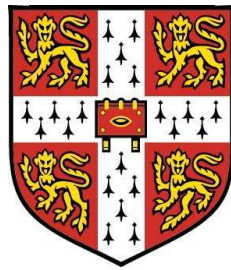# Application of Mixed-Integer Programming in Chemical Engineering

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Ἔν τζεῖνον τῆ τσιλιᾶς πάσ' στὸ βολίτζιν

Εἴδεν ἕναν τζι' ἔπεψεν τὸγ γιόν του να σπουδάση. Ἄμαν ἤρτεμ ποὺ τὲς
σπουδές του, ἐκαρτέραν τον ὁ τζύρης του τὴν ἄλλη ἡμέραν νὰ σηκωστῆ
νὰ μπουκκώσουν ... ἐκαρτέραν, ἐκαρτέραν ... τίποτε. ≪Νὰ πάω, λαλεῖ,
να δοῦμεν εἴντα' μ κάμνει.≫

Πάει, θωρεῖ τον, γράφει τζαὶ σβήννη, τζαὶ τὸ δεῖν του πάσ' στὴβ βολίκωσην.

- Εἴντα 'μ ποὺ κάμνεις, γιέ μου, λαλεῖ του, τζι' ἐν ἔρκεσαι νὰ μπουκκώσουμεν;

- Ἄης' με, παπᾶ λαλεῖ του, τζι' ἔτο κάμνω λοαρκούς νὰ δω εἴντα λοῆς
ἐκόρτωσεν ὁ βοῦς τὸγ κῶλον του τζι' ἐπῆρεν τῆ τσιλιάν του πάσ' τζεῖν
το βολίτζιν.

- Κρῖμα στὰ ρϊάλια, γιέ μου, λαλεῖ του, ποὺ ξόκιασα νὰ σὲ σπουδάσω.
Ἔτο τὸ βολίτζιν εἴσεμ πάνω του τῆ τσιλιάν τζι' ὁ χτίστης ἔβαλέν το
πάσ' στὴβ βολίκωσην, χωρίς νὰ τὸ καθαρίση.

Cypriot fable

≪Όχι! Όχι! Ποτέ μην αναγνωρίσεις τα σύνορα του ανθρώπου! Να σπας
τα σύνορα! Ν' αρνιέσαι ό,τι θωρούν τα μάτια σου. Να πεθαίνεις και να
λες: Θάνατος δεν υπάρξει!≫

Ασκητική, Νίκος Καζαντζάκης
(The Saviours of God: Spiritual Exercises, Nikos Kazantzakis)

Preface

The work in this dissertation was undertaken at the Department of Chemical Engineering and Biotechnology, University of Cambridge, between October 2009 and November 2012. It is the original work of the author, except where specifically acknowledged in the text, and includes nothing that is the outcome of work done in collaboration. No part of this dissertation has been submitted for a degree, diploma or other qualification at any other university.

The dissertation is approximately 47000 words in length, including figures, tables, references, equations and the appendix. It contains exactly 30 figures.

Thomas A. Pogiatzis
29 November 2012

Acknowledgements

Abstract

Mixed-Integer Programming has been a vital tool for the chemical engineer in the recent decades and is employed extensively in process design and control. This dissertation presents some new Mixed-Integer Programming formulations developed for two well-studied problems, one with a central role in the area of Optimisation, the other of great interest to the chemical industry. These are the Travelling Salesman Problem and the problem of scheduling cleaning actions for heat exchanger networks subject to fouling.

The Travelling Salesman Problem finds a plethora of applications in many scientific disciplines, Chemical Engineering included. None of the mathematical programming formulations proposed for solving the problem considers fewer than $\mathcal{O}(n^2)$ binary degrees of freedom. The first part of this dissertation introduces a novel mathematical description of the Travelling Salesman Problem that succeeds in reducing the binary degrees of freedom to $\mathcal{O}(n\lceil \log_2(n)\rceil)$. Three Mixed-Integer Linear Programming formulations are developed and the computational performance of these is tested through computational studies.

Sophisticated methods are now available for scheduling the cleaning actions for networks of heat exchangers subject to fouling. In the majority of these, only one form of cleaning is used, which restores the performance of the exchanger back to its clean level. Ishiyama *et al.* [2011b] recently revised the scheduling problem for the case where there are several cleaning methods available. The second part of this dissertation extends their approach, developed for individual units, to heat exchanger networks and explores the concept of selection of cleaning techniques further. Mixed-Integer Programming formulations are proposed for the scheduling task, for two fouling scenarios: (i) chemical reaction fouling and (ii) biological fouling. A series of results are presented for the implementation of the scheduling formulations to networks of different sizes.

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Nomenclature

Roman Symbols

A	set of arcs in Part I; area in Part II
a	constant in equation (4.5)
B	binary tree
b	constant in equation (4.6)
B^k	set of binary variables that are equal to one at iteration k
C	cost matrix in Part I; constant defined by equation (5.5) in Part II; cost vector in Part II
c	constant in equation (4.9)
ch	index denoting chemical action
c_{ijk}	cost in time dependent formulation of the travelling salesman problem
c_{ij}	length of arc (i, j)
C^k	set of binary variables that are equal to zero at iteration k
c^m	cost of cleaning action m
$C_{p,c}$	specific heat capacity of cold stream
$C_{p,h}$	specific heat capacity of hot stream

d_E	Euclidean distance
cd	index denoting chemical disinfection
d_M	Manhattan distance (rectilinear metric)
E	set of elements
e_{ijl}	continuous variable indicating whether cities i and j have the same or opposite directions at level l of binary tree representation
F	configuration correction factor
f	function
f_e	energy cost
fl	index denoting water flush cleaning
G	graph
g	function
h	function
h_{cold}	film heat transfer coefficient of cold stream
h_{hot}	film heat transfer coefficient of hot stream
h^k	length of time element k
i	general index; index of vertex (city) in Part I; index of unit in Part II
I_1	integral of process costs
j	general index; index of vertex (city) in Part I; index of time period in Part II
K	set of iterations in Generalised Benders Decomposition algorithm

k	general index; index of leaf in Part I; index of element in Part II; index of iteration in Generalised Benders Decomposition; constant rate introduced in equation (7.2)
k_c	coke formation rate
k_g	gel formation rate
L	set of levels for a binary tree
l	general index; index of level in Part I; index of node in Part II
l'	index in Theorem 3.1
l''	index in proof of Theorem 3.1
l_∞	infinity norm
$l_k^{(x)}$	x-distance between leaves k and $k+1$ of binary tree
$l_k^{(y)}$	y-distance between leaves k and $k+1$ of binary tree
M	set of cleaning actions
m	general index; index of cleaning mode in Part II; maintenance costs function in Part II
$\dot{m}_c$	mass flow rate of cold stream
me	index denoting mechanical action
$\dot{m}_h$	mass flow rate of hot stream
n	general index; number of vertices in graph (cities in travelling salesman problem); exponent in equation (7.4)
nl	number of levels of a binary tree
np	number of leaves of a binary tree in Part I; number of time periods in Part II

n_{RH}	number of periods in receding horizon heuristic procedure
nu	number of units
n_x	dimension of vector x
n_y	dimension of vector y
O	set of collocation nodes
P	set of leaves for a binary tree in Part I; set of time periods in Part II
p	general index; function of process costs in Part II
pos_i	position of city i in decimal base
Q	set of vertices (cities) in Part I; heat duty in Part II
Q_0	heat duty for a clean heat exchanger
q_i	Lagrange interpolation polynomial
r_c	coke formation rate
R_f	thermal fouling resistance
r_f	function defined by equation (7.7)
$R_{f,\mathrm{cold}}$	thermal fouling resistance of layer deposited on the cold side of the heat transfer wall
$R_{f,\mathrm{hot}}$	thermal fouling resistance of layer deposited on the hot side of the heat transfer wall
$R_{f\infty}$	asymptotic value of thermal fouling resistance
$R_{f,\mathrm{tot}}$	total thermal fouling resistance
r_g	gel formation rate
r_{ijk}	binary variable in time dependent formulation of the travelling salesman problem

r_{il}	binary variable indicating the direction of city i at level l of the binary tree
R_w	thermal resistance of heat transfer wall
t	time
t_0	starting time
t_{ch}	duration of chemical cleaning
$T_{c,in}$	inlet temperature of cold stream
t_{cl}	cleaning time
$T_{c,o}$	outlet temperature of cold stream
T_f	final temperature of cold stream
t_f	time horizon
T_f^{limit}	lower limit on final temperature of cold stream
$T_{h,in}$	inlet temperature of hot stream
$T_{h,o}$	outlet temperature of hot stream
t_I	initiation or induction time
t_{kl}	parameter defining the target binary strings in the proposed mathematical description of the travelling salesman problem
t_{le}^{ch}	leap time after chemical cleaning
t_{le}^{fl}	leap time after water flush cleaning
t_{me}	duration of mechanical cleaning
t_{op}	operating time
T_{target}	target temperature for cold stream

U overall heat transfer coefficient

U' set of units

U_0 overall heat transfer coefficient for a clean heat exchanger

u_i continuous variable in sequential formulation of the travelling salesman problem

V set of vertices (cities)

v continuous variable

w function

w_{ij} continuous variable in multi-commodity formulation of the travelling salesman problem

x x-coordinate in Part I; continuous variable in Part II

$x_i^{(0)}$ x-coordinate of city i

x_{ij} binary variable in Chapter 2/continuous variable in Chapter 3 indicating the presence of arc (i, j) in travelling salesman's tour

x_k x-coordinate of leaf k of the binary tree

y binary vector

$y_i^{(0)}$ y-coordinate of city i

y^{ijm} binary variable indicating the cleaning of unit i at period j with action m

y_k y-coordinate of leaf k of the binary tree

z objective variable

z^* optimal objective function value

z_{GBD}^* best objective function value found by the Generalised Benders Decomposition algorithm

z_{ij}	continuous variable in single commodity formulation of the travelling salesman problem
z_{ik}	continuous variable indicating the allocation of city i on leaf k of the binary tree
z_{IP}	optimal objective function value for integer programming problem
$z_{\mathrm{LP}}^{\mathrm{rel}}$	optimal objective function value for linear programming relaxation problem
z_{no}	objective function value for the no-cleaning situation
z_{Pr}^{k}	objective variable in primal problem (NLP-Pr) at iteration k
z_R	objective variable in relaxed problem (NLP-R)
z_{RH}	objective function value by the receding horizon heuristic procedure

Greek Symbols

α	function defined by equation (3.12)
β	function defined by equation (3.13)
δ	thickness
δ_c	thickness of coke layer
δ_g	thickness of gel layer
ΔT_{lm}	logarithmic mean temperature difference
θ^k	objective variable in master problem (MILP-M) at iteration k
λ_c	thermal conductivity of coke layer
λ_c^k	Lagrange multiplier at iteration k
λ_g	thermal conductivity of gel layer
λ_g^k	Lagrange multiplier at iteration k

τ	collocation time
τ_k	collocation node k
t^{ijkl}	sigmoid time

Acronyms

ATSP	asymmetric travelling salesman problem
BM	basic model for asymmetric travelling salesman problem
CPU	central processing unit
DFJ	Dantzig, Fulkerson and Johnson travelling salesman problem formulation
ER	equality relaxation
GBD	generalised Benders decomposition
GG	Gavish and Graves travelling salesman problem formulation
IP	integer programming
LP	linear programming
MILP	mixed-integer linear programming
MINLP	mixed-integer nonlinear programming
MIP	mixed-integer programming
MPC	model predictive control
MTZ	Miller, Tucker and Zemlin travelling salesman problem formulation
NLP	nonlinear programming
NP	non-deterministic polynomial class of problems
OA	outer approximation

P   polynomial class of problems

RH   receding horizon

TDTSP   time dependent travelling salesman problem

TSP   travelling salesman problem

Chapter 1

Introduction

Mathematical programming has become an indispensable tool for the chemical engineer over the past 40 years. Optimisation is widely used in process design, process control, process identification, model development [Biegler, 2010] and more recently in product and molecule design [Pistikopoulos *et al.*, 2010].

The class of optimisation problems that involve both continuous variables and discrete variables are generally known as Mixed-Integer Programming problems. Mixed-Integer Programming finds a plethora of applications in Chemical Engineering. These include the scheduling of batch processes, the synthesis of complex reactor networks and the retrofit of heat exchanger networks [Floudas, 1995].

In this work, some new Mixed Integer Programming formulations are presented for two very different problems, one of great theoretical and practical value, and the other a real industrial problem. The dissertation is divided into two parts:

   I. Travelling Salesman Problem

  II. Scheduling cleaning actions for heat exchanger networks subject to fouling

The Travelling Salesman Problem has a central role in Mathematical Programming. It was the systematic study of the problem that led to the development of the areas of Integer Programming and Mixed-Integer Programming and directed the way for the discovery of many rigorous and heuristic optimisation tools. Today, the problem finds numerous applications across all scientific

disciplines. Those related to Chemical Engineering include the vehicle routing problem, machine scheduling problem and genome mapping.

Hitherto, all existing mathematical formulations of the Travelling Salesman Problem have required $\mathcal{O}(n^2)$ binary degrees of freedom or more. The aim of the current work is the development of a mathematical description for the problem that involves fewer than $\mathcal{O}(n^2)$ binary variables.

Chapter 2 reviews the basic aspects of the Travelling Salesman Problem. A major part of the chapter is devoted to the description of some well-accepted formulations found in the literature. The basic rigorous algorithms used to identify optimal tours are introduced briefly and some successful tour searching heuristic procedures are mentioned.

Chapter 3 introduces the novel mathematical description of the Travelling Salesman Problem. A new class of mathematical programming formulations is developed, based on work in Binary Arithmetic. The detailed presentation of the proposed Mixed-Integer Programming formulations is followed by computational studies, which aim to test their computational performance in practice. At the end of the chapter, their relationship to other well-known formulations is discussed.

The second part of this dissertation revisits the problem of scheduling the cleaning actions for heat exchanger networks subject to fouling. Fouling remains a long-standing problem in industrial process heat transfer. It dominates the performance of heat transfer devices and causes acute financial losses. An effective mitigation strategy for the rectification of the negative effects of fouling is the regular cleaning of the dirty devices. In recent years, decision-making tools have been used to schedule the cleaning actions in an attempt to minimise the associated losses.

A novel scheduling study, presented by Ishiyama *et al.* [2011b] for an isolated heat exchanger, introduced the important problem of competition between two alternative cleaning techniques on the basis of length, cost and effectiveness. The aims of the current work are to extend the approach of Ishiyama *et al.* [2011b] to heat exchanger networks and to explore the concept of choice of cleaning methods further.

Chapter 4 introduces the phenomenon of fouling and discusses its negative im-

pact on heat transfer processes. The focus is primarily on heat exchangers. Subsequent sections of the chapter review previous scheduling approaches presented for isolated heat exchangers or networks of units. It is decided to investigate the problem of scheduling the cleaning actions for: (i) heat exchanger networks subject to chemical reaction fouling and (ii) heat exchanger networks subject to biological fouling.

Chapter 5 describes in detail the Mixed-Integer Programming formulation proposed for the scheduling task for networks subject to chemical reaction fouling. The chapter includes a description of the fouling model used to quantify the negative effect of the deposits on heat transfer performance. It concludes with a discussion regarding appropriate solution methods for the scheduling problem.

In Chapter 6 the proposed scheduling formulation is tested in practice. Case studies are presented where it is used to generate cleaning schedules for an isolated unit and two heat exchanger networks. A series of results is presented in each case, considering the impact of variations in the fouling parameters.

Chapter 7 is concerned with the novel study of scheduling cleaning actions for heat exchanger networks subject to biological fouling. Two Mixed-Integer Programming formulations are presented for this scheduling task, which involves the choice between three cleaning methods. A series of results are obtained for a small network, using one of the scheduling formulations. These are presented and discussed at the end of the chapter.

Chapter 8 presents conclusions and recommendations for future work.

Part I

Travelling Salesman Problem

Chapter 2

Basic aspects of the problem

This chapter reviews the basic aspects of the Travelling Salesman Problem. The first section presents a brief history of the problem. Section 2.2, which is of prime interest for this work, focuses on the mathematical description of the problem and an overview of some well-established Mathematical Programming formulations is provided. Subsequent sections give a short description of some of the most important solution methods and establish the importance of the problem in the areas of Applied Mathematics, Engineering and Computer Science. Some applications of the problem related to Chemical Engineering are also provided.

