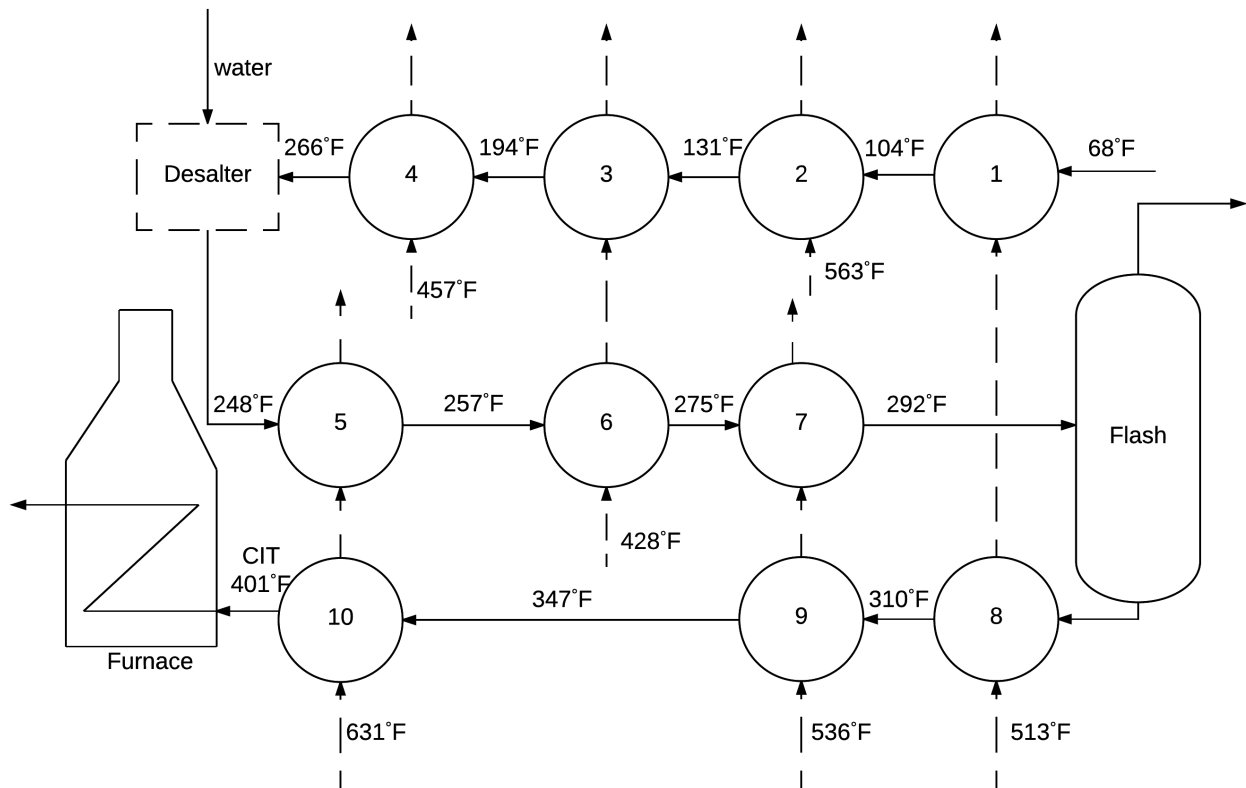


Figure 2: 10 unit HEN case. Temperature values are given for initial, clean condition. Adapted from Lavaja and Bagajewicz, 2004.