2.1   History of problem

"Given a finite set of discrete points and the distance between each pair of them, find the shortest route to visit all of them exactly once and return to the starting point". This humble-sounding task is one of the most notorious and intensively studied problems of computational mathematics, namely the Travelling Salesman Problem (TSP). It remains unknown who coined this nifty name for the problem. In the paragraphs that follow, some of the most important moments in the development of the TSP are retraced. The source is the detailed historical survey by Cook [2011].

Leonard Euler was the first person to study tour problems while trying to solve a puzzle known as 'The Bridges of Königsberg'. Euler also studied the re-

lated Knight's Tour problem in chess, where one needs to find a closed tour for the knight to visit all the squares in the board and return to its initial position. Naturally, he managed to solve both puzzles and in doing so he laid the foundations for Graph Theory [Aldous and Wilson, 2000]. One century later, another mathematician, Sir William Rowan Hamilton, was investigating possible tours through all twenty corners of a dodecahedron. He drew the construction known as the Icosian graph and was trying to identify closed walks that touched all the vertices (corners) only once. Such a tour is called a Hamiltonian circuit. Following this, the salesman's problem is defined, in mathematical terminology, as the task of finding the Hamiltonian circuit of minimum weight on a given graph.

Graph Theory is esoteric for the salesman on the road. For him, the search for the shortest possible tour still continues. To his aid came the Austrian mathematician Karl Menger, who was the person who introduced the TSP to the mathematical community. Menger, in the 1920s, began investigating the closely-related problem of finding the shortest path without the need to return to the initial point. He called this the 'Messenger Problem'. It is speculated that Menger exchanged ideas on the matter with the American mathematician Hassler Whitney during a visit at Harvard University. Afterwards, Whitney posed the problem to the mathematical community at one seminar given in Princeton University, and, by the late 1940's, it was a recognised challenge.

The first systematic treatment of the TSP appeared in [Dantzig *et al.*, 1954], where the authors presented the first mathematical formulation for the problem and crafted a computational method to solve it. These prominent mathematicians identified the shortest route for travelling through the capitals of all 49 states of the U.S. This was a challenge that had beset the research community for 15 years.

The interest of a wider research community was sparked by a TV commercial in 1962 by Procter & Gamble, which promoted a competition with a $10000 prize, enough money to buy a house at the time. The task was to identify the shortest route starting from Chicago, travelling through 32 destinations across the U.S. and finally return back to the starting point. The research community responded enthusiastically to the challenge and at the end there was a tie between a number of contestants.

Until today, the travelling salesman problem remains an open challenge and

the interest of researchers has increased rather than diminished. The validity of the statement is apparent when one considers the numerous articles written on the problem every year.

2.2   Problem formulations

Adopting the notation employed in Graph Theory, the task is to find the Hamiltonian circuit of minimum weight for a graph $G = (V, A)$, where $V = \{1, 2, \ldots, n\}$ is the set of vertices (cities) and $A = \{(i, j) : i, j \in V\}$ the set of arcs (connecting lines).

Let us focus our interest on the different formulations proposed for the Asymmetric Travelling Salesman Problem (ATSP). In this variant of the problem the length of an arc depends on the direction in which it is travelled. This is the general case and it includes the special case of the symmetric problem where the distance between two cities is independent of the direction of travel.

There are a number of excellent reviews in the literature, such as [Langevin *et al.*, 1990], [Orman and Williams, 2007] and [Öncan *et al.*, 2009], which describe and compare the large number of proposed formulations. This section considers a selection of the most well-known.

It is essential at this point to review the terms Integer Programming (IP), Linear Programming (LP) and Mixed Integer Programming (MIP). An IP problem involves only integer variables, whereas an MIP one involves both continuous and integer variables. Finally, an LP problem involves only continuous variables which are related to each other by linear constraints only.

The basic model (BM) [Dantzig *et al.*, 1954] for the ATSP is as follows:

$$\text{min.} \quad \sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij} x_{ij} \tag{2.1}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} x_{ij} = 1 \tag{2.2}$$

$$\sum_{j=1}^{n} x_{ij} = 1 \tag{2.3}$$

$$x_{ij} = \{0, 1\}; \quad i, j = 1, 2, \ldots, n \tag{2.4}$$

$$\{(i, j) : x_{ij} = 1, \ i, j = 2, 3, \ldots, n\} \quad \text{does not contain subtours} \tag{2.5}$$

where the binary variables x_{ij} are equal to 1 if and only if the arc (i, j) is present in the optimal solution and c_{ij} is the length of arc (i, j). Constraints (2.2), (2.3) and (2.5) eliminate subtours for all vertices.

The key aspect of a TSP formulation is how to formulate the constraints that break subtours. A subtour is a closed loop that does not contain all the cities. The majority of TSP formulations have this basic model in common and the only difference is found at the subtour elimination constraints. There are however some formulations, such as the time-dependent models, that do not follow this line drawn by Dantzig *et al.* [1954]. In the description of the various formulations that follows, the objective function is given only when the (BM) does not apply.

2.2.1 Classical formulation

The classical TSP formulation was proposed by Dantzig *et al.* [1954] (DFJ formulation). The set of elimination constraints for their IP model is given by

$$\sum_{i \in Q}^{n} \sum_{j \in Q}^{n} x_{ij} \leq |Q| - 1 \quad \text{for all } Q \subseteq \{1, 2, \ldots, n\} \quad \text{and } 2 \leq |Q| \leq n - 1. \tag{2.6}$$

Equation (2.6) defines $\mathcal{O}(2^n)$ constraints, a very large number even for small problems (~ 1 million for 20 cities). Nevertheless, the ingenuity of their proposal lies in the fact that only a relatively small number of these facet defining inequalities [Grötchel and Padberg, 1985] needs to be added progressively to the model to reach the optimal solution. Dantzig *et al.* [1954] managed to solve by hand a 42-cities problem by incorporating only 9 inequalities out of a two trillion set of constraints.

2.2.2 Sequential formulations

An extended category of formulations is based on a model first presented by Miller *et al.* [1960] (MTZ formulation) for a vehicle routing problem. Firstly, there is

the need to introduce $\mathcal{O}(n)$ supplementary continuous variables, u_i, which denote the sequence in which vertex i is visited. The elimination constraints take the form:

$$u_i - u_j + (n-1)x_{ij} \leq n-2; \quad i,j = 2,3,\ldots,n; \; i \neq j. \tag{2.7}$$

There are $\mathcal{O}(n^2 - n + 2)$ constraints defined in equation (2.7). One can introduce simple bounds on the continuous variables, but this is not necessary. This is an MIP model. Many improvements of the MTZ formulation have appeared in the literature over the years, such as those by Desrochers and Laporte [1991], Gouveia and Pires [2001] and Sherali and Driscoll [2002].

2.2.3 Commodity flow formulations

The class of commodity flow formulations follows from the work of Gavish and Graves [1978]. This class is further divided to: (i) single-commodity flow; (ii) two-commodity flow and (iii) multi-commodity flow models. The earliest single-commodity flow model introduced by Gavish and Graves [1978] (GG formulation) and the first multi-commodity flow model that belongs to Wong [1980] (Wong formulation) are presented here. An example of a two-commodity flow model is that by Finke *et al.* [1984], but Langevin *et al.* [1990] subsequently showed that it is equivalent to the GG formulation.

Before stating the constraints for the GG model, first there is the need to introduce $\mathcal{O}(n^2)$ continuous variables z_{ij} which describe the flow of a single commodity to vertex 1 from every other vertex. The elimination constraints are given by

$$\sum_{j=1}^{n} z_{ji} - \sum_{j=2}^{n} z_{ij} = 1; \quad i = 2,3,\ldots,n \tag{2.8}$$

$$0 \leq z_{ij} \leq (n-1)x_{ij}; \quad i = 1,2,\ldots,n, \; j = 2,3,\ldots,n. \tag{2.9}$$

The above set has $\mathcal{O}(n^2)$ constraints. The GG model belongs to the MIP class.

Wong [1980] formulated the first multi-commodity flow model using additional

$\mathcal{O}(n^3)$ continuous variables to describe the flow of $2(n-1)$ commodities between vertex 1 and the other vertices. A set of $\mathcal{O}(2n^3)$ elimination constraints is defined by

$$\sum_{j=1}^{n} w_{ij}^{(1,l)} - \sum_{j=1}^{n} w_{ji}^{(1,l)} = 0; \quad i, l = 2, 3, \ldots, n; \ i \neq l \tag{2.10}$$

$$\sum_{j=2}^{n} w_{1,j}^{(1,l)} - \sum_{j=2}^{n} w_{j,1}^{(1,l)} = 1; \quad l = 2, 3, \ldots, n \tag{2.11}$$

$$\sum_{j=1}^{n} w_{ij}^{(1,i)} - \sum_{j=1}^{n} w_{ji}^{(1,i)} = -1; \quad i = 2, 3, \ldots, n \tag{2.12}$$

$$\sum_{j=1}^{n} w_{ij}^{(k,1)} - \sum_{j=1}^{n} w_{ji}^{(k,1)} = 0; \quad i, k = 2, 3, \ldots, n; \ i \neq k \tag{2.13}$$

$$\sum_{j=2}^{n} w_{1,j}^{(k,1)} - \sum_{j=2}^{n} w_{j,1}^{(k,1)} = -1; \quad k = 2, 3, \ldots, n \tag{2.14}$$

$$\sum_{j=1}^{n} w_{ij}^{(i,1)} - \sum_{j=1}^{n} w_{ji}^{(i,1)} = 1; \quad i = 2, 3, \ldots, n \tag{2.15}$$

$$0 \leq w_{ij}^{(1,l)} \leq x_{ij}; \quad i, j = 1, 2, \ldots, n; \ l = 2, 3, \ldots, n \tag{2.16}$$

$$0 \leq w_{ij}^{(k,1)} \leq x_{ij}; \quad i, j = 1, 2, \ldots, n; \ k = 2, 3, \ldots, n. \tag{2.17}$$

This is also a MIP model. Another well-accepted multi-commodity flow formulation is that by Claus [1984], which uses only $(n-1)$ commodities. For the sake of brevity, it is not described here. Finally, multi-commodity formulations are, among others, the ones presented by Gouveia and Pires [2001] and Sherali *et al.* [2006].

2.2.4   Time dependent formulations

The next category of formulations originates from the work of Fox *et al.* [1980]. Here, the classical problem is generalized as a time-dependent scheduling problem where the cost of any given arc is related to its position in the tour [Gouveia and Voß, 1995]. The problem is known as the Time Dependent TSP (TDTSP) and it

is equivalent to the single machine scheduling problem.

A single machine is at the initial state, where job 1 is being processed. A number of $(n-1)$ jobs must be performed before the machine returns to the initial state. The cost of a task depends on its position in the sequence and the preceding job. Thus, a cost c_{ijk} is incurred when job j is processed directly after job i in the kth position and the corresponding binary variable r_{ijk} will be equal to 1. The optimisation problem is stated as follows:

$$\text{min.} \quad \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{n} c_{ijk} r_{ijk} \tag{2.18}$$

$$\text{s.t.} \quad \sum_{j=1}^{n}\sum_{k=1}^{n} r_{ijk} = 1; \quad i = 1, 2, \ldots, n \tag{2.19}$$

$$\sum_{i=1}^{n}\sum_{k=1}^{n} r_{ijk} = 1; \quad j = 1, 2, \ldots, n \tag{2.20}$$

$$\sum_{i=1}^{n}\sum_{j=1}^{n} r_{ijk} = 1; \quad k = 1, 2, \ldots, n \tag{2.21}$$

$$\sum_{j=1}^{n}\sum_{k=2}^{n} k r_{ijk} - \sum_{j=1}^{n}\sum_{k=1}^{n} k r_{jik} = 1; \quad i = 2, 3, \ldots, n \tag{2.22}$$

$$r_{ijk} = \{0, 1\}; \quad i, j, k = 1, 2, \ldots, n \tag{2.23}$$

This formulation requires $\mathcal{O}(n^3)$ binary variables and $\mathcal{O}(4n)$ constraints and it belongs to the IP class. Other TDTSP formulations can be found in the work of Picard and Queyranne [1978] and Gouveia and Voß [1995].

2.2.5 Comparison of TSP formulations

Travelling Salesman Problem formulations are compared in terms of computational efficiency. The solution of TSP instances is computationally intense, especially as the number of cities increases. Therefore, it is beneficial to define an efficiency scale where the formulations which require the least computational effort are placed at the top, and those which force the solver into an endless run at the bottom. The criterion for the classification is the LP-relaxation of each

formulation [Gouveia and Voß, 1995; Langevin *et al.*, 1990; Öncan *et al.*, 2009].

The LP-relaxation of an IP (or MIP) model is simply the IP (or MIP) model itself without the integrality conditions. Thus, the integer variables of IP (or MIP) are now continuous (with lower and upper bounds) in the LP-relaxation. Removing the integrality conditions means that the optimal solution of the LP-relaxation, z_{LP}^{rel}, cannot exceed (since we are performing a minimisation) the optimal solution of the IP model, z_{IP}. Hence, the solution of the relaxation provides a lower bound on the solution of the original model ($z_{IP} \geq z_{LP}^{rel}$). Moreover, an LP-relaxation is said to be strong if the gap between z_{LP}^{rel} and z_{IP} is relatively small. A good IP (or MIP) formulation must have a strong LP-relaxation since in general less computational effort will be required by the solver to reach the optimal solution. For that to happen the LP-relaxation must be well-constrained.

The most recent comparative analysis of a number of well-known TSP formulations is that by Öncan *et al.* [2009]. The authors have summarized results obtained by previous researchers and they also established new relationships, where non-existent, between the examined formulations. Herein, the interest is focused on the models detailed above. Table 2.1 summarises the number of binary variables, continuous variables and constraints for the described formulations and Table 2.2 shows the relationships between these models [Öncan *et al.*, 2009]. Each model in the first column is classified as stronger, weaker or equivalent with respect to the models in the first row. The word "Unknown" denotes that a relationship is yet to be established between two formulations.

Table 2.1: Size of different ATSP formulations

Formulation	Binary Variables	Continuous Variables	Constraints
DFJ	$\mathcal{O}(n^2)$	-	$\mathcal{O}(2^n)$
MTZ	$\mathcal{O}(n^2)$	$\mathcal{O}(n)$	$\mathcal{O}(n^2)$
GG	$\mathcal{O}(n^2)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^2)$
Wong	$\mathcal{O}(n^2)$	$\mathcal{O}(n^3)$	$\mathcal{O}(2n^3)$
FGG	$\mathcal{O}(n^3)$	-	$\mathcal{O}(4n)$

On the efficiency scale, the DFJ and Wong formulations are placed at the top, whereas the GG and MTZ formulations are located at the bottom. To date, the

Table 2.2: Comparison of ATSP formulations

	DFJ	MTZ	GG	Wong	FGG
DFJ	-	Stronger	Stronger	Equivalent	Unknown
MTZ	Weaker	-	Weaker	Weaker	Weaker
GG	Weaker	Stronger	-	Weaker	Weaker
Wong	Equivalent	Stronger	Stronger	-	Unknown
FGG	Unknown	Stronger	Stronger	Unknown	-

relationship of the FGG formulation to the DFJ and Wong formulations has yet to be established.

2.3   Searching for an optimal tour

The TSP has acted as an engine of discovery for many rigorous and heuristic optimisation approaches. To date, these methods are used to solve many different decision problems.

2.3.1   Exact methods

There are two rigorous methods for the exact solution of TSP instances, namely the cutting-plane technique and the branch-and-bound technique. These techniques are applicable to IP and MIP problems as well. The general framework of the two methods is briefly described below. This is essential background for understanding the computational studies presented in Chapter 3.

2.3.1.1   Cutting-plane method

The main idea of the cutting-plane approach was introduced by Dantzig *et al.* [1954]: the LP-relaxation of the IP problem is solved iteratively while progressively adding violated constraints, such as subtour elimination constraints, until the solution produced is a closed tour. The name cutting-plane derives from the fact that these added constraints act as cuts which progressively restrict the feasible region containing the optimal solution.

The cuts added at each step are relevant to the solution of the LP-relaxation at that step. A valid cut must satisfy two criteria: (i) it excludes no feasible integer solution and (ii) it is violated by the current solution. The difficulty of applying this solution technique lies with the fact that the number of valid cuts can be very large [Cook, 2011].

An extended catalogue of valid cuts, *e.g.* the constraints defined by (2.6), exists for the travelling salesman problem. Nevertheless, using the library is not an easy task. Sorting out the cuts that violate the solution of the LP problem at each step is a great challenge. Correspondingly, much of the ongoing research on the topic is focused on finding effective ways to identify possible cuts from the catalogue.

Shortly after the fundamental work of Dantzig *et al.* [1954], the method was generalised for the larger class of IP problems by Gomory [1958]. Gomory's algorithm gave birth to what we call today the general cutting-plane method. The importance of his work is due to the fact that he described a routine for generating the desired cuts automatically. Thus, the added constraints are named *Gomory cuts*. The solution procedure can be summarized as follows: the LP-relaxation of the IP problem is solved at each iteration while progressively adding *Gomory cuts* until the optimal basic solution acquires integer values.

The cutting-plane method, general or TSP associated, has one drawback: the number of added cuts can become very large. As a result, the solution of the LP-relaxation at each step will become computationally expensive.

2.3.1.2 Branch-and-Bound method

The branch-and-bound method was first presented by Land and Doig [1960] and was given its name by Little *et al.* [1963]. The method applies a "divide and conquer" scheme which can be visualised using a binary tree structure. The use of the method is illustrated using a small problem. The IP problem is:

$$\text{min.} \quad z = 5x_1 + 6x_2 + 4x_3 + 11x_4 \tag{2.24}$$

$$\text{s.t.} \quad 5x_1 + 8x_2 + 6x_3 + 4x_4 \geq 12 \tag{2.25}$$

$$x_1, x_2, x_3, x_4 = \{0, 1\}. \tag{2.26}$$

The solution procedure is as follows.

1. Solve the LP-relaxation of the problem. This yields the solution:

$$\text{(node 0)} \quad x_1 = 0, \ x_2 = 0.75, \ x_3 = 1, \ x_4 = 0, \ z_{\text{rel}} = 8.5$$

which violates the integrality conditions. Variable x_2 has a fractional value, therefore it must be forced to take an integer value. Accordingly, the problem is divided into two sub-problems, one for $x_2 = 0$ and one for $x_2 = 1$. The variable x_2 is called the *branching* variable.

2. Apply integrality conditions on x_2 at node 0. Enforcing $x_2 = 0$ and solving the corresponding LP-relaxation gives

$$\text{(node 1)} \quad x_1 = 1, \ x_2 = 0, \ x_3 = 1, \ x_4 = 0.25, \ z_{\text{rel}} = 11.75$$

which is not an integer solution. Enforcing $x_2 = 1$ and solving the corresponding LP-relaxation yields

$$\text{(node 2)} \quad x_1 = 0, \ x_2 = 1, \ x_3 = 0.67, \ x_4 = 0, \ z_{\text{rel}} = 8.67$$

which is also a fractional solution. As noticed, the objective value at nodes 1 and 2 is greater than the objective value at node 0. This was expected to happen since more constraints were added. In general, as more constraints are added, the objective value is expected to get worse (increase) or at least remain unchanged. It can never be improved. The progress of the branch-and-bound procedure is illustrated in Figure 2.1.

At this point there are two unacceptable solutions, each of which involves a variable with fractional value. Obviously, a choice needs to be made: which of the two will be the next *branching* variable? This is an important decision since it can have a large effect on how quickly the problem is solved [Williams, 1993]. A number of heuristic rules exist in the bibliography. Here, after an arbitrary choice, branching is applied on variable x_4. This means that the tree is developed further past node 1.
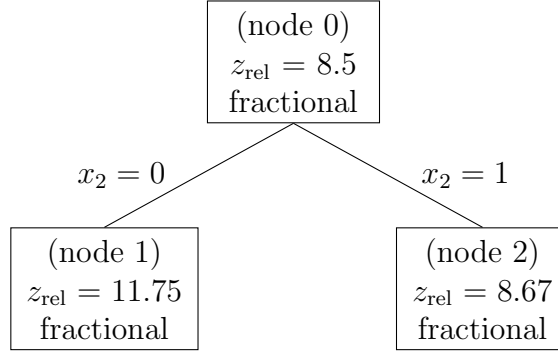
Figure 2.1: Branch-and-bound example: solution tree after stage 2

3. Apply integrality conditions on x_4 at node 1, recalling that $x_2 = 0$. Setting $x_4 = 0$ and solving the corresponding LP-relaxation results in an infeasible solution (node 3). Setting $x_4 = 1$ and solving the LP-relaxation gives the fractional solution:

$$\text{(node 4)} \quad x_1 = 0.4, \ x_2 = 0, \ x_3 = 1, \ x_4 = 1, \ z_{\text{rel}} = 17.$$

Figure 2.2 shows the updated solution tree.
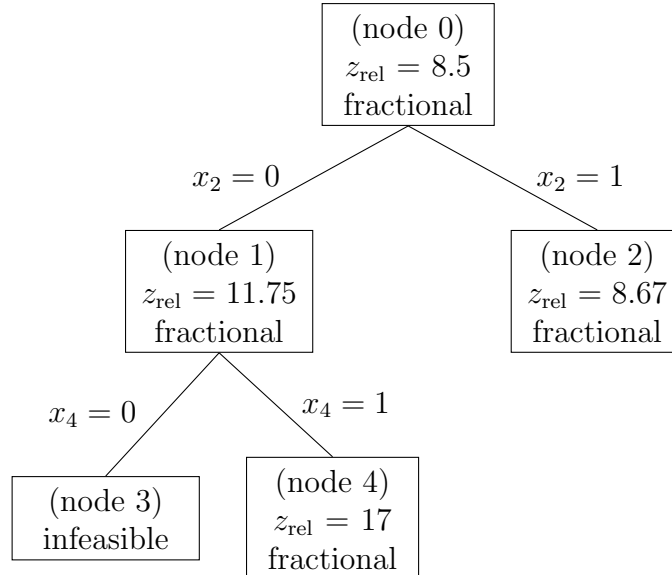
Figure 2.2: Branch-and-bound example: solution tree after stage 3

Up to this point, an integer solution has yet to be obtained. Let us now

return to node 2 and select x_3 as the next branching variable.

4. Apply integrality conditions on x_3 at node 2, with $x_2 = 1$. Solving the LP problem for $x_3 = 0$ gives

$$\text{(node 5)} \quad x_1 = 0.8, \ x_2 = 1, \ x_3 = 0, \ x_4 = 0, \ z_{\text{rel}} = 10.$$

which again is a fractional solution. On the other hand, solving the LP-relaxation for x_3 results in

$$\text{(node 6)} \quad x_1 = 0, \ x_2 = 1, \ x_3 = 1, \ x_4 = 0, \ z_{\text{rel}} = 10$$

which is an integer solution. This is a significant step forward since the integer solution identified provides an upper bound for the optimal objective value of the IP problem. Any node that has an objective value greater or equal to 10 can now be eliminated from the solution procedure. Further development of such nodes will not provide any improvement. In branch-and-bound jargon, it is said that these nodes can be *fathomed*. In this fashion, the waiting nodes 4 and 5 are *fathomed*. Moreover, node 3 is also *fathomed* since the associated LP-relaxation is found to be infeasible. Therefore, it is now proven that the solution at node 6 is the optimal integer solution. At this point, the search is terminated. The solution tree after stage 4 is shown in Figure 2.3.

During the solution of this example, only the case where just one variable took a fractional value at an examined node was encountered. Unfortunately this is not the case in most real problems. Fortunately though, contemporary branch-and-bound solvers include heuristic strategies for the selection of the next branching variable and the selection of the next node to be developed.

One very important feature, which is also the main disadvantage of the branch-and-bound method, is that it requires the solution of a series of LP-relaxations of the initial IP problem. The LP-relaxation of a given node provides a lower bound on the objective value of all subordinate nodes. If the LP-relaxations solved in the course of the procedure are strong, then fewer nodes will be examined and the optimal solution is obtained more quickly [Williams, 1990]. Therefore, it is
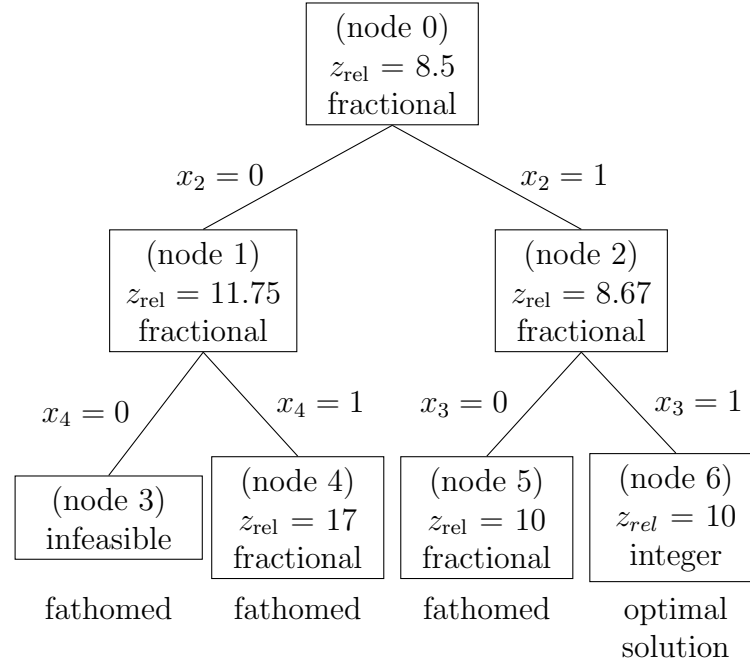
Figure 2.3: Branch-and-bound example: solution tree after stage 4

crucial that the LP-relaxations are well-constrained [Williams, 1993], or "tight" in branch-and-bound jargon.

An explicit enumeration of the example requires the solution of 2^4 LP problems (number of nodes for the full solution tree). However, using the branch-and-bound method the optimal point was identified after solving seven LP problems. For this reason, the method is also called implicit enumeration.

2.3.1.3 Hybrid methods

State-of the art algorithms for IP problems utilise a hybrid of the cutting-plane and branch-and-bound methods. These hybrid algorithms are called branch-and-cut and are proven to be the most successful in terms of computational efficiency. The cutting-plane scheme is applied at the top and at the nodes of the branch-and-bound tree. Adding cutting planes during the branch-and-bound search can speed up the solution procedure considerably [Mitchell, 2002]: the LP-relaxations solved at each node of the tree will be better constrained and therefore provide better (tighter) bounds.

2.3.2 Heuristic approaches

In the class of heuristic approaches the undisputed leader is a search technique developed by Lin and Kernighan [1973]. This tour improvement method is known as the Lin-Kernighan heuristic and it takes as an input a complete tour and tries to modify it in order to produce an alternative solution of lower cost. The Lin-Kernighan heuristic is widely used in conjunction with exact algorithms when attacking large problems, because it can successfully provide initial tours which are very close to the optimal solution. In fact, in many cases these initial tours are proven to be the optimal solutions. A variant of the initial heuristic developed by Helsgaun [2009] was the first to identify the optimal solution for the largest TSP instance (85900 cities) solved to date, at the time of writing this dissertation.

Another popular heuristic that is used in computational studies of TSP is simulated annealing. A 400-city problem was solved by Kirkpatrick *et al.* [1983] as a test problem in the paper that introduced the method to the scientific community. Finally, another well-established heuristic which is widely used in optimisation, the neural network technique reported by Hopfield and Tank [1985], was also tested using two travelling salesman problems.

2.4 Travelling Salesman & Computational Complexity Theory

One of the reasons the TSP has been studied so extensively is its relation to Computational Complexity Theory. This area is common ground for theoretical Computer Science and Mathematics and is concerned with the inherent difficulty of computational problems.

Before moving on, let us introduce the notions of polynomial (P) and non-deterministic polynomial (NP) problems. For the class P of computational problems there exist algorithms that solve them in polynomial time, whereas, roughly speaking, for class NP problems no such algorithms are known (yet?). To formally define the NP class one can say that it consists of all the decision problems ('yes' or 'no' problems) for which if the answer is positive, a certificate of correctness can be issued in polynomial time. However, if the answer is negative it is not

known whether the correctness can be checked in polynomial time.

Within the NP class there are the NP-complete problems. Now, an NP problem is NP-complete if every problem in NP can be reduced to it in polynomial time. The travelling salesman problem is NP-complete. Proving that an NP-complete problem can be solved in polynomial time, and therefore, P=NP, will fetch an award of one million dollars from the Clay Institute of Mathematics. Every year, tens of research articles appear in the bibliography claiming the award. A large percentage of these, base their proof on the discovery of a polynomial-time running algorithm that solves the TSP. None of them has survived close examination. The search continues.

2.5   Applications in Chemical Engineering

The TSP is found in a large number of applications across many scientific areas [Applegate *et al.*, 2007; Gutin and Punnen, 2002]. Those related to Chemical Engineering are the following:

a) Vehicle routing problem

TSP models are used to calculate optimal itineraries for vehicles that need to travel between a number of destinations. These can be delivery or pick-up trucks, laundry vans, school buses or a helicopter connecting the onshore base of an oil company to the offshore platforms [Cook, 2011]. A taxonomic review of the literature that refers to the problem can be found in [Eksioglu *et al.*, 2009].

b) Machine scheduling problem

The scheduling of repeated tasks to be carried out by industrial machines is a common setting for TSP applications. The different versions of the problem, along with other aspects, are described by Chen *et al.* [1998].

c) Genome mapping

An interesting application was reported by [Agarwala *et al.*, 2000]. The authors utilised TSP models to order chromosome markers while reconstructing genome maps.

d) X-ray diffractometer aiming in crystallography

A TSP model was used by Bland and Shallcross [1989] to determine sequences of X-ray diffraction measurements in crystallography. The travel costs in this case refer to the time required to reposition the crystals and to aim the X-ray instrument.

2.6   Conclusions

The Travelling Salesman Problem is a well-studied fundamental problem in the area of Mathematical Programming. The study of the problem led to the development of the disciplines of Integer and Mixed-Integer Programming. It has also acted as an engine of discovery for some important optimisation methods.

Today the problem holds a central role in Computational Complexity theory. Nevertheless, its importance is not only theoretical since it is found in numerous practical applications such as vehicle routing, machine scheduling and data organisation.

The development of a robust solution framework for attacking large travelling salesman problems remains an open challenge. The two essential components of a successful framework are: a tight mathematical formulation and an efficient solution algorithm.

This work is not concerned with the discovery of a novel solution method but rather with the development of a new modelling approach for the problem. A number of different mathematical formulations have been proposed for the TSP, some more well-accepted than others. None of the existing formulations includes fewer binary degrees of freedom than $O(n^2)$. It is the primary aim of the current work to develop a mathematical formulation which uses fewer than $O(n^2)$ binary variables.

Chapter 3

Formulations & computational studies

A general overview of the Travelling Salesman Problem was presented in Chapter 2. Among the various relevant aspects, a number of different mathematical programming formulations of the problem were presented. The choice of formulation is critically essential since the TSP belongs to the NP-complete class and the solution of large problems requires intense computational effort. Thus, it is crucial to model the problem in a fashion that will ease the computational burden on the solver.

Towards that end, a new family of formulations is presented in this chapter, which attempts to reduce the complexity of the problem by reducing the number of binary degrees of freedom. The computational efficiency of the proposed formulations is then tested and the results of the computational studies are presented at the end of the chapter.

3.1   Inspiration

The primary aim is to propose a mathematical description for the TSP that involves fewer binary variables than $O(n^2)$. The approach taken is based on work in Binary Arithmetic, and binary tree structures in particular.