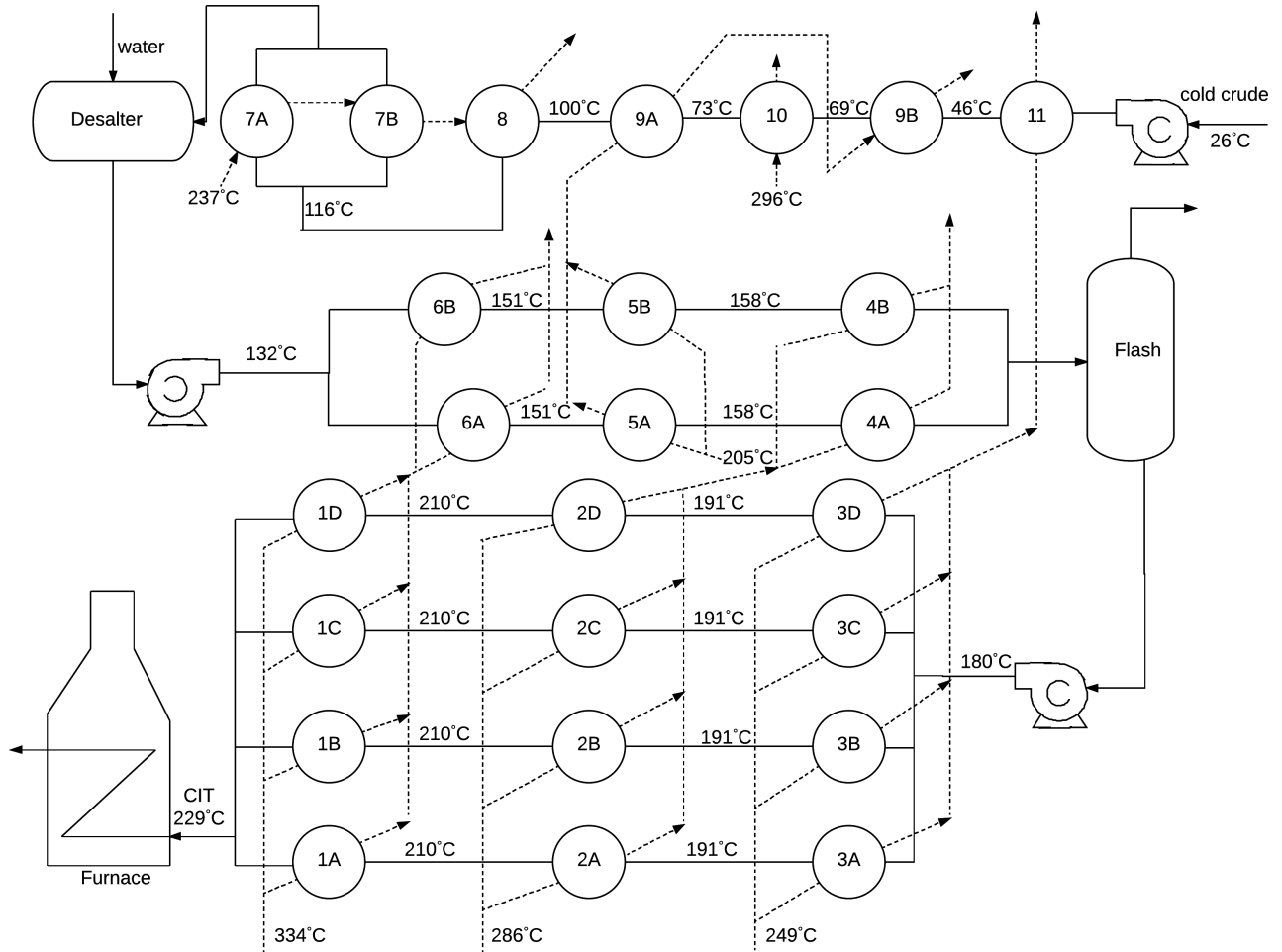


Figure 3: 25 unit HEN case. Solid lines, cold (crude) streams; dashed lines, hot streams; CIT, crude inlet temperature to furnace. Temperature values are given for initial, clean condition. Adapted from Smaïli et al., 2002a.

313 The cleaning schedules featuring the best objective, *i.e.* lowest overall cost, are reported  
 314 for each case. The optimal cleaning schedules are presented in tables 11 to 16 alongside  
 315 those obtained by Lavaja and Bagajewicz (2004) and Smaïli et al. (2002a). In the economic  
 316 comparison, we placed the cleaning schedules obtained by Lavaja and Bagajewicz (2004) and  
 317 Smaïli et al. (2002a) into our model to evaluate the cost. Tables 7 to 10 show the economic  
 318 comparison.

319 Fouling rates directly impact the performance of heat exchangers. The asymptotic fouling  
 320 cases have larger initial fouling rates, causing a rapid decay in the hot stream temperatures  
 321 through the network, resulting in a much larger objective value for the uncleaned case (*e.g.*

Table 1: Data for single heat exchanger case. Adapted from Lavaja and Bagajewicz, 2004.

Parameter	Value
$F_h$ [lb/h]	208000
$F_c$ [lb/h]	649000
$C_h$ [Btu/lb°F]	0.67
$C_c$ [Btu/lb°F]	0.57
$U_c$ [Btu/hft <sup>2</sup> °F]	88.1
$U_0$ [Btu/hft <sup>2</sup> °F]	88.1
$A$ [ft <sup>2</sup> ]	1257
$a$ (linear fouling) [ft <sup>2</sup> °F/Btu]	$3.88 \times 10^{-7}$
$R_f^\infty$ (asymptotic fouling) [hft <sup>2</sup> °F/Btu]	$6.73 \times 10^{-3}$
$\tau$ (decay constant) [month]	4
$\Delta t^{cl}$ [month]	0.20
$\Delta t^{op}$ [month]	0.80
$\eta_f$	0.75

322 £317k vs. £203k for the single unit case shown in table 7). Consequently, one would expect  
 323 more cleaning actions in all the asymptotic fouling model cases than the corresponding linear  
 324 ones due to the early loss of exchanger efficiencies. This is evident in table 11 with the cleaning  
 325 actions increasing from 3 to 5 in both this work’s solution and the solution of Lavaja and  
 326 Bagajewicz (2004). Similar observations to Lavaja and Bagajewicz (2004) are seen in the  
 327 single unit case, where cleaning actions are cyclic (table 11). For linear fouling, the number  
 328 of cleaning actions as well as the schedules are very similar: however the cleanings in our  
 329 model are performed 1 month earlier than in Lavaja and Bagajewicz ’s schedule.

330 For the four heat exchanger case, the number of cleaning actions are the same as Lavaja  
 331 and Bagajewicz ’s model and the schedule for the 12 month operating horizon is the same,  
 332 meanwhile the schedule for the 18 month duration differs. No pattern is evident when the  
 333 schedules are compared, with some cleaning actions occurring earlier in some cases and later  
 334 in others.

335 In the majority of our cases our model produced similar overall costs to those reported  
 336 by Lavaja and Bagajewicz (2004), the only differences being (i) the 4 heat exchanger case  
 337 over 18 months, where the cost of our schedule is slightly smaller than that reported, with  
 338 the difference in savings being only <1.5%; and (ii) the 10 unit HEN case with asymptotic

Table 2: Data for four heat exchangers case. Reproduced from Lavaja and Bagajewicz, 2004.

Parameter	Heat Exchanger			
	1	2	3	4
$F_h$ [lb/h]	141000	73800	423000	429000
$C_h$ [Btu/lb°F]	0.67	0.70	0.62	0.62
$A$ [ft <sup>2</sup> ]	465	287	1192	1488
$a$ (linear fouling, $\times 10^7$ ) [ft <sup>2</sup> F/Btu]	3.07	3.27	3.68	3.88
$F_c$ [lb/h]	721000			
$C_c$ [Btu/lb°F]	0.46			
$U_c$ [Btu/hft <sup>2</sup> F]	88.1			
$U_0$ [Btu/hft <sup>2</sup> F]	88.1			
$\Delta t^{cl}$ [month]	0.20			
$\Delta t^{op}$ [month]	0.80			

Table 3: Data for 10 unit HEN case. Adapted from Lavaja and Bagajewicz, 2004.

Parameter	Heat Exchanger									
	1	2	3	4	5	6	7	8	9	10
$F_h$ [lb/h]	141000	73800	423000	429000	208000	423000	210000	141000	283000	208000
$F_c$ [lb/h]	721000	721000	721000	721000	721000	721000	721000	649000	649000	649000
$C_h$ [Btu/lb°F]	0.67	0.70	0.62	0.62	0.67	0.62	0.69	0.67	0.69	0.67
$C_c$ [Btu/lb°F]	0.46	0.46	0.46	0.46	0.55	0.55	0.55	0.57	0.57	0.57
$A$ [ft <sup>2</sup> ]	465	287	1192	1488	183	546	492	437	885	1257
$a$ (linear fouling, $\times 10^7$ ) [ft <sup>2</sup> °F/Btu]	1.23	1.84	1.23	1.64	3.07	2.25	3.07	3.27	3.68	3.88
$R_f^\infty$ (asymptotic fouling, $\times 10^3$ ) [hft <sup>2</sup> °F/Btu]	1.61	2.41	1.61	2.14	4.02	2.95	4.02	4.29	4.82	5.09
$U_c$ [Btu/hft <sup>2</sup> °F]	88.1									
$U_0$ [Btu/hft <sup>2</sup> °F]	88.1									
$\Delta t^{cl}$ [month]	0.20									
$\Delta t^{op}$ [month]	0.80									
$\tau$ (decay constant) [month]	4									
$\eta_f$	0.75									

Table 4: Operational constraints for 10 unit HEN case.

only one unit of exchangers 1-4 can be cleaned in each period	$y_{1p} + y_{2p} + y_{3p} + y_{4p} \geq 3 \forall p$
only one unit of exchangers 5-7 can be cleaned in each period	$y_{5p} + y_{6p} + y_{7p} \geq 2 \forall p$
temperature drop across desalter	$T_{c,5p}^{in} = T_{c,4p}^{out} - 18 \forall p$

Table 5: Data for 25 unit HEN case. Adapted from Smaïli et al., 2002a.