Let us consider the binary tree in Figure 3.1. This is a directed graph where

the circles denote the vertices. The root vertex is at level 0 and the leaves of the tree are the vertices at level 3. The vertices in levels 1 and 2 are called intermediate vertices. An edge that connects the parent vertex with the left child is assigned the value 0 and it is assigned the value 1 if it reaches the right child. Thus, starting from the root, to get to leaf-1 one must follow the edge-sequence 000. Similarly, to reach leaf-6 the only way is to follow the path 101.
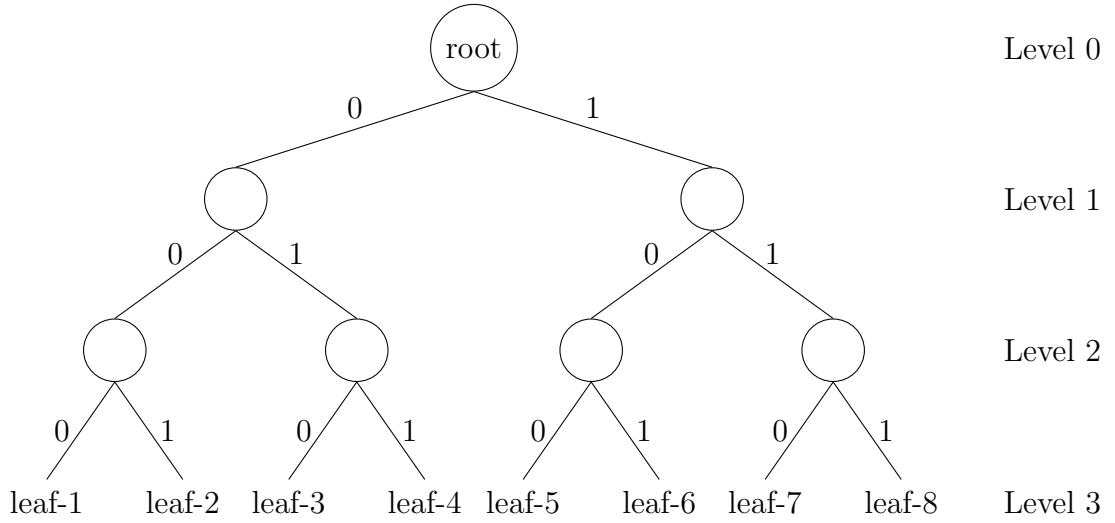
Figure 3.1: Binary tree with 8 leaves

The binary tree in Figure 3.1 is *regular* because each intermediate vertex has two children, and it is *full* because all its leaves are at the same level. All binary trees considered in this work are *regular* and *full*.

It is apparent that one can store up to 8 objects on the leaves of this tree to create a binary data structure. The position of a certain object will be described by a binary string. Can these objects be the cities of a travelling salesman problem? Yes, the cities can be placed sequentially on the leaves according to their position in the tour.

Let us explore the scheme where the set of cities is repeatedly partitioned into left-right orientation from the root to the last level of a binary tree, where the cities are allocated on the leaves according to their order in the optimal tour. The proposed formulation is explained in detail in the following section.

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3.2 Novel formulation

Let us consider the graph $G = \{V, A\}$, where $V = \{1, 2, \ldots, n\}$ is the set of vertices (cities) and $A = \{(i, j) : i, j \in V\}$ the set of arcs, on which the Hamiltonian cycle of minimum cost has to be identified. The length of the arcs is given by the cost matrix $C = \{c_{ij} : (i, j) \in A\}$. Also, consider the binary tree $B = \{L, P\}$ where $L = \{1, 2, \ldots, nl\}$ is the set of levels and $P = \{1, 2, \ldots, np\}$ is the set of leaves (available positions for the allocation of objects). It is a property of binary trees that

$$np = 2^{nl}. \tag{3.1}$$

Now, for the binary tree structure to have enough positions to store the sequence of vertices for the optimal cycle, it is required that $np \geq n$. If n is an exact power of 2 then obviously $np = n$. For the rest of the analysis the general case where n is not an exact power of 2 is considered. Thus, $np > n$ and the number of levels is equal to

$$nl = \lceil log_2(n) \rceil \tag{3.2}$$

where the ceiling function $\lceil . \rceil$, applied on a real number, returns the smallest integer number greater than the real number.

3.2.1 Basics

Here the basics of the proposed formulation are discussed. As already mentioned, the position of a city on the tree will be coded by a binary string. For that purpose, let us introduce the binary variables r_{il}, for $i \in V$; $l \in L$, such that:

$$r_{il} = \begin{cases} 0, & \text{if city } i \text{ is directed left at level } l \\ 1, & \text{if city } i \text{ is directed right at level } l. \end{cases} \tag{3.3}$$

At each level l of the tree, every city is allocated a left or right orientation. Therefore, $n\lceil log_2(n) \rceil$ of these binary variables are needed to describe the position of all the cities. Decoding the binary string, the position of vertex i on the cycle is given in decimal base by

$$pos_i = 1 + \sum_{l=1}^{nl} 2^{nl-l} r_{il}; \quad i = 1, 2, \ldots, n \tag{3.4}$$

Assuming that the starting point of the tour is always vertex 1:

$$r_{1,l} = 0; \quad l = 1, 2, \ldots, nl \tag{3.5}$$

and, since there are more leaves than cities the position of the remaining vertices on the optimal tour is restricted by

$$1 \leq \sum_{l=1}^{nl} 2^{nl-l} r_{il} \leq n - 1; \quad i = 2, 3, \ldots, n \tag{3.6}$$

To determine the partitioning of cities to left-right branching at each level, the following set of constraints is necessary:

$$\sum_{i=1}^{n} r_{il} = \sum_{k=1}^{n} t_{kl}; \quad l = 1, 2, \ldots, nl \tag{3.7}$$

The parameters t_{kl} are calculated using Algorithm 3.1 which defines the 'target' binary strings since the number of leaves of the tree is generally greater than the number of cities in the problem.

Algorithm 3.1: Nodal binary string analysis

  for $k = 1$ to n **do**
    $temp = k - 1$
    for $l = nl$ to 1 **do**
      $t_{kl} = temp \mod 2$
      $temp = \lfloor temp/2 \rfloor$
    end for
  end for

As an aside, the set of constraints given by Equation (3.7) is equivalent to

$$\sum_{i=1}^{n} r_{il} = \frac{n}{2}; \quad l = 1, 2, \ldots, nl \tag{3.8}$$

when the cardinality of set V is an exact power of 2.

The constraints defined in equation (3.7) are not sufficient to allocate a unique binary string to a city. For this reason, the variables z_{ik}, for $i \in V$; $k \in P$, are defined such that:

$$
z_{ik} = \begin{cases} 0, & \text{if city } i \text{ is not allocated on leaf } k \\ 1, & \text{if city } i \text{ is allocated on leaf } k. \end{cases} \tag{3.9}
$$

The z_{ik} variables are continuous and constrained within $[0, 1]$. They will be forced to take the value of 0 or 1 by the binary variables r_{il}, *viz.*

$$
z_{ik} \leq \alpha(t_{kl}) + \beta(t_{kl})r_{il}; \quad i, k = 1, 2, \ldots, n; \; l = 1, 2, ..., nl \tag{3.10}
$$

$$
z_{ik} \geq 1 - \sum_{l=1}^{nl} [\alpha(1 - t_{kl}) + \beta(1 - t_{kl})r_{il}]; \quad i, k = 1, 2, \ldots, n. \tag{3.11}
$$

where the functions $\alpha(v)$ and $\beta(v)$ are defined as

$$
\alpha(v) = \begin{cases} 1, & \text{if } v = 0 \\ 0, & \text{if } v = 1 \end{cases} \tag{3.12}
$$

$$
\beta(v) = \begin{cases} -1, & \text{if } v = 0 \\ 1, & \text{if } v = 1. \end{cases} \tag{3.13}
$$

Finally, it is necessary to use the variables x_{ij}, for $i, j \in V$, such that:

$$
x_{ij} = \begin{cases} 0, & \text{if arc } (i, j) \text{ is not present in the optimal tour} \\ 1, & \text{if arc } (i, j) \text{ is present in the optimal tour} \end{cases} \tag{3.14}
$$

Unlike existing formulations, the variables x_{ij} are continuous and constrained within $[0, 1]$ in this work. These variables can be forced to take binary values using the following constraints [Millar and Cyrus, 2000]:

$$
z_{ik} + z_{j,k+1} - 1 \leq x_{ij}; \quad i, j = 1, 2, \ldots n; \; k = 1, 2, \ldots, n - 1 \tag{3.15}
$$

$$z_{i,n} + z_{j,1} - 1 \leq x_{ij}; \quad i, j = 1, 2, \ldots, n \tag{3.16}$$

Constraints (3.15) – (3.16) force the variables x_{ij} to take the value of 1 if arc (i, j) is included in the optimal tour. Otherwise, the lower bound is inactive. Due to the fact that variables x_{ij} appear in the objective function multiplied by positive coefficients, they will be driven to their lower bound, which is 0, if the constraints do not enforce a value of 1.

Equations (3.15) – (3.16) define $\mathcal{O}(n^3)$ constraints. The issue of reducing the number of these adjacency constraints is examined next.

3.2.2 Adjacency of binary leaves

Consider two cities i and j, for $i, j \in V$, which occupy consecutive positions on the leaves of a binary data structure. Assuming that city j is positioned immediately after city i, it is true that:

$$pos_j - pos_i = 1 \tag{3.17}$$

or using equation (3.4):

$$\sum_{l=1}^{nl} 2^{nl-l}(r_{jl} - r_{il}) = 1 \tag{3.18}$$

A link between equation (3.18) and the x_{ij} variables must be established, such that:

$$x_{ij} = 1, \quad \text{if} \quad \sum_{l=1}^{nl} 2^{nl-l}(r_{jl} - r_{il}) = 1 \tag{3.19}$$

$$0 \leq x_{ij} \leq 1, \quad \text{if} \quad \sum_{l=1}^{nl} 2^{nl-l}(r_{jl} - r_{il}) \neq 1 \tag{3.20}$$

It is desired to reduce the order of adjacency constraints (3.15) – (3.16) to less than $\mathcal{O}(n^3)$. To achieve this, the constraints must be derived using the three indices $i, j \in V$ and $l \in L$. Recall that the cardinality of set V is n and that of set L is $nl = \lceil log_2(n) \rceil$.

Theorem 3.1. *Given two cities i and j and the binary representation of their positions, pos_i and pos_j, in the tour by variable sets $r_{il}, r_{jl} \in \{0, 1\}$ with $l =$*

$1, 2, \ldots nl$, *then if and only if the cities are allocated adjacently such that the position of city j is greater by 1 from the position of city i, $pos_j = pos_i + 1$, the following properties hold:*

Property A:

There exists exactly one and only one $l' \in L$ such that

$$r_{il'} = 0 \ \text{ and } \ r_{jl'} = 1 \tag{3.21}$$

Property B:

For $1 \le l < l'$ $(l = 1, 2, \ldots, (l' - 1))$

$$r_{il} = r_{jl} \ \text{ (either both 0, or both 1)} \tag{3.22}$$

Property C:

For $l' < l \le nl$ $(l = (l' + 1), (l' + 2), \ldots, nl)$

$$r_{il} = 1 \ \text{ and } \ r_{jl} = 0 \tag{3.23}$$

The converse is also true: if the three properties do not hold simultaneously for a pair of cities i and j, then these are not placed on adjacent leaves of the binary tree (i.e. the arc (i, j) is not present in the tour).

The following lemma:

Lemma 3.1. *If and only if $pos_j = pos_i$ then $r_{il} = r_{jl}$, $\forall \, l \in L$.*

Lemma 3.2. *If and only if $pos_j > pos_i$ then there exists an $l' = \min\limits_{l \in L} l$ for which $r_{il'} = 0$, $r_{jl'} = 1$ and $r_{il''} = r_{jl''}$, with $l'' = 1, 2, \ldots, l' - 1$.*

and the formulae given below are used to prove the theorem.

$$\sum_{i=1}^{k} 2^{k-i} = 2^k - 1 \tag{3.24}$$

$$\sum_{i=1}^{m} 2^{k-i} = 2^k - 2^{k-m} \tag{3.25}$$

$$\sum_{\substack{i= \\ m+1}}^{k} 2^{k-i} = \sum_{i=1}^{k} 2^{k-i} - \sum_{i=1}^{m} 2^{k-i} = 2^{k-m} - 1 \tag{3.26}$$

Proof. Let $pos_j > pos_i$. If properties A, B & C hold simultaneously then

$$pos_j - pos_i = \sum_{l=1}^{l'-1} 2^{nl-l}(r_{jl} - r_{il}) - 2^{nl-l'}(r_{jl} - r_{il}) + \sum_{l=l'+1}^{nl} 2^{nl-l}(r_{jl} - r_{il})$$

$$= 2^{nl-l'} - \sum_{l=l'+1}^{nl} 2^{nl-l} = 2^{nl-l'} - (2^{nl-l'} - 1) = 1.$$

The converse must also be true. Consider the three cases:

1. Property A does not hold

   Taking into account Lemmas 3.1 – 3.2, property A does not hold when $r_{il''} = 0$ and $r_{jl''} = 1$ for one or more $l'' \in [l'+1, nl]$. This also violates property C.

   Let us examine the case where this happens only for one index l''. Thus,

   $$r_{il'} = 0, \ r_{jl'} = 1$$
   $$r_{il''} = 0, \ r_{jl''} = 1.$$

   The difference between the two positions is:

   $$pos_j - pos_i = \sum_{l=1}^{l'-1} 2^{nl-l}(r_{jl} - r_{il}) + 2^{nl-l'}(r_{jl'} - r_{il'}) + \sum_{l=l'+1}^{l''-1} 2^{nl-l}(r_{jl} - r_{il}) +$$

   $$2^{nl-l''}(r_{jl''} - r_{il''}) + \sum_{l=l''+1}^{nl} 2^{nl-l}(r_{jl} - r_{il})$$

   $$= 2^{nl-l'} + \sum_{l=l'+1}^{l''-1} 2^{nl-l}(r_{jl} - r_{il}) + 2^{nl-l''} + \sum_{l=l''+1}^{nl} 2^{nl-l}(r_{jl} - r_{il}).$$

   The minimum of this subtraction is achieved when $r_{il} = 1$ and $r_{jl} = 0$ in both summations. Hence,

   $$pos_j - pos_i \geq 2^{nl-l'} - \sum_{l=l'+1}^{l''-1} 2^{nl-l} + 2^{nl-l''} - \sum_{l=l''+1}^{nl} 2^{nl-l}$$

$$\geq 2^{nl-l'} - (\sum_{l=1}^{nl} 2^{nl-l} - \sum_{l=1}^{l'} 2^{nl-l} - \sum_{l=l''}^{nl} 2^{nl-l}) +$$

$$2^{nl-l''} - (2^{nl-l''} - 1)$$

$$\geq 2^{nl-l'} - (2^{nl} - 1) + (2^{nl} - 2^{nl-l'}) + (2^{nl-(l''-1)} - 1) + 1$$

$$\geq 2 \cdot 2^{nl-l''} + 1$$

$$\geq 3.$$

In the same fashion, the statement $pos_j - pos_i > 1$ can be proven to be true if the above occurs for more than one index l''. Thus, if property A is violated, the cities are not placed in consecutive order.

2. Property B does not hold. It follows from Lemma 3.2 that if property B does not hold then properties A and C do not hold either.

3. Property C does not hold. For this to happen, there are two possible scenarios:

   (a) There is at least one $l'' \in [l'+1, nl]$ for which $r_{il''} = 0$ and $r_{jl''} = 1$. This violates property A.

   (b) There exists at least one $l'' \in [l'+1, nl]$ for which $r_{il''} = r_{jl''}$.

   Let us assume that there is only one such index l''. The difference between the two positions is:

$$pos_j - pos_i = \sum_{l=1}^{l'-1} 2^{nl-l}(r_{jl} - r_{il}) + 2^{nl-l'}(r_{jl'} - r_{il'}) + \sum_{l=l'+1}^{l''-1} 2^{nl-l}(r_{jl} - r_{il}) +$$

$$2^{nl-l''}(r_{jl''} - r_{il''}) + \sum_{l=l''+1}^{nl} 2^{nl-l}(r_{jl} - r_{il})$$

$$= 2^{nl-l'} + \sum_{l=l'+1}^{l''-1} 2^{nl-l}(r_{jl} - r_{il}) + \sum_{l=l''+1}^{nl} 2^{nl-l}(r_{jl} - r_{il})$$

   The minimum of this subtraction is achieved when $r_{il} = 1$ and $r_{jl} = 0$

in both summations. Thus,

$$pos_j - pos^i \geq 2^{nl-l'} - (2^{nl} - 1) + (2^{nl} - 2^{nl-l'}) +$$
$$(2^{nl-(l''-1)} - 1) - (2^{nl-l''} - 1)$$
$$\geq 2 \cdot 2^{nl-l''} - 2^{nl-l''} + 1$$
$$\geq 2^{nl-l''} + 1$$
$$\geq 2.$$

Similarly, the statement $pos_j - pos_i > 1$ can be proven to be true if the above occurs for more than one index l''. It is obvious that if property C does not hold then the cities are not allocated on adjacent leaves.