<i>HEX</i>	$F_h$ (kg s <sup>-1</sup> )	$F_c$ (kg s <sup>-1</sup> )	$C_h$ (kJ kg <sup>-1</sup> K <sup>-1</sup> )	$C_c$ (kJ kg <sup>-1</sup> K <sup>-1</sup> )	$U_c$ (kW m <sup>-2</sup> K <sup>-1</sup> )	$A$ (m <sup>2</sup> )	$a \times 10^{11}$ (m <sup>2</sup> KJ <sup>-1</sup> )
1A	8.7	23	2.8	2.4	0.5	21.3	1.9
2A	11.4	23	2.9	2.4	0.5	29.7	1.8
3A	4.8	23	2.8	2.4	0.5	31.4	1.6
1B	8.7	23	2.8	2.4	0.5	21.3	1.9
2B	11.4	23	2.9	2.4	0.5	29.7	1.8
3B	4.8	23	2.8	2.4	0.5	31.4	1.6
1C	8.7	23	2.8	2.4	0.5	21.3	1.9
2C	11.4	23	2.9	2.4	0.5	29.7	1.8
3C	4.8	23	2.8	2.4	0.5	31.4	1.6
1D	8.7	23	2.8	2.4	0.5	21.3	1.9
2D	11.4	23	2.9	2.4	0.5	29.7	1.8
3D	4.8	23	2.8	2.4	0.5	31.4	1.6
4A	23	47.4	2.8	2.3	0.5	26.7	1.5
5A	28	47.4	2.6	2.3	0.5	35.4	1.1
6A	17.4	47.4	2.9	2.3	0.5	79.1	1.5
4B	23	47.4	2.8	2.3	0.5	29.2	1.6
5B	28	47.4	2.6	2.3	0.5	35.4	1.1
6B	17.4	47.4	2.9	2.3	0.5	79.1	1.5
7A	25	47.4	2.6	1.92	0.5	60.8	0.8
7B	25	47.4	2.6	1.92	0.5	80.3	0.8
8	49.6	95	2.6	1.92	0.5	129	0.8
9A	55.8	95	2.6	1.92	0.5	110	0.9
9B	55.8	95	2.6	1.92	0.5	96.6	0.9
10	3.3	95	2.9	1.92	0.5	8.5	0.6
11	19.1	95	2.8	1.92	0.5	56.6	0.6



Table 6: Operational constraint for 25 unit HEN case.

vacuum residue rundown temperature target	$y_{1A,p} + y_{1B,p} + y_{1C,p} + y_{1D,p} + y_{6A,p} + y_{6B,p} \geq 5$
atmospheric middle pump-around target	$y_{2A,p} + y_{2B,p} + y_{2C,p} + y_{2D,p} + y_{4A,p} + y_{4B,p} \geq 5$
side-stream rundown temperature target	$y_{3A,p} + y_{3B,p} + y_{3C,p} + y_{3D,p} + y_{11,p} \geq 4$
atmospheric top pump-around target	$y_{5A,p} + y_{5B,p} + y_{9A,p} + y_{9B,p} \geq 3$
vacuum pump-around target	$y_{7A,p} + y_{7B,p} + y_{8,p} \geq 2$
one hot end exchanger is allowed to be cleaned at a time	$y_{1A,p} + y_{2A,p} + y_{3A,p} \geq 2$
	$y_{1B,p} + y_{2B,p} + y_{3B,p} \geq 2$
	$y_{1C,p} + y_{2C,p} + y_{3C,p} \geq 2$
	$y_{1D,p} + y_{2D,p} + y_{3D,p} \geq 2$
flash temperature is required to be maintained	$y_{4A,p} + y_{5A,p} + y_{6A,p} \geq 2$
	$y_{4B,p} + y_{5B,p} + y_{6B,p} \geq 2$
maintenance of the desalter temperature	$y_{7A,p} + y_{7B,p} + y_{8,p} + y_{9A,p} + y_{9B,p} + y_{10,p} + y_{11,p} \geq 6$
temperature drop across desalter	$T_{c,9p}^{\text{in}} = T_{c,7p}^{\text{out}} - 10$

339 fouling, where there is an insignificant difference in savings. This is because of the existence  
340 of multiple local optima. It is noteworthy that Lavaja and Bagajewicz’s (2004) MILP model  
341 is solved to global optimality whereas our model, being a non-convex MINLP model, is not.  
342 Despite this, we still obtain similar results.

343 For the 10 unit HEN (tables 14 and 15), although a general relation is seen in Lavaja  
344 and Bagajewicz’s schedule where cleaning actions increase in the asymptotic fouling case *vs.*  
345 the linear one (from 10 to 11 cleanings), this drops down by 4 cleaning actions in our model  
346 as shown in tables 14 and 15. Only the last 3 units are cleaned here whilst there is a more  
347 distributed cleaning of units in the schedule of Lavaja and Bagajewicz, with half the units  
348 in the network undergoing cleaning during the operational horizon. Consequently, the cost  
349 of their schedule is slightly less than ours (£484k versus £493k as shown in table 9). This is  
350 a small difference of just over 1.5% in savings.

351 For all reported schedules there is an absence of cleaning actions near the start and the end  
352 of the operating horizon as there is little incentive to clean a relatively clean unit and there is  
353 little time for the cost of cleaning to be recovered towards the end of the operating horizon.  
354 If one were to increase the cost of cleaning further, this would limit the number of cleaning  
355 actions even more and increase the objective further. This can be used to determine which  
356 cleaning actions and/or exchangers are more important. For the 10 unit HEN, from tables  
357 14 and 15, it can be seen that exchangers 9 and 10 are cleaned most frequently, indicating  
358 that these exchangers are more important in the network, while exchangers 1 and 2 in the  
359 linear and asymptotic models are not cleaned at all. Exchangers 9 and 10 are cleaned more  
360 often as they have the highest fouling rates as shown in table 3. The fouling rate is not the  
361 only criterion that determines how often cleaning is done. For instance as shown in table 3  
362 in Lavaja and Bagajewicz’s (2004) schedule, despite the similar asymptotic fouling rates of  
363 exchangers 5 and 7, the former is not cleaned at all while the latter is cleaned twice during  
364 the operating horizon. This is due to network sensitivity.

365 An important point to note is the bang-bang nature of these problems. The solutions

366 of the relaxed models are completely integer *i.e.* a bang-bang control solution. Thus, the  
367 proposed rounding up scheme was not performed here. A number of schedules with similar  
368 objective values but different order of cleaning actions are obtained where very few fractional  
369 binary variables occur. These solutions are termed bang-singular. For the majority of cases,  
370 the range of objective values obtained in the 50 runs is quite narrow as shown in table 17,  
371 where the objective values only vary from as little as £3k up to £15k in the first 5 case  
372 studies. For the 10 unit asymptotic HEN case study, this range widens up to to £42k with a  
373 minimum of £493k to a maximum of £535k, and up to £28k for the 25 unit HEN case study  
374 with a variation of £902k to £930k. Hence, for less complex networks and/or fouling models  
375 many runs at different starting points are not required to obtain a good solution.

376 A cost comparison only makes sense in the case studies appearing in Lavaja and Baga-  
377 jewicz (2004) where the objective value for the no cleaning scenarios are similar (see tables  
378 7 to 9). For the 25 unit HEN case studies, Smaïli et al. (2002a) reported a lower objective  
379 associated with the no cleaning scenario representing <11% difference (see table 10). This is  
380 partly attributed to our model retaining the fouling expressions in their dynamic form, which  
381 is more accurate. Smaïli et al. (2002a) discretised the system equations and thus assumed  
382 that variables such as temperature of hot and cold stream are fixed within each sub-period  
383 which is not a good approximation for large complex networks with extensive feedback of  
384 hot/cold streams. Temperatures in our model are interpreted continuously over time. The  
385 difference in the objective for the no cleaning scenario in the 25 unit HEN is also attributed  
386 to the different numerical methods used to the solve the equation sets.

387 For the 25 unit HEN case study our solution yields a saving of 36.2% with an overall  
388 cost of £902k, whereas the best reported cost produced by Smaïli et al. (2002a) using their  
389 BTA algorithm is £917k. Smaïli et al. (2002a) were unable to generate a solution using the  
390 OA method. Our schedules have a small number of cleaning actions, in common with that  
391 of Smaïli et al.. As in the 4 units over 18 months case study, no pattern is evident in the  
392 cleaning actions for the Smaïli et al. (2002a) method. More cleaning actions are performed

393 in our schedule (37 versus 34, table 16). Some features in common are that most exchangers  
394 are cleaned the same number of times as our schedule and certain exchangers are not cleaned  
395 at all (*e.g.* exchanger 10).

396 In terms of the distribution of the objective values for the 50 runs performed in each case,  
397 the results for each of the cases is narrowly dispersed around its associated mean value. The  
398 relative standard deviation (RSD) of the local optima for each of the cases considered lies in  
399 a narrow range of 0.8 to 1.5% (table 17). Furthermore, the difference between the maximum  
400 and minimum cost value is only £3k for the 4 unit heat exchanger case over a 12 month  
401 operating horizon, whereas this difference is the highest for the 10 unit HEN case subject to  
402 asymptotic fouling, at £42k. For the 10 unit HEN case subject to asymptotic fouling, the  
403 worst run results in a saving of 3.6% compared to 11.2% for the best solution achieved, while  
404 for the 4 unit heat exchanger case over a 12 month length of operation this is a saving of  
405 19.3% in the worst case compared to 21.5% in the best case scenario.