□

The challenge to face now is how to utilise the results of Theorem 3.1. At first, it is essential to construct a test in order to check if two cities follow the same branch of the tree at a given level. For this purpose, the variables e_{ijl}, for $i, j \in V; \ l \in L \setminus \{nl\}$ are defined as follows:

$$e_{ijl} = \begin{cases} 0, & \text{if cities } i \text{ and } j \text{ follow opposite branches at level } l \\ 1, & \text{if cities } i \text{ and } j \text{ follow the same branch at level } l. \end{cases} \quad (3.27)$$

The variables e_{ijl} are continuous and constrained within $[0, 1]$, but can be forced to take binary values by using the following set of constraints:

$$1 - (r_{il} + r_{jl}) \leq e_{ijl}; \quad i, j = 1, 2, \ldots, n; \ i \neq j; \ l = 1, 2, \ldots, nl - 1 \quad (3.28)$$
$$(r_{il} + r_{jl}) - 1 \leq e_{ijl}; \quad i, j = 1, 2, \ldots, n; \ i \neq j; \ l = 1, 2, \ldots, nl - 1. \quad (3.29)$$

Constraints (3.28) – (3.29) will force the variable e_{ijl} to take the value of 1 if the binary variables r_{il} and r_{jl} of the two cities i and j, respectively, are equal at level l. If this is not the case, the variable is left loose within its bounds, and, due to the fact that it is associated with variables x_{ij} (see equations (3.30) – (3.32)), it will attain the value of its lower bound which is 0. The equality test is not required for the last level, $l = nl$.

The ultimate goal is to impose lower bounds equal to 1 on the x_{ij} variables, if the properties of Theorem 3.1 are met for each pair of cities i and j. To achieve that, the following logical checks are employed:

$$x_{ij} \geq \underbrace{[(1 - r_{i,1}) + r_{j,1} - 2]}_{\text{Property A}} +$$

$$\underbrace{\left[\sum_{l=2}^{nl} [r_{il} + (1 - r_{jl})] - 2(nl - 1) \right]}_{\text{Property C}} + 1;$$

$$i, j = 1, 2, \ldots, n \qquad (3.30)$$

$$x_{ij} \geq \underbrace{[(1 - r_{il'}) + r_{jl'} - 2]}_{\text{Property A}} +$$

$$\underbrace{\left[\sum_{l=1}^{l'-1} e_{ijl} - (l' - 1) \right]}_{\text{Property B}} +$$

$$\underbrace{\left[\sum_{l=l'+1}^{nl} [r_{il} + (1 - r_{jl})] - 2(nl - (l' + 1) + 1) \right]}_{\text{Property C}} + 1;$$

$$i, j = 1, 2, \ldots, n; \ l' = 2, 3, \ldots, (nl - 1) \qquad (3.31)$$

$$x_{ij} \geq \underbrace{[(1 - r_{i,nl}) + r_{j,nl} - 2]}_{\text{Property A}} +$$

$$\underbrace{\left[\sum_{l=1}^{nl-1} e_{ijl} - (nl - 1) \right]}_{\text{Property B}} + 1;$$

$$i, j = 1, 2, \ldots, n \qquad (3.32)$$

Constraints $(3.30) - (3.32)$ impose the adjacency properties and are used for $nl \geq 3$. For $nl \leq 2$ only the set of constraints given by (3.30) is required.

3.2.3 Asymmetric Travelling Salesman model

It is now time to put the various components together and build the asymmetric TSP model. Two new formulations are suggested. The only difference between the two are the adjacency constraints. The basic formulation is as follows:

$$\text{min.} \quad \sum_{i=1}^{n}\sum_{j=1}^{n} c_{ij}x_{ij} \tag{3.33}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} x_{ij} = 1; \quad j = 1, 2, ..., n \tag{3.34}$$

$$\sum_{j=1}^{n} x_{ij} = 1; \quad i = 1, 2, ..., n \tag{3.35}$$

$$\sum_{i=1}^{n} z_{ik} = 1; \quad k = 1, 2, ..., n \tag{3.36}$$

$$\sum_{k=1}^{n} z_{ik} = 1; \quad i = 1, 2, ..., n \tag{3.37}$$

$$z_{ik} \leq \alpha(t_{kl}) + \beta(t_{kl})r_{il}; \quad l = 1, 2, ..., nl; \ i, k = 1, 2, ..., n \tag{3.38}$$

$$z_{ik} \geq 1 - \sum_{l=1}^{nl} [\alpha(1 - t_{kl}) + \beta(1 - t_{kl})r_{il}]; \quad i, k = 1, 2, ..., n \tag{3.39}$$

$$x_{i,1} = z_{i,n}; \quad i = 1, 2, ..., n \tag{3.40}$$

$$\sum_{i=1}^{n} r_{il} = \sum_{k=1}^{n} t_{kl}; \quad l = 1, 2, ..., nl \tag{3.41}$$

$$r_{1,l} = 0; \quad l = 1, 2, \ldots, nl \tag{3.42}$$

$$1 \leq \sum_{l=1}^{nl} 2^{nl-l} r_{il} \leq n - 1; \quad i = 2, 3, ..., n \tag{3.43}$$

$$0 \leq x_{ij} \leq 1; \quad i, j = 1, 2, ..., n \tag{3.44}$$

$$0 \leq z_{ik} \leq 1; \quad i, k = 1, 2, ..., n \tag{3.45}$$

$$r_{il} = \{0, 1\}; \quad i = 1, 2, ..., n; \ l = 1, 2, ..., nl \tag{3.46}$$

$$+ \ \text{adjacency constraints.}$$

It is required that city $i = 1$ is the starting and finishing point of the tour.

Thus, constraint (3.40) is used to close the loop. Moreover, the self-looping arcs are eliminated by setting $c_{ii} = \infty$. Constraints (3.34) – (3.35) ensure that each city is the end-point of one outgoing arc and the start-point of one incoming arc. Also, constraints (3.36) – (3.37) guarantee the uniqueness of the allocation of each city to each position and vice versa. In addition, the tightening constraints (3.43) are included. These constraints are redundant, but they can be used in order to tighten the feasible domain.

On one hand, for the first formulation named Tree-1, the adjacency constraints are given by equations (3.15) – (3.16), thus constraint (3.40) is excluded. On the other hand, the adjacency constraints for the second formulation called Tree-2 are defined by equations (3.28) – (3.32). Table 3.1 shows the number of binary and continuous variables for the two formulations and the cardinality of the constraints set.

Table 3.1: Size of proposed ATSP formulations

Formulation	Binary variables	Continuous variables	Constraints
Tree-1	$\mathcal{O}(n\lceil log_2(n)\rceil)$	$\mathcal{O}(n^2)$	$\mathcal{O}(n^3)$
Tree-2	$\mathcal{O}(n\lceil log_2(n)\rceil)$	$\mathcal{O}(n^2\lceil log_2(n)\rceil)$	$\mathcal{O}(n^2\lceil log_2(n)\rceil)$

3.2.4   Manhattan Travelling Salesman model

Let us now consider the asymmetric TSP where the distance between the cities is calculated using the rectilinear metric. This is referred to as the Manhattan-TSP. The distance between two points in the rectilinear metric is commonly known as the Manhattan distance. With reference to Figure 3.2, the Manhattan distance between points 1 and 2 (solid line) is given by

$$d_M = |x_1 - x_2| + |y_1 - y_2| \tag{3.47}$$

whereas the Euclidean distance (dashed line) is given by

$$d_E = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2}. \tag{3.48}$$
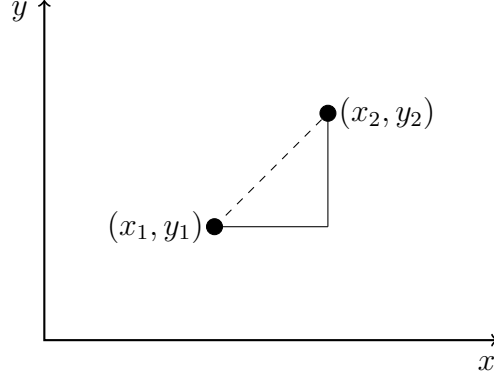
Figure 3.2: Manhattan distance on a system of Cartesian coordinates

Let us assume that the pair of coordinates $(x_i^{(0)}, y_i^{(0)})$ for each city is available. It is then easy to assign coordinates (x, y) to a leaf of the binary tree according to which city is placed there:

$$x_k = \sum_{i=1}^{n} x_i^{(0)} z_{ik}; \quad k = 1, 2, \ldots, n \tag{3.49}$$

$$y_k = \sum_{i=1}^{n} y_i^{(0)} z_{ik}; \quad k = 1, 2, \ldots, n. \tag{3.50}$$

The pair of variables (x_k, y_k) represents the coordinates of pos_k. It follows that the rectilinear distance between two adjacent leaves, k and $k+1$, can be calculated by

$$d_{M_k} = l_k^{(x)} + l_k^{(y)}; \quad k = 1, 2, \ldots, n \tag{3.51}$$

where

$$l_k^{(x)} \equiv |x_k - x_{k+1}|; \quad k = 1, 2, \ldots, n-1 \tag{3.52}$$

$$l_k^{(y)} \equiv |y_k - y_{k+1}|; \quad k = 1, 2, \ldots, n-1. \tag{3.53}$$

Equations (3.52) – (3.53) can be replaced by the following inequalities:

$$-l_k^{(x)} \leq x_k - x_{k+1} \leq l_k^{(x)}; \quad k = 1, 2, \ldots, n-1 \tag{3.54}$$

$$-l_k^{(y)} \leq y_k - y_{k+1} \leq l_k^{(y)}; \quad k = 1, 2, \ldots, n-1. \tag{3.55}$$

Following the above, a unique formulation for the Manhattan-TSP may be constructed if the coordinates of all the cities are known. The proposed formulation is:

$$\text{min.} \quad \sum_{k=1}^{n} (l_k^{(x)} + l_k^{(y)}) \tag{3.56}$$

$$\text{s.t.} \quad \sum_{i=1}^{n} z_{ik} = 1; \quad k = 1, 2, ..., n \tag{3.57}$$

$$\sum_{k=1}^{n} z_{ik} = 1; \quad i = 1, 2, ..., n \tag{3.58}$$

$$z_{ik} \leq \alpha(t_{kl}) + \beta(t_{kl}) r_{il}; \quad l = 1, 2, ..., nl; \; i, k = 1, 2, ..., n \tag{3.59}$$

$$z_{ik} \geq 1 - \sum_{l=1}^{nl} [\alpha(1 - t_{kl}) + \beta(1 - t_{kl}) r_{il}]; \quad i, k = 1, 2, ..., n \tag{3.60}$$

$$\sum_{i=1}^{n} r_{il} = \sum_{k=1}^{n} t_{kl}; \quad l = 1, 2, ..., nl \tag{3.61}$$

$$1 \leq \sum_{l=1}^{nl} 2^{nl-l} r_{il} \leq n - 1; \quad i = 2, 3, ..., n \tag{3.62}$$

$$x_k = \sum_{i=1}^{n} x_i^{(0)} z_{ik}; \quad k = 1, 2, \ldots, n \tag{3.63}$$

$$y_k = \sum_{i=1}^{n} y_i^{(0)} z_{ik}; \quad k = 1, 2, \ldots, n \tag{3.64}$$

$$-l_k^{(x)} \leq x_k - x_{k+1} \leq l_k^{(x)}; \quad k = 1, 2, \ldots, n - 1 \tag{3.65}$$

$$-l_n^{(x)} \leq x_n - x_1 \leq l_n^{(x)} \tag{3.66}$$

$$-l_k^{(y)} \leq y_k - y_{k+1} \leq l_k^{(y)}; \quad k = 1, 2, \ldots, n - 1 \tag{3.67}$$

$$-l_n^{(y)} \leq y_n - y_1 \leq l_n^{(y)} \tag{3.68}$$

$$x_k, y_k, l_k^{(x)}, l_k^{(y)} \geq 0; \quad k = 1, 2, \ldots, n \tag{3.69}$$

$$0 \leq z_{ik} \leq 1; \quad i, k = 1, 2, \ldots, n \tag{3.70}$$

$$r_{il} = \{0, 1\}; \quad i = 1, 2, \ldots, n; \; l = 1, 2, \ldots, nl \tag{3.71}$$

Constraints (3.66) and (3.68) are used to close the route. The Manhattan formulation features $\mathcal{O}((n\lceil \log_2(n) \rceil))$ binary variables, $\mathcal{O}(n^2)$ continuous variables

and $\mathcal{O}(n^2)$ constraints.

3.3 Computational studies

The computational performance of the proposed formulations is tested in practice using small instances of the problem. Furthermore, the efficiency of Tree-1 and Tree-2 formulations is compared against the efficiency of the MTZ formulation [Miller *et al.*, 1960] and the Wong formulation [Wong, 1980], on the basis of the strength of their LP relaxation. For the computational studies, the problems are modelled in GAMS™ [Brooke *et al.*, 1992] and solved using CPLEX® 10.1.1 [GAMS, 2010] on an ASUS™ Chassis computer with 2.21 GHz CPU. The CPLEX® 10.1.1 solver employs a hybrid of the branch-and-bound and cutting plane methods, *i.e.* a branch-and-cut algorithm.

3.3.1 ATSP case studies

The ATSP formulations, Tree-1 and Tree-2, are applied to three small problems: (i) $n = 8$; (ii) $n = 10$ and (iii) $n = 12$. The asymmetric cost matrices for (i) and (ii) are produced using a random-number generator. For the third problem the cost matrix is symmetric and the data are part of the *gr17* instance reported by Reinelt [1991]. The cost matrices of all three problems are given in Appendix A. Table 3.2 summarises the optimal solutions of the three instances. The number of nodes refers to the nodes of the solution tree (branch-and-bound tree) examined.

The three problems are also modelled according to Miller *et al.* [1960]. The tours reported in Table 3.2 are in agreement with the optimal tours obtained when solving the MTZ models.

Let us now observe closely the results reported in Table 3.2. The Tree-1 formulation emerges as superior to the Tree-2 formulation in terms of computational performance. Firstly, the solver successfully produced a solution for the largest instance tested, $n = 12$, when using the Tree-1 formulation, whereas for the Tree-2 case it failed to converge after 1 day of execution time. Moreover, the solver requires considerably less CPU time to converge for cases $n = 8$ and $n = 10$ when implementing Tree-1. The large gap in performance becomes more

Table 3.2: Solution report for ATSP case studies

Formulation	Optimal tour	Nodes	CPU time (s)
	$n = 8$		
Tree-1	31	3	0.3
Tree-2	31	78	1.8
	$n = 10$		
Tree-1	70	2	0.4
Tree-2	70	602	33.7
	$n = 12$		
Tree-1	1799	3200	362.8
Tree-2	not solved after 1 day of execution		

apparent when comparing the nodes examined during the branch-and-cut scheme for the two formulations. For $n = 10$ the solver visits 2 and 602 nodes for Tree-1 and Tree-2, respectively.

This difference arises due to one crucial factor on which the computational performance of a branch-and-bound algorithm (and correspondingly of a branch-and-cut algorithm) depends. This is the quality of the LP-relaxations solved at each node of the solution tree. If these LP-relaxations are strong, then the solver will examine fewer nodes and will converge to the optimal solution faster [Williams, 1990].

Clearly, Tree-1 produces stronger LP-relaxations than the Tree-2 formulation. This is due to the fact that the adjacency constraints $(3.30) - (3.32)$ which are part of Tree-2 formulation involve a large number of binary variables and continuous variables in comparison to the adjacency constraints $(3.15) - (3.16)$ which are included in the Tree-1 formulation. Hence, the former constraints are not as tight as the latter.

The formulations were also applied to larger instances ($12 < n \leq 20$) without any success. The solver failed to converge after one day of execution. For all intents and purposes, the running time for small instances like the ones

examined here should not be more than a few minutes, as reported elsewhere [Applegate *et al.*, 2007].

3.3.2 Manhattan-TSP case studies

The Manhattan formulation is applied to two problems with $n = 8$ and $n = 10$ cities. The coordinates for the two problems are those of real cities and are given in Appendix A. The computational performance of the Manhattan formulation is compared against the performance of the Tree-1 formulation. When implementing Tree-1, the cost matrix was calculated using the set of coordinates prior to the execution of the solution algorithm. Table 3.3 shows the solution report for the aforesaid computational studies. The optimal itineraries for the two instances are presented in Figures 3.3(a) and 3.3(b).