406 The resource usage varies depending on fouling type, method used and problem size.  
407 Reasonable time for convergence is achieved for cases studies appearing in Lavaja and Baga-  
408 jewicz (2004) and resource usage is practical even for the worst case: the 10 unit HEN with  
409 asymptotic fouling model required 942 CPU s (15.7 CPU min), with the corresponding best  
410 case for this model being a modest 91 CPU s. Lavaja and Bagajewicz (2004) stated that the  
411 time to solve the 10 unit HEN case was impractical, therefore in addition to reformulating  
412 their model into a MILP problem they used a decomposition procedure to decrease the com-  
413 putational time. They also stated that they kept the linearity of the expressions with the  
414 aim of having better chances of capturing the global optimum. From our findings, neither of  
415 these are required. In comparison, the resource usage becomes expensive for the 25 unit HEN  
416 case study. This required 55,243 CPU s (15.3 CPU hr) with 38,603 function evaluations in  
417 the worst case. This is due to the implementation approach whereby gradients are estimated  
418 using finite differences in the MATLAB<sup>®</sup> optimiser.

419 The computational cost is proportional to the number of finite difference calculations

420 required, with each finite difference calculation requiring a full dynamic system simulation;  
421 for larger problems, this leads to a significant computational cost. For example, for the single  
422 heat exchanger case under linear fouling for an operating horizon of 24 periods, an average of  
423 11 gradient calculations is required with each one requiring 24 finite difference calculations,  
424 as shown in Table 17. This accounts for the average computational cost of 30 CPU s. In  
425 the case of the 25 unit heat exchanger network under linear fouling over 36 periods results  
426 in a much larger average computational time of 39,611 CPU s (11 CPU hr). In this case,  
427 there is an average of 31 gradient calculations each of them requiring 900 finite difference  
428 calculations.

429 Future applications of the multistage optimal control approach will include the reduction  
430 of CPU time such that it becomes significantly smaller in larger and more complex networks.  
431 This will be achieved through gradient estimation using sensitivity equations. Furthermore,  
432 future work will involve extending the range of case studies in HENs to include pressure  
433 drop constraints, variable throughput, and optimisation of operating conditions such as the  
434 consumption of utilities. This approach is not limited to HENs, and future work will focus  
435 on the optimisation of general scheduling maintenance problems.

## 436 6. Critique

437 This work has demonstrated that the heat exchanger cleaning scheduling problem as  
438 posed, considering all potential cleaning actions, can be solved for large networks and larger  
439 numbers of actions than previously achieved through the recognition of the task as an optimal  
440 control problem where the solutions fit bang-bang characteristics. We here review which  
441 aspects of the scheduling problem which may be encountered in practice have been included  
442 in the work, and those which have not, in order to identify the scope and potential for further  
443 development.

444 Aspects which have been included are the distribution of heat duties within networks in  
445 response to cleaning actions, and their evolution; linear and nonlinear (asymptotic) fouling

Table 7: Economic chart for the single heat exchanger case. All values in k£.

Case	This work's model		Lavaja and Bagajewicz's (2004) model	
	This work's solution (relaxed MIOCP)	203	Lavaja and Bagajewicz's (2004) solution	203
No cleaning, linear fouling	203	203	Lavaja and Bagajewicz's (2004) solution	203
No cleaning, asymptotic fouling	317	317		316
Cleaning cost=£4k, linear fouling	103 (103*)	102		102
Cleaning cost=£4k, asymptotic fouling	226 (226*)	225		225
* relaxed MIOCP completely integer <i>i.e.</i> feasible solution				

Table 8: Economic chart for the four heat exchangers case. All values in k£.

Case	This work's model		Lavaja and Bagajewicz's (2004) model
	This work's solution (relaxed MIOCP)	Lavaja and Bagajewicz's (2004) solution	
No cleaning, linear fouling, 12 months	135	135	Not reported
No cleaning, linear fouling, 18 months	289	289	Not reported
Cleaning cost = £4k, linear fouling, 12 months	106 (106*)	106	106
Cleaning cost = £4k, linear fouling, 18 months	179 (179*)	183	183
* relaxed MIOCP completely integer <i>i. e.</i> feasible solution			

Table 9: Economic chart for the 10 unit HEN case. All values in k£.

Case	This work's model		Lavaja and Bagajewicz's (2004) model	
	This work's solution (relaxed MIOCP)	Lavaja and Bagajewicz's (2004) solution	Lavaja and Bagajewicz's (2004) solution	Lavaja and Bagajewicz's (2004) solution
No cleaning, linear fouling	361	361		361
No cleaning, asymptotic fouling	555	555		554
Cleaning cost = £4k, linear fouling	259 (259*)	258		258
Cleaning cost = £4k, asymptotic fouling	493 (493*)	484		482

\* relaxed MIOCP completely integer *i.e.* feasible solution



Table 10: Economic chart for the 25 unit HEN case. All values in k£.

Case	This work's model		Smaïli et al.'s (2002a) model	
	Smaïli et al.'s (2002a) OA method solution	1413	Smaïli et al.'s (2002a) BTA algorithm solution	1413
No cleaning, 36 months	1413	1413	Not reported	1261
Cleaning cost = £5k, 36 months	902 (902*)	Smaïli et al. unable to solve	917	819
* relaxed MIOCP completely integer <i>i.e.</i> feasible solution				

Table 11: Cleaning schedule for the single heat exchanger case (linear and asymptotic fouling).

Case	Time (months)																								No. of cleaning actions			
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	+	○		
Linear fouling, cleaning cost=£4000						+	○					+	○					+	○								+	○
Asymptotic fouling, cleaning cost=£4000					⊕			⊕					⊕				○	⊕			⊕						5	6
cleaning actions: + this work; ○ Lavaja and Bagajewicz; ⊕ common																												

Table 12: Cleaning schedule for the four heat exchanger case (duration 12 months, linear fouling, cleaning cost = £4000)

Exchanger No.	Time (months)												No. of cleaning actions	
	1	2	3	4	5	6	7	8	9	10	11	12	+	○
1													0	0
2													0	0
3						⊕							1	1
4							⊕						1	1
cleaning actions: + this work; ○ Lavaja and Bagajewicz; ⊕ common														
													2	2

Table 13: Cleaning schedule for the four heat exchanger case (duration 18 months, linear fouling, cleaning cost = £4k)

Exchanger No.	Time (months)																		No. of cleaning actions			
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	+	○		
1									+	○									1	1		
2										⊕									1	1		
3					○		+			○				+					2	2		
4						⊕						⊕							2	2		
cleaning actions: + this work; ○ Lavaja and Bagajewicz; ⊕ common																					6	6

Table 14: Cleaning schedule for the 10 unit HEN case (linear fouling, cleaning cost = £4k).  
Time (months)

Exchanger No.	Time (months)																		No. of cleaning actions			
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	+	○		
1																			0	0		
2																			0	0		
3								⊕											1	1		
4									⊕										1	1		
5								○	+										1	1		
6							○			+									1	1		
7								+	○										1	1		
8									⊕										1	1		
9													⊕						2	2		
10						⊕						⊕							2	2		
cleaning actions: + this work; ○ Lavaja and Bagajewicz; ⊕ common																					10	10

Table 15: Cleaning schedule for the 10 unit HEN case (asymptotic fouling, cleaning cost = £4k).

Exchanger No.	Time (months)																		No. of cleaning actions			
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	+	○		
1																			0	0		
2																			0	0		
3																			0	0		
4											○								0	1		
5																			0	0		
6																			0	0		
7						○					○								0	2		
8							○			+		○							1	2		
9				○		+		○	+				○						2	3		
10				+	○			+		○		+			○				3	3		
cleaning actions: + this work; ○ Lavaja and Bagajewicz; ⊕ common																					6	11



Table 17: Solution metrics for all case studies.

Case Study	Objective (in k£)		RSD (in %)				No. of iterations				No. of function evaluations ( <i>i.e.</i> simulations)				CPU time (in s)		
	Min	Max	Mean	Max	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	Min	Max	Mean	
Single, linear fouling, 24 months	103	109	105	1.3	5	18	11	145	467	286	15	48	30				
Single, asymptotic fouling, 24 months	226	241	233	1.4	2	15	7	72	388	192	9	47	25				
4 units, linear fouling, 12 months	106	109	107	0.9	5	12	8	270	592	404	22	48	34				
4 units, linear fouling, 18 months	179	189	182	1.1	11	22	15	835	1609	1141	97	190	132				
10 unit HEN, linear fouling, 18 months	259	270	264	1.0	9	25	16	1581	4322	2782	298	822	535				
10 unit HEN, asymptotic fouling, 18 months	493	535	512	1.5	2	19	7	343	3292	1298	91	942	343				
25 unit HEN, linear fouling, 36 months	902	930	915	0.8	25	43	31	21944	38603	28042	30670	55243	39611				



446 behaviour; and constraints on the selection of combination of cleaning actions representing  
447 pump-around targets, rundown temperature targets, flash temperature maintenance, *etc.*  
448 Aspects presented by other workers which could be included without loss of generality, but  
449 requiring more detailed modelling and therefore solution time, include the choice between  
450 two cleaning actions (Pogiatzis et al., 2011) and temperature target constraints (*e.g.* desalter  
451 temperature, see Ishiyama et al. (2010)).

452 Those not included can be grouped as follows:

453 (i) Nonlinearity arising from fouling phenomena. Fouling rates are known to depend  
454 strongly on temperature, and will therefore vary in an exchanger over time as fouling changes  
455 the temperature distribution within a network. This level of detailed modelling can be  
456 incorporated in greedy (Ishiyama et al., 2009a) and genetic algorithm approaches (Rodriguez  
457 and Smith, 2007), at the expense of ensuring global optimality, as well as in these total  
458 horizon approaches.