Table 3.3: Solution report for Manhattan-TSP case studies

Instance	Optimal tour	Nodes	CPU time (s)
	$n = 8$		
Manhattan	4630.74	132	1.8
Tree-1	4630.74	49	1.2
	$n = 10$		
Manhattan	289.1	3861	127.6
Tree-1	289.1	16	1.1

On the basis of the above examples, the computational performance of the Manhattan model appears to be worse than that of Tree-1. For the former, the solver visits many more nodes of the solution tree and, also, it requires more CPU time to converge.

As an aside, the solver failed to converge when the Manhattan model was tested for instances with $(12 < n \leq 20)$. During the solution of an instance of $n = 15$ cities the memory demand for the storage of the solution tree exceeded 100 megabytes.

(a) $n = 8$

(b) $n = 10$
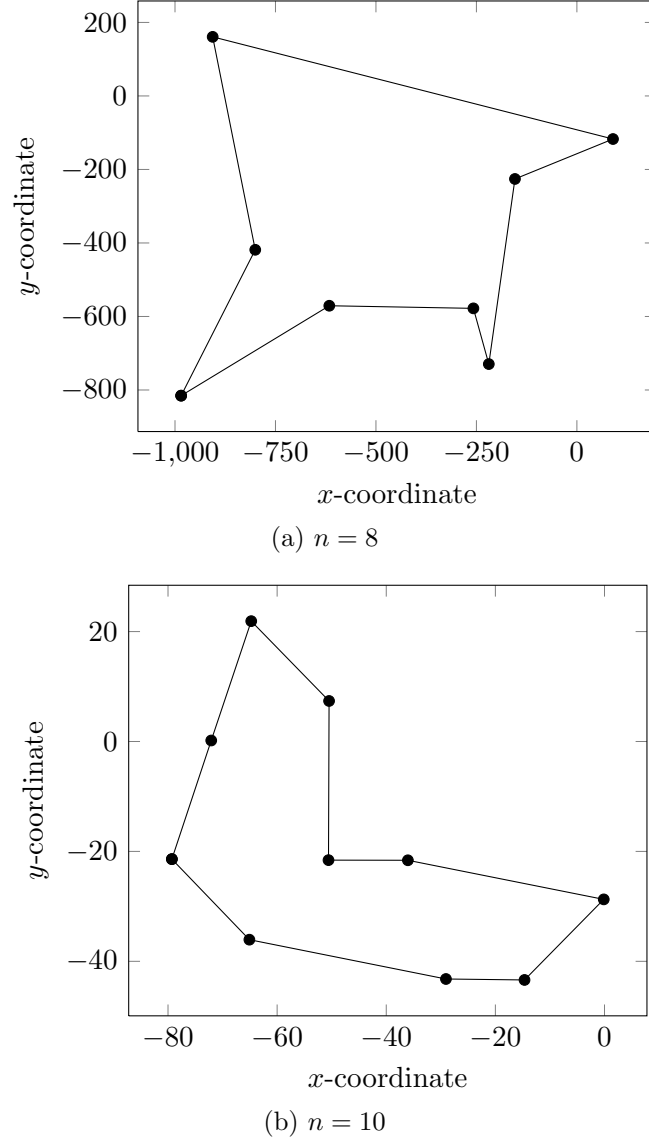
Figure 3.3: Optimal itinerary for Manhattan-TSP case studies

3.3.3 Comparison with existing formulations

The next step in the evaluation of the proposed formulations is to compare their computational efficiency with those of existing formulations. Let us focus our interest on the more general ATSP formulations, Tree-1 and Tree-2. The Manhattan formulation is not included in the analysis.

It is customary to conduct such a comparison by using the LP-relaxations of

the examined formulations. The Tree-1 and Tree-2 formulations are compared against the MTZ formulation [Miller *et al.*, 1960] and the Wong formulation [Wong, 1980]. The MTZ formulation is proven to be one of the weakest among the existing formulations, while the Wong formulation is proven to be one of the strongest [Öncan *et al.*, 2009]. Three TSP instances found in TSPLIB [Reinelt, 1991] are modelled with respect to the four formulations. The LP relaxation of all four models is solved and the optimal value of the relaxed objective function, z_{LP}^{rel} is reported in Table 3.4. The length of the optimal tour of each problem is also given in Table 3.4.

Table 3.4: Comparison of LP-relaxations: optimal objective function value

Problem	z_{LP}^{rel}				Optimal tour
	Tree-1	Tree-2	MTZ	Wong	
gr17	1652	1652	1656	2085	2085
fri26	833	833	835.48	937	937
dantzig42	533	532	535.65	697	699

It is helpful to recall our discussion in Section 2.2.5: for an efficient formulation, the gap between the optimal objective value of the LP-relaxation, z_{LP}^{rel}, and the optimal objective value of the original problem should be small. The results of Table 3.4 confirm that Wong is more efficient than MTZ. It is notable that for Wong the gap for *gr17* and *fri26* is 0% and it is only 2.8% for the *dantzig42* problem.

As for the proposed formulations, they are ranked in the last two places. The LP-relaxations of Tree-1 and Tree-2 are shown to be slightly weaker than those of MTZ for all three instances. Hence, it is safe to place them at the bottom of the computational efficiency scale of the existing TSP formulations. Tree-1 and Tree-2 are proved to be poorly constrained.

The values of the LP-relaxations for the two smaller problems are equal for Tree-1 and Tree-2. Nevertheless, as already seen in Section 3.3.1 the Tree-1 formulation is more computationally efficient than Tree-2.

3.4 Conclusions

A novel family of mathematical formulations, originating from work in Binary Arithmetic and binary tree structures in particular, was developed for the Travelling Salesman Problem. The proposed mathematical description succeeds in decreasing the binary degrees of freedom for the problem to $O(n\lceil\log_2(n)\rceil)$.

The three new formulations are named Tree-1, Tree-2 and Manhattan. The first two apply to the general case of the asymmetric TSP while the third applies only to the Manhattan-TSP case (the distance between two cities is calculated on the basis of the rectilinear metric).

The results of test studies suggest that the computational performance of the new formulations in practice is poor. Computational tests have shown that using the three formulations to model problems with a number of cities $12 < n \leq 20$ leads to excessive computational effort.

In comparison to Tree-1, the Tree-2 formulation emerges as inferior in terms of computational performance. When implementing Tree-2 the solver requires notably more CPU time and it visits far more nodes of the solution tree than when implementing Tree-1, on the same problems. Also, the results in Section 3.3.2 suggest that it is safe to discard the Manhattan formulation in favour of Tree-1.

The computational efficiency of the Tree-1 and Tree-2 formulations was compared to that of the Wong formulation [Wong, 1980] and to that of the MTZ formulation [Miller *et al.*, 1960]. The criterion for the comparison was the strength of the LP-relaxation of the formulations. Both Tree-1 and Tree-2 are shown to have weaker LP-relaxations than those of Wong and MTZ.

The comparison revealed a major disadvantage: the proposed formulations are not tightly constrained. In turn, the larger feasible region forces the solver to span a large portion of the solution tree before yielding the optimal tour. This is the reason why the formulations can only be applied to very small TSP instances. To overcome this drawback, additional constraints need to be added to the formulations. Finding appropriate constraints is not a trivial task but it is the only recourse for continuing this work.

Part II

Scheduling cleaning actions for heat exchanger networks subject to fouling

Chapter 4

Background

The first part of this dissertation was dedicated to a central problem of Mathematical Programming, namely the Travelling Salesman Problem. The problem is considered to be the cornerstone on which the areas of Integer Programming and Mixed-Integer Programming developed.

Mixed-Integer Programming is used in the second part of this dissertation to optimise the operation of heat transfer devices. The study of heat transfer and the operation of heat transfer units is a matter of great industrial importance and it lies at the core of Chemical Engineering.

This chapter introduces a major industrial problem: fouling of heat transfer surfaces. The negative impact of fouling is described and the physical/chemical mechanisms that lead to the formation of fouling layers are outlined briefly. One of the main fouling mitigation methods for industrial heat transfer units is regular cleaning. Subsequent sections review the use of decision-making tools in scheduling cleaning actions for process heat transfer devices subject to fouling.

4.1 Fouling & heat transfer processes

Fouling is a phenomenon prevalent in many industrial heat transfer processes: it is the deposition of unwanted materials on heat transfer surfaces. The thermal conductivity of such dirt-deposits is low [Müller-Steinhagen, 2000] and as a result, fouling has a negative impact on the efficiency of heat transfer.

To counter-balance the reduction in heat transfer efficiency the operator needs to provide additional energy to the process by increasing the consumption of combustible fuels or increasing the flow of utility, with associated financial penalties. Adequate control measures must be taken to mitigate the negative effect of fouling.

To avoid high operating cost the engineer must take precautionary measures or apply effective mitigation strategies. For the former the heat transfer units must be over-designed: the engineer takes into account the thermal inefficiencies caused by fouling by assigning extra heat transfer surface to the device. This strategy results in additional capital expenditure. Alternatively, the units might be replaced with expensive non-fouling devices if these are available. The mitigation of fouling is achieved through the use of anti-fouling chemicals and/or the regular on-line or off-line cleaning of the heat exchangers. These lead to high maintenance costs as well as loss of production during the cleaning period.

The reduction of heat transfer efficiency is not the only result of fouling. The presence of dirt layers in the channels of a heat transfer device causes a reduction in the flow area, which leads to an increase in pressure drop. In turn this results in reduced throughput and loss of production if the pumping power is limited. To avoid such a scenario more pumping power and additional electricity costs are required. Also, additional capital expenditure is required since the devices must be designed to operate at high pressure.

Despite the fact that fouling is a well-established problem in many industries it has only received detailed attention in the last forty years [Bott and Melo, 1997]. It is a problem that necessitates careful energy and financial management.

4.2   Fouling in heat exchangers

A heat exchanger is a device whose purpose is to transfer thermal energy from a hot stream to a cold stream. Real-life processes sometimes involve networks of heat exchangers in serial and/or parallel configurations. A simplified schematic representation of such a device is shown in Figure 4.1.

Thermal energy is transferred from the hot stream to the cold stream through the heat exchanger wall. The two streams can flow in co-current mode, as in
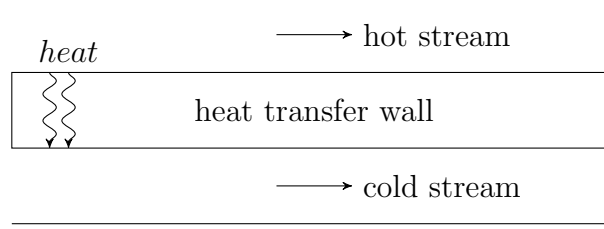
Figure 4.1: Simplified representation of a heat exchanger, co-current flow

Figure 4.1, or in other configurations such as counter-current mode and cross-flow. The amount of heat, Q, recovered from the hot stream for single phase heat transfer (none of the streams changes phase) is given by

$$Q = FUA\Delta T_{lm} \tag{4.1}$$

where F is the configuration correction factor, U is the overall heat transfer coefficient, A is the heat transfer area and ΔT_{lm} is the logarithmic mean temperature difference between the streams. The overall heat transfer coefficient for a clean heat exchanger, assuming that the cold and hot side areas of the tubes are the same, is given by

$$\frac{1}{U} = \frac{1}{h_{\text{hot}}} + \frac{1}{h_{\text{cold}}} + R_w \tag{4.2}$$

where h_{hot} and h_{cold} are the film heat transfer coefficients of the hot and cold stream, respectively, and R_w is the thermal resistance of the wall. If, however, the heat exchanger suffers from fouling, equation (4.2) is modified to include the thermal resistance of the deposits on both sides of the wall, *viz.*

$$\frac{1}{U} = \frac{1}{h_{\text{hot}}} + \frac{1}{h_{\text{cold}}} + R_w + R_{f,\text{hot}} + R_{f,\text{cold}} \tag{4.3}$$

The thermal fouling resistances $R_{f,\text{hot}}$ and $R_{f,\text{cold}}$ depend on the thickness and the thermal conductivity of each layer. The overall thermal fouling resistance, $R_{f,\text{tot}}$, is given by

$$R_{f,\text{tot}} = R_{f,\text{cold}} + R_{f,\text{hot}}. \tag{4.4}$$

An accurate prediction of the fouling resistances is very difficult since reliable estimation models are usually not available [Ishiyama *et al.*, 2009].

The main reason for the lack of robust estimation models is the number and the complexity of different mechanisms responsible for the formation of the fouling layers. Epstein [1983] identified five fouling types based on the key physical/chemical mechanism causing the formation of the deposit. In each case, fouling involves five successive steps, any one of which (or combination thereof) can be rate-determining.

4.2.1 Mechanisms of heat exchanger fouling

The taxonomy of fouling mechanisms into five major classes is accepted by many researchers in the field. The classes are:

a) Crystallisation fouling

It is a broad class that can be divided into two categories. For the first category, the formation of the fouling layer is caused by the growth of salt crystals on the heat transfer surface. The salts (the term salts is also taken to include non-mineral species such as fats and waxes) are originally dissolved in the bulk fluid. Normal-solubility salts crystallise when cooled below their solubility limit, while inverse-solubility salts crystallise when heated above the limit. Furthermore, supersaturation may arise if an amount of solvent evaporates or when two streams are mixed. For the second category, formation of the fouling layer is caused by the cooling of a pure liquid or melt below its freezing point: solid material is then generated at the cold wall. This is often termed 'freezing fouling'.

b) Particulate fouling

The process stream contains suspended particles which deposit on the heat transfer surface. Fine particles may accumulate on surfaces of any orientation while relatively large particles settle on lower horizontal surfaces due to gravity.

c) Chemical reaction fouling

Chemical reactions between some components of the stream generate fouling precursors in the bulk fluid and/or on the heat transfer surface. The surface material is not one of the reactants but may play a role as a catalyst. This

type of fouling is common in petroleum refineries, polymer production and food processing.

d) Corrosion fouling

The heat transfer wall is involved in a chemical reaction, often a corrosion mechanism, which generates a fouling layer. If the corrosion products are removed from the surface fouling does not occur (but the mechanical integrity is compromised).

e) Biological fouling (biofouling)

The fouling layer is caused by the attachment and growth of micro-organisms (micro-biofouling) such as bacteria, fungi and algae or macro-organisms (macro-biofouling) such as mussels and barnacles. In some cases, biofouling is a serious risk for human health. However, in other cases it can be useful: it is a key feature of waste water treatment.

Many industrial fouling problems involve a combination of these mechanisms [Bott, 1988]. Nonetheless, the classification scheme helps decompose this complicated phenomenon into topics that can be studied separately in order to provide fundamental understanding of the causes of the problem.

To assist the detailed study of each mechanism, Epstein [1983] also proposed five sequential events that occur during the formation of a fouling layer. The consecutive steps are:

1. Initiation

The formation of a fouling layer of appreciable thickness on a clean heat transfer surface often occurs after a delay. A crucial factor for the occurrence of this delay period is the cleanliness of the heat transfer surface [Epstein, 1988]. The length of the initiation period can vary from few seconds to several days [Müller-Steinhagen, 2000] depending on the dominant fouling mechanism. For crystallisation fouling the delay period is associated with the crystal nucleation process. In cases of biological fouling it is linked with the conditioning of the surface (colonisation) to favour micro-organism or macro-organism attachment. Blöchl and Müller-Steinhagen [1990] reported that no initiation occurs for particulate fouling.

2. Mass transport

   At least one of the key components involved in the formation of the fouling layer is transported from the fluid bulk to the heat transfer surface.

3. Attachment

   After a key component is transported to the surface region to form fouling precursors, these attach to the surface where the fouling layer is formed.

4. Growth retardation

   The growth of the fouling layer can be decelerated by several mechanisms such as increasing surface repulsion due to electrical interactions or decreasing oxygen diffusion rate as the corrosion layer thickens [Epstein, 1983]. Furthermore, the growth of the layer can be hindered by the removal of parts of the deposit.

5. Ageing

   The physical/chemical properties of the fouling layer are altered due to prolonged exposure to process conditions. Considering the effect of ageing on fouling layers is an important aspect of this work, as explained below.

4.2.2 Ageing

Ageing has been for many years the least understood and the least investigated step of fouling formation [Müller-Steinhagen, 2000]. Until recently, it was usually ignored in modelling attempts and in the analysis of experimental data. It has attracted the interest of fouling researchers in the last decade and the advances in the subject have been reviewed by Wilson *et al.* [2009].

The effect of ageing on the physical/chemical properties of a deposit depends on the formation mechanism. For most mechanisms the aged deposit is stronger than the fresh deposit: it has a more cohesive structure. For crystallisation fouling, it has been reported by Brahim *et al.* [2003] that the initial porous crystalline matrix becomes denser over time to yield a more stable material. In chemical reaction fouling, experimental studies conducted by Fan and Watkinson [2006] showed the structural evolution of fluid-coker deposits from an amorphous conglomerate to a coherent graphitic arrangement. On the other hand, in some cases

of biological fouling, ageing can weaken the initial fouling layer and cause deposit sloughing [Müller-Steinhagen, 2000].

The structural properties of the fouling layer have a direct impact on the choice of the appropriate cleaning method. The extent of ageing can determine the ease with which a fouling layer can be removed: harder (stronger) deposits are more difficult to remove from surfaces [Pogiatzis *et al.*, 2012]. Also, an increase in the deposit hardness is usually accompanied by an increase in the thermal conductivity [Ishiyama *et al.*, 2011a].

Experimental results reported by Er and Lee [2010] (reproduced with permission by Pogiatzis *et al.* [2012]), for fouling layer gums formed by auto-oxidation of linseed oil, show such an increase in thermal conductivity as the initial deposit ages. The change in thermal conductivity has significant consequences on the dynamics of fouling formation and the efficiency of the heat transfer process. The increase in thermal conductivity with time changes the thermal resistance of the deposit layer and thereby the temperature distribution across the layer [Pogiatzis *et al.*, 2012]. The deposit/bulk-fluid interface temperature is recognized to be a key variable influencing fouling kinetics [Ishiyama *et al.*, 2010a].

4.2.3   Fouling models

The purpose of a fouling model is to assist the designer or the operator of a heat exchanger to make an assessment of the impact of fouling on the performance of the unit [Bott, 1995]. In that respect, the two idealised curves shown in Figure 4.2 have been proposed for the prediction of the thermal fouling resistance, R_f, of a fouling layer over time. These curves are often observed in practice on laboratory units and on process units [Epstein, 1983].

The parameter t_I represents the length of the initiation period. An initiation period may not always occur or it may be so short as to be negligible. It is usually ignored in modelling approaches as it is very difficult to predict [Bott, 1995].

Curve A on Figure 4.2 represents situations where the thickness of the deposit increases steadily with time. The evolution of the overall thermal fouling resistance is given by

$$R_f = at \qquad (4.5)$$
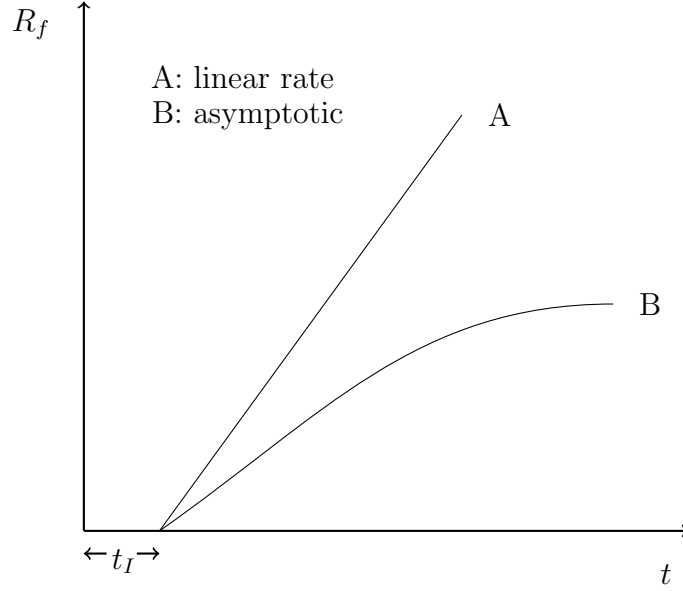
Figure 4.2: Idealised evolution of thermal fouling resistance

where t is time and a the slope of the line.

Curve B exemplifies the asymptotic fouling behaviour. The growth of the layer is decelerated due to auto-retardation mechanisms [Epstein, 1988] which cause a gradual decrease of the deposition rate, *e.g.* ever-reducing wall catalysis of chemical reaction fouling as the deposit layer builds on the wall or because of a decrease in the deposit/bulk-fluid interface temperature. Eventually a steady state is reached when there is no net increase of the thickness of the fouling layer. At that point the asymptotic value of the thermal fouling resistance, $R_{f\infty}$, is attained. The model proposed by Kern and Seaton [1959] is commonly used to describe the asymptotic fouling behaviour:

$$R_f = R_{f\infty}(1 - e^{-t/b}) \tag{4.6}$$

where b is a time constant and t is the time elapsed since fouling started.

The idealised curves shown in Figure 4.2 may fail to describe the fouling process. In a real-life application, an ideal situation may not be achieved. Parts of the deposit may be removed due to periodic weakening [Epstein, 1988]. Changes in crystal structure, chemical degradation, the development of thermal stresses or

the slow poisoning of micro-organisms can all be causes for weakening the deposit [Epstein, 1988].

The fouling behaviour and kinetics depend on the following operating parameters [Müller-Steinhagen, 2000]: (i) foulant concentration in stream; (ii) surface temperature; (iii) surface roughness and (iv) flow velocity.

4.2.4 Cleaning fouled heat exchangers

Fouling and cleaning are symbiotic processes, as outlined by Wilson [2005]. The periodic cleaning of heat exchangers is essential in order to maintain the heat recovery efficiency within desirable limits. The removal of unwanted deposits is necessary even for well-designed devices because the operating conditions may deviate considerably from the design conditions [Müller-Steinhagen, 2000].

Cleaning techniques can be categorized into chemical and mechanical methods. Chemical cleaning methods attempt to remove the fouling layer using chemical agents that react with the deposit layer causing it to dissolve, soften or detach from the heat transfer surface, while mechanical methods remove the deposit by applying shear forces (other mechanisms exist, *e.g.* ultrasound). The former have certain advantages: chemical techniques are relatively quick, less costly, do not damage the surfaces of the exchanger if the correct agent is chosen and can be performed in situ. In contrast, mechanical methods are usually more effective in removing resilient deposits and there is less need to handle dangerous chemicals or dispose of chemical waste. Mechanical methods usually require direct access to the fouled surface so the dirty heat exchanger must be disassembled. For the recirculation of chemical agents there is no need to dismantle the unit if it has been designed for cleaning-in-place.

An effective mitigation strategy may include a combination of both cleaning types. The choice of the appropriate method relies on the physical/chemical characteristics of the fouling layer and the costs associated with each cleaning technique. For optimal energy and financial management the choice of method and the timing of cleaning require the use of decision-making tools.

4.3   Scheduling of cleaning actions

Let us firstly define the term heat exchanger cycle. The operation of a fouled heat exchanger is succeeded by a maintenance period during which the unit is cleaned in order to restore the heat recovery efficiency (partially or completely, depending on the cleaning method). Hence, a heat exchanger cycle is divided in two periods: the operating period and the cleaning period. The duration of the cleaning period will depend on the severity of fouling and the type of cleaning.

Let us consider now the maintenance decisions the operator needs to make. When the process involves only a single heat exchanger, then she needs to decide the length of the operating period and the cleaning method (if more than one are available). If, however, the process involves a network of interacting heat exchangers, then she also needs to choose which units are to be cleaned at a given time. There might be a restriction in the number of units that can be cleaned at the same time. Other constraints, such as key target temperatures or heat transfer duties, may also exist.

The optimal management of the heat transfer process is achieved through the minimisation of energy losses and maintenance expenditure. It would be beneficial for the minimisation to be performed over the life cycle of the process or the time span between process shut-downs. Hence, the existence of a function that captures the process and maintenance costs is essential. This cost function is then minimized over the desired time horizon with respect to the decision variables (cleaning and timing choices) to yield the optimal cleaning schedule.

The effect of fouling on the heat recovery process is quantified by the heat duty which is related to the thermal fouling resistances. It has not yet been possible to apportion a single measurement of the overall thermal fouling resistance, $R_{f,\text{tot}}$, between the two sides of the wall. In all the studies presented below it is assumed that fouling occurs only on one side of the heat transfer surface (*i.e.* that one process stream is 'clean').

Let us assume that the duration of the cleaning period is fixed. The general

form of the cost function is the following:

$$z = \int_0^{t_f} p(t)\mathrm{d}t \; + \; m(y) \tag{4.7}$$

where function $p(t)$ refers to process costs: energy losses due to fouling and lost-production opportunity due to cleaning, integrated over a time horizon of length t_f. The energy losses due to fouling depend on the timing of cleaning actions (timing decisions). Function $m(y)$ refers to maintenance costs and y is the array of cleaning decisions. The cleaning choices correspond to 'yes' or 'no' decisions (should we clean exchanger i? / should we clean using a chemical method?) which can be expressed by binary variables. Therefore, y is an array of binary values.

The next section reviews the research already conducted on the subject. To facilitate the discussion, the work on single units is presented first before moving on to the more general case of heat exchanger networks. In all the approaches described below two common assumptions are made: (i) there is only one available cleaning action and (ii) the properties of the fouling layer are uniform and constant.

4.3.1 Single heat exchanger

Let us consider the case of a single heat exchanger and assume that a cleaning action which removes the deposits completely is available. Since the cleaning action restores the effectiveness of the unit, the minimisation needs only to be performed over one heat exchanger cycle. This optimised cycle is then repeated over again. The time horizon is given by

$$t_f = t_{op} + t_{cl} \tag{4.8}$$

where t_{op} is the length of the operating period (decision variable) and t_{cl} is the duration of the cleaning period (fixed, only one cleaning action is available). Hence, the operator needs only to calculate the optimal length of the operating

period t_{op}. The simplified objective function is the following:

$$z = \int_0^{t_{op}+t_{cl}} p(t)\mathrm{d}t \ + \ c \tag{4.9}$$

where c is the fixed maintenance cost.

The scheduling problem as described above was first considered by Epstein [1979] who devised an analytical solution for determining the optimal heat exchanger cycle for an evaporator subject to fouling. The optimal duration of the operating period can be calculated analytically using the first derivative, *viz.*

$$\frac{dz}{dt_{op}} = 0 \tag{4.10}$$

The solution of equation (4.10) provides an analytical result for the calculation of the optimal operating period length, t_{op}^*. Epstein [1979] assumed that the amount of deposit at a given time t was proportional to the amount of heat transferred up to that time.

Casado [1990] extended the analytical approach of Epstein [1979] to a single-phase counter-current heat exchanger used in a crude oil preheat train. He presented a detailed economic model and explored the major operating trade-offs that dictate the existence of a minimum cost. Casado [1990] also presented an algorithm for computer implementation where the analytical formula was solved using a trial-and-error procedure.

Zubair *et al.* [1992] argued that stochastic fouling models must be used to capture the true performance of a heat exchanger. In that vein, Sheikh *et al.* [1996] introduced uncertainty in the linear fouling model and presented a reliability-based cleaning strategy.

4.3.2 Heat exchanger networks

Scheduling the cleaning actions for heat exchanger networks subject to fouling is the main topic of this work. The scheduling framework developed for a network should be readily applicable to the special case of a single unit.

Let us assume that a cleaning action is available, which removes the deposits

completely. The cost function is given by equation (4.7), where the binary array y corresponds to unit choices. The cost function is non-differentiable and, hence, an analytical formulae cannot be derived. The optimal cleaning schedule for the network can only be obtained using numerical optimisation tools.

Let us now examine the scheduling problem with respect to mathematical programming theory. The presence of the binary array y means the problem is described by a Mixed-Integer Programming (MIP) formulation. It is desirable for the MIP formulation to be convex as the identification of the global solution is guaranteed for convex formulations. Nevertheless, identifying the global solution for convex MIP problems can be very expensive computationally. For non-convex formulations, it is not always possible to issue a certificate of global optimality.

4.3.2.1 Non-convex formulations

The scheduling problem is described by a non-convex Mixed-Integer Nonlinear Programming (MINLP) formulation, primarily due to equation (4.1). The thermal fouling resistance may also be nonlinearly related to some other variable depending on the complexity of the fouling model. Smaïli *et al.* [1999] were the first to formulate the problem as a non-convex MINLP while trying to optimise the performance of a network of 11 units, representing a preheat train in a sugar refinery, over a horizon of 120 days. Subsequently, Smaïli *et al.* [2001] presented an improved MINLP formulation which was used to obtain cleaning schedules for two oil refinery networks over a time-horizon of three years. Smaïli *et al.* [2001] used two different models to estimate the thermal fouling resistance: the linear and the asymptotic.

To calculate the process costs, $p(t)$, the operation of the network must be simulated in time. In that respect, Smaïli *et al.* [2001] discretised time: the horizon was divided into periods of fixed and equal length. Each period was further divided into an operating sub-period and a cleaning sub-period (both of fixed length). If a cleaning action was selected, it was performed during the cleaning sub-period while the other units continued to operate normally. In this case, the binary array y corresponds to unit and timing decisions (*e.g.* the value of y^{ij} denotes if unit i is cleaned at period j or not).

The length of the operating sub-period can also be allowed to vary, *e.g.* [Markowski and Urbaniec, 2005]. It will then be a decision variable for the MINLP problem. Such an MINLP formulation is highly non-convex [Markowski and Urbaniec, 2005] and it may be impossible to solve (depending on how many variables and constraints are involved).

Smaïli *et al.* [1999], Smaïli *et al.* [2001] and Markowski and Urbaniec [2005] attempted to optimise the MINLP formulations they constructed using rigorous optimisation methods developed for convex problems. Applying such exact algorithms to non-convex programming problems is a heuristic approach. An alternative path is to use heuristic solution techniques which usually require less computational effort than exact algorithms to yield a sub-optimal solution.

In that fashion, Smaïli *et al.* [2001] proposed a simple greedy solution procedure to act as a competitor to the rigorous optimisation algorithm. The greedy solver considers cleaning actions in the current period and the effect of those actions over a 'sliding' horizon (selected number of periods in the future). The difference between the costs when the exchanger is cleaned and when no cleaning occurs is calculated for each unit. The heat exchanger that exhibits the largest return, given that it is greater than a predetermined threshold, is chosen to be cleaned. The greedy solver was found to produce worse solutions than the exact algorithm.

Calculating the return for each heat exchanger at each period requires the simulation of the operation of the network several times. Ishiyama *et al.* [2009] proposed the use of a 'merit list' to identify favourable candidates to be compared in a full simulation in order to reduce the computational effort. Furthermore, they included model-based representations of the fouling kinetics and considered the impact of fouling on the hydraulic performance of crude oil preheat train networks.

Ishiyama *et al.* [2010b] extended the above scheduling approach to deal with the problem of controlling the inlet temperature of a de-salter. A de-salter is an essential device on an oil refinery: it removes inorganic substances from the crude oil to prevent damages such as the deactivation of catalysts used in the process. The operation of the de-salter depends on the upstream temperature, which varies due to deposits' build-up in the exchangers. The inlet temperature

is also affected by cleaning actions performed on heat exchangers upstream in the network.

Smaïli *et al.* [2002] proposed a variant of simulated annealing [Kirkpatrick *et al.*, 1983] for optimising the cleaning schedule for two networks of 14 and 25 heat exchangers, respectively. The best schedules found were compared to solutions obtained using an exact algorithm. The values of the heuristic and exact objective (total cost) were found to be very close for both networks. In fact, for the larger network the heuristic solver identified a solution which was slightly better. Furthermore, for the same network the heuristic solver generated the solution with considerably less computational effort. Here, a linear fouling model was used.

Sanaye and Niroomand [2007] scheduled the cleaning actions for a heat exchanger network used in ammonia and urea production. The authors neglected to describe the heuristic technique they used to schedule the cleaning actions.

Rodriguez and Smith [2007] used simulated annealing [Kirkpatrick *et al.*, 1983] to simultaneously optimise the cleaning schedule and the operating conditions to mitigate the negative effect of fouling on an oil refinery network. According to the 'fouling threshold' concept [Panchal *et al.*, 1999] which the authors employed, the deposition rate for chemical reaction fouling in crude oil heat exchangers depends on the bulk velocity and the surface temperature. Optimising the profile of these two operating variables can reduce the amount of fouling significantly. Rodriguez and Smith [2007] controlled the stream splitters and bypasses to manipulate the fluid velocity and in turn surface temperature.

4.3.2.2 Convex formulations

Georgiadis and co-workers [Georgiadis *et al.*, 1999, 2000] presented a Mixed-Integer Linear Programming (MILP) formulation where they tried to avoid the drawbacks associated with non-convex models. The linearisation of the model was achieved by replacing the logarithmic temperature difference in equation (4.1) with the arithmetic mean average. The authors considered a linear fouling model and created time profiles for the overall heat transfer coefficient, U, of each unit. Hence, U was a parameter in their formulation and not a variable. The

MILP formulation was used to schedule the cleaning actions for heat exchanger networks used for the sterilisation of milk.

Following the approach of Georgiadis *et al.* [2000], Lavaja and Bagajewicz [2004] used the time profiles of the overall heat transfer coefficient, U, to devise an MILP formulation for the problem without introducing any linear approximation to the nonlinear heat duty equation (4.1). They considered only the linear fouling model but stated that the approach is easily extended to the case of asymptotic fouling. The MILP formulation of Lavaja and Bagajewicz [2004] is examined more carefully in Chapter 5.

4.4   Motivating study

The scheduling studies reviewed in the previous section considered the physical/chemical properties of the fouling deposits to remain constant throughout the operation of a heat exchanger. However, it is probable that the properties of a foulant will change over time due to the prolonged exposure to process conditions. The ageing of the deposit might result in structural changes as well as changes in thermal conductivity (see Section 4.2.2). Furthermore, in all previous studies it was assumed that an available cleaning action restores the unit to its original performance (completely clean state): the selection between different cleaning methods was not considered.

Ishiyama *et al.* [2011a] were the first to introduce the economic competition between two cleaning methods in a scheduling study. In their novel work, fouling was defined as the combination of deposition and ageing phenomena and the selection of the appropriate cleaning method relied on the extent of ageing.

The study focused on an isolated evaporator operating under chemical reaction fouling and included the selection between solvent (chemical) cleaning and mechanical cleaning. There, it was assumed that ageing converts the initial deposit into a harder and more conductive form which is not susceptible to removal by the chemical cleaning method. A simple heuristic search that favoured the selection of the method with the lowest daily average cost was used to obtain mixed cleaning schedules.

In summary, Ishiyama *et al.* [2011b] investigated the benefits of applying

mixed cleaning strategies rather than cleaning using only one technique. In addition, they incorporated, for the first time, the effects of ageing on fouling and cleaning dynamics in a scheduling study. This work aims to extend their approach to heat exchanger networks.

4.5 Conclusions

Fouling is identified as a major problem in industrial process heat transfer. It is responsible for large energy and throughput losses resulting in financial penalties.

Fouling is a complicated phenomenon. Epstein [1983] presented a classification scheme that describes the formation of a fouling layer as the result of five different deposition mechanisms, acting separately or in synergy. Furthermore, he suggested that the formation of a fouling layer can be decomposed to five sequential steps: initiation, mass transport, attachment, growth retardation and ageing.

One of the main mitigation strategies for industrial heat transfer devices subject to fouling is regular cleaning. The cleaning of fouled units involves the formulation and optimisation of a scheduling problem. The goal is to minimise the maintenance costs and the process losses, which include energy losses due to fouling and lost-production opportunity during the cleaning intervals.

A number of scheduling studies have been presented for isolated heat exchangers or heat exchanger networks subject to fouling. Various mathematical formulations have been proposed for the scheduling problem and different optimisation tools have been used to obtain cleaning programs. All studies that preceded the work of Ishiyama *et al.* [2011b] considered the physical/chemical properties of the fouling deposits to remain constant in time, and that a cleaning action restores the heat exchanger to its original clean condition. None of these studies has taken under consideration the effect of ageing on fouling and cleaning dynamics or the competition between cleaning methods.

Motivated by the work of Ishiyama *et al.* [2011a], the current work focuses on developing optimal mixed cleaning campaigns for heat exchanger networks. The situation where more than one method is available, giving different degrees of cleaning, is investigated. Two scenarios are studied: (i) heat exchanger networks

subject to chemical reaction fouling and (ii) heat exchanger networks subject to biofouling.

For the first scenario, the scheduling approach proposed by Ishiyama *et al.* [2011b] for a single evaporator is extended to accommodate heat exchanger networks. Here, the extent of ageing has a direct impact on the selection between two competing cleaning methods: the more conductive aged material can be removed only by a mechanical action, while chemical actions are capable of removing only the 'softer' fresh deposit.

The second scenario refers to the novel study of scheduling the cleaning actions for heat exchanger networks subject to biological fouling. The scheduling problem features the selection between three cleaning methods: (i) a simple water flush, which removes most of the biofilm but leaves the surface colonised and ready to restart growth when process operation resumes; (ii) chemical cleaning, which removes all biofilm and imposes a short initiation period and (iii) chemical cleaning followed by disinfection, which resets the unit to its original clean state.

The scheduling formulation for the chemical reaction fouling scenario is described in Chapter 5 along with the proposed solution methods. Chapter 7 introduces two mathematical programming formulations for the biological fouling scenario.

Chapter 5

Chemical reaction fouling: formulation & solution methods

The previous chapter introduced the negative effect of fouling on industrial heat transfer. It also established the importance of using optimisation tools to schedule the cleaning actions for heat exchanger networks subject to fouling. Two scenarios were identified, based on the fouling mechanism and the selection between available cleaning techniques.

The current chapter describes the scheduling problem for the chemical reaction fouling scenario. Firstly, after a brief heat transfer analysis, the two-layer fouling model used to calculate the thermal resistance of the deposits is introduced. The main part of the chapter is dedicated to the description of the mathematical programming formulation. This includes the time representation, the constraints and the objective function of the scheduling problem.

The last section discusses the suitability of an existing numerical solver for the type of mathematical programming problem proposed. Subsequently, two alternative solution procedures are suggested as more suitable. The first applies Generalised Benders Decomposition while the second is inspired by Model Predictive Control.

5.1 Heat transfer analysis

The scheduling model is developed for networks of single-pass shell-and-tube heat exchangers. Figure 5.1 shows the schematic representation of such a unit, operating in counter-current mode. The model can be easily modified to accommodate different types of heat exchangers and other flow configurations.
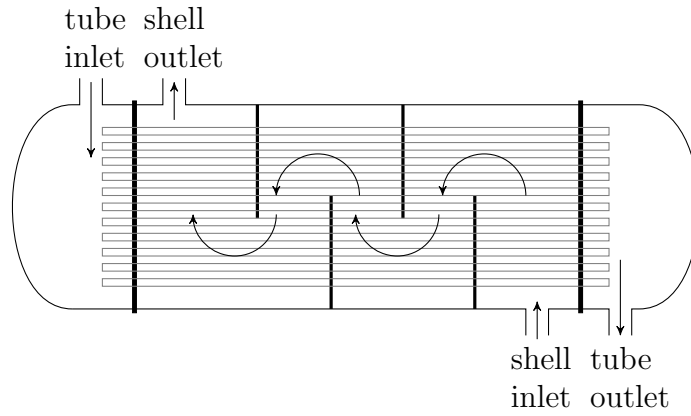
Figure 5.1: Schematic representation of a shell-and-tube heat exchanger (counter-current mode)

For a unit in operation, the following assumptions are made:

a) it is in counter-current mode; consequently the configuration correction factor, F, is equal to one;

b) the cold stream flows on the tube side and the hot stream on the shell side;

c) neither of the streams changes phase within the unit;

d) the specific heat capacities of the streams are constant;

e) the mass flow rate of both streams remains constant.

The rate of heat transfer of a shell-and-tube heat exchanger operating in counter-current mode is given by equation (4.1). The logarithmic mean temperature difference for the unit is calculated as follows:

$$\Delta T_{lm} = \frac{(T_{h,o} - T_{c,in}) - (T_{h,in} - T_{c,o})}{\ln[(T_{h,o} - T_{c,in})/(T_{h,in} - T_{c,o})]} \tag{5.1}$$

where T is the temperature with subscripts c, h, in and o referring to cold, hot, inlet and outlet stream, respectively. Equation (4.1) can then be rewritten as follows:

$$Q = UA \frac{(T_{h,o} - T_{c,in}) - (T_{h,in} - T_{c,o})}{\ln[(T_{h,o} - T_{c,in})/(T_{h,in} - T_{c,o})]}. \tag{5.2}$$

The energy balance for the unit is

$$Q = \dot{m}_c C_{p,c}(T_{c,o} - T_{c,in}) = \dot{m}_h C_{p,h}(T_{h,in} - T_{h,o}) \tag{5.3}$$

where $\dot{m}$ represents the mass flow rate and C_p is the specific heat capacity. Combining equations (5.2) and (5.3) yields

$$T_{h,o} = T_{c,in} + (T_{h,in} - T_{c,o}) \exp(UAC) \tag{5.4}$$

with C given by

$$C = \frac{\dot{m}_h C_{p,h} - \dot{m}_c C_{p,c}}{\dot{m}_h C_{p,h} \dot{m}_c C_{p,c}}. \tag{5.5}$$

The negative effect of fouling on the heat transfer process is quantified through equation (5.4). Accumulation of deposits will cause a decrease of the overall heat transfer coefficient U.

5.2   Fouling analysis

The key requirement is to be able to track the effect of fouling on heat recovery and on cleaning effectiveness. A two-layer model is used to estimate the thermal fouling resistance. The two layers are: the fresh deposit and the aged material. The fresh deposit is susceptible to removal by both mechanical action and chemical action. On the other hand, the more resilient aged material can only be removed by mechanical cleaning. Hence, a mechanical action restores the efficiency of a unit fully, while a chemical action does not.

The concept of a two-layer model was described by Atkins [1962] while considering fouling in crude oil preheat trains. Atkins [1962] proposed that there are two discrete events taking place during the formation of fouling. At first, a layer of soft material is deposited, which is then converted to a harder layer due to

ageing. The transition from soft to hard layer was modelled as a phase change so that the growth of the aged layer followed a moving front.

Crittenden and Kolaczkowski [1979] extended the concept proposed by Atkins [1962] and presented the first quantitative two-layer model. The conversion of fresh deposit to hard material was assumed to be first order in foulant concentration and to follow an Arrhenius-type temperature dependency.

The two-layer concept was used by Ishiyama *et al.* [2011a] for the investigation of the thermal and hydraulic aspects of ageing on heat exchangers. The authors used the terms 'gel' and 'coke', borrowed from the crude oil fouling literature, to describe the fresh deposit and aged material, respectively. The same terminology is used in the current study. Ishiyama *et al.* [2011a] compared the evolution of the thermal fouling resistance over time for different ageing kinetic schemes under constant heat flux operation and under constant wall temperature operation.

In their scheduling approach Ishiyama *et al.* [2011b] used the simplest possible form of the two-layer model, where the rates of gel formation and coke formation are constant. The same model is used here. Before introducing the model, the following assumptions are made:

a) deposition occurs only on the tube side of the heat transfer wall (the shell side is free of fouling). It is recognised that in practice both streams may give rise to fouling but this scenario is not considered in this work.

b) The formation of foulant is entirely due to chemical reactions between the components of the stream.

c) The duration of the initiation period is negligible.

d) The gel and coke formation rates are uniform at all locations along the tubes of the heat exchanger.

e) The density of the two layers remains constant.

f) The coke layer is more thermally conductive than the gel layer.

The growth of the gel layer is expressed as the competition between gel for-

mation and coke formation, *viz.*

$$\frac{d\delta_g}{dt} = k_g - k_c \tag{5.6}$$

where δ_g the thickness of the gel layer, k_g the gel formation rate and k_c the coke formation rate. The growth of the coke layer is given by

$$\frac{d\delta_c}{dt} = \begin{cases} k_c, & \text{if } \delta_g > 0 \\ 0, & \text{if } \delta_g = 0 \end{cases} \tag{5.7}$$

where δ_c is the thickness of the aged deposit. Figure 5.2 shows the growth of the two layers as moving fronts in time.
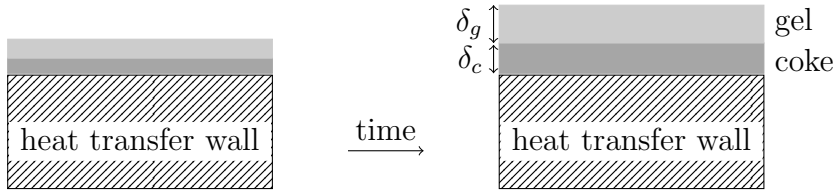
Figure 5.2: Growth of gel and coke layers in time

Recall that fouling occurs only on the cold side of the shell-and-tube heat exchanger. Treating the two layers as a pair of thin insulating slabs, the thermal fouling resistance, R_f, for the unit is as follows:

$$R_f = \frac{\delta_g}{\lambda_g} + \frac{\delta_c}{\lambda_c} \tag{5.8}$$

where λ_g and λ_c are the thermal conductivities of the gel layer and coke layer, respectively. The aged material is more conductive than the fresh deposit: $\lambda_g < \lambda_c$.

Equation (4.3) can be rewritten as follows:

$$\frac{1}{U} = \frac{1}{U_0} + R_f = \frac{1}{U_0} + \frac{\delta_g}{\lambda_g} + \frac{\delta_c}{\lambda_c} \tag{5.9}$$

where U_0 is the overall heat transfer coefficient for a foulant-free heat exchanger

given by

$$\frac{1}{U_0} = \frac{1}{h_{\text{hot}}} + \frac{1}{h_{\text{cold}}} + R_w. \tag{5.10}$$

The growth of the two layers in the tubes of a heat exchanger will cause a reduction in flow area and this will lead to an increase in pressure drop. If fouling is severe, this will affect the pumping capacity as it is assumed that the mass flow rate of the cold stream is maintained constant. The effects of fouling on pressure drop are not considered in this work.

5.3   Time representation

The optimisation of the cleaning schedule for a heat exchanger network operating under fouling requires the calculation of the process costs $p(t)$ as noted in Section 4.3.2.1. To calculate the process costs the operation of the network must be simulated.

The system to be simulated is dynamic due to equations (5.6) – (5.7). Hence, an integration scheme is required to obtain numerical solutions for the differential equations and to integrate the process costs $p(t)$ over the examined time horizon. For that purpose, orthogonal collocation is chosen for its precision and its need for relatively few discretisation points [Biegler, 2010]. Among the different collocation schemes, Radau collocation is chosen due to the fact that it allows large time steps for systems with slow time scales [Biegler, 2010].

Let us assume that the cleaning actions are scheduled over a time horizon t_f. To achieve discretisation, the time horizon is divided into a finite number of periods, n_p, of fixed length. In turn, each period is divided into three elements of fixed length each of which contains four collocation nodes. Figure 5.3 shows the graphic representation of a discrete period.

The first element considered to be the operating sub-period has length t_{op}, which is assumed to be constant in this work. Elements 2 and 3 correspond to the cleaning sub-periods and their added length corresponds to the duration of a mechanical cleaning, t_{me}. The length of the third element corresponds to the duration of a chemical cleaning, t_{ch}. The duration of both cleaning actions is assumed to be constant and independent of the thickness of the layers. The
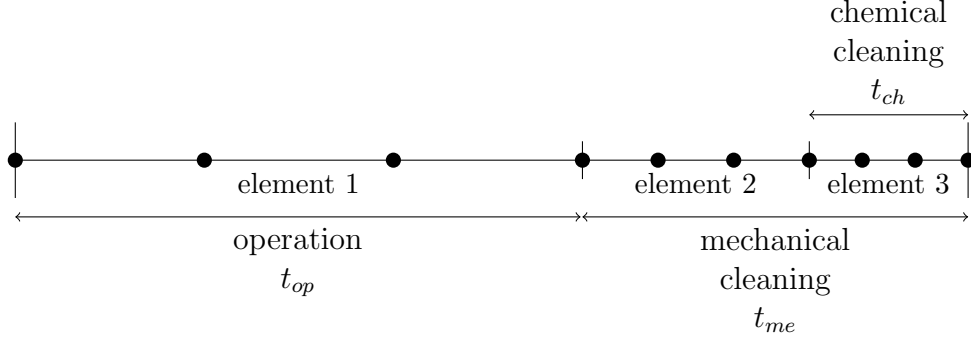
Figure 5.3: Schematic representation of a discrete time period (filled circles: collocation