459 (ii) Nonlinearity arising from network dynamics. Fouling deposits change the pressure  
460 drop across a heat exchanger as well as its heat transfer performance. The network model  
461 presented here assumes constant stream flow rates, but fouling in practice can give rise to flow  
462 redistribution between parallel streams as well as throughput reduction as a result of pumping  
463 limitations (Yeap et al., 2004; Ishiyama et al., 2008). Changes in flow rate affect both local  
464 fouling rates and the objective function, and network models incorporating pressure drop and  
465 throughput dynamics have been constructed. The relationship between fouling resistance,  
466 pressure drop and throughput is not linear: depending on the network configuration, it can  
467 feature a threshold followed by a quasi-parabolic region. The heat duty in the objective  
468 function (equation (24)) then contains a product of two variables ( $\dot{F}_c$  and CIT), and with an  
469 appropriate formulation, this is amenable to this total horizon approach.

470 (iii) Uncertainty in fouling models and model parameters. Wilson et al. (2017) recently  
471 reviewed the progress in quantitative fouling models for crude oil fouling. They reported  
472 three areas where systematic uncertainty arise in models for predicting the fouling rates in

473 crude oil as related to the problems presented here:

474 (a) The fouling models are semi-empirical and the relationship to crude oil composition  
475 and characteristics has yet to be established, so one cannot predict, for example, whether  
476 linear or asymptotic fouling will be observed in a given unit.

477 (b) Fouling rates for complex fluids such as crude oil are rarely studied under controlled  
478 conditions. In practice many operators used fouling models constructed from reconciliation  
479 and interpretation of plant fouling data. These are subject to uncertainties in measurement  
480 and calculation, so the accuracy of the fouling rate data is low.

481 (c) The relationship between fouling rates and crude composition is unknown. In most  
482 applications the crude being processed varies with time so the rate(s) will also vary. This is  
483 one of the reasons why plant fouling data, used to quantify fouling model parameters, contain  
484 noticeable scatter and variation. These areas mean that, in practice, scheduling calculations  
485 must be able to consider a range of likely fouling rates.

486 There is a conflict between aspects (i) and (ii), and (iii): the increased model complexity in  
487 the former means that multiple condition testing, as required by (iii), will require considerable  
488 resource. The desire to account for known, deterministic phenomena must be balanced  
489 against the limitations to tractability introduced by those phenomena. From an engineering  
490 perspective, the question to be asked is which essential features of the problem must be  
491 included, at a suitable level of detail, to achieve the desired outcome.

492 Aspects (i) and (ii) will require special reformulation to be incorporated in a suitable level  
493 of detail for some practical cases with total horizon approaches, such as the one described  
494 in this work. These approaches are, however, ideally suited for combination with algorithms  
495 for designing heat exchanger networks as they can generate estimates for expecting optimal  
496 operating performance, including considerations of uncertainty in fouling (and operating  
497 parameters).

498 For the case of a crude preheat train, the initial network design would yield temperature  
499 and flow rate conditions for which fouling rates could be estimated. The operation of this

500 network, with cleaning schedules calculated for a portfolio of fouling rates, could then be  
501 quantified (and key exchangers identified for design attention), and this information used  
502 to update the design. Wang and Smith (2013) employed simulated annealing approaches  
503 to identify fouling resistant preheat train designs but did not incorporate cleaning aspects  
504 in their consideration of network performance: the current work now makes this a tractable  
505 problem and one worthy of attention. Current network complexities may prohibit application  
506 of a full optimisation based methodology for the scheduling of cleaning, and hence currently  
507 the preference in industry is to use heuristic or greedy approaches. However, the contribution  
508 of this work is to show that optimisation based methodologies can be general enough to  
509 encapsulate both complexity and different operating modes and this will be explored further  
510 in future work.

## 511 7. Conclusions

512 An alternative methodology to the solution of the HEN cleaning scheduling problem is  
513 presented here by recognising, for the first time, that this optimisation model is in actuality  
514 a MIOCP which exhibits bang-bang behaviour. This proves to be an efficient and robust  
515 approach and has been compared with 3 different methods: a direct MINLP approach (OA),  
516 reformulation of the MINLP to an MILP model, and a stochastic optimisation technique  
517 (BTA algorithm).

518 The multistage optimal control formulation using the feasible path approach does not  
519 suffer from failures in convergence and is thus reliable, contrary to the OA method which  
520 fails to produce a solution in larger and more complex networks. The feasible path approach  
521 as implemented is shown to be very competitive. Optimal solutions reported here are all  
522 bang-bang in the controls. As a result, these particular case studies did not require any  
523 heuristic approaches to be applied. In comparison to the classical methods, economic values  
524 are similar and in some instances better than those obtained. The cleaning schedules showed  
525 several conventional characteristics, with key exchangers being cleaned more often. However,

526 the allocation of cleaning actions was often not systematic, *i.e.* unpredictable.

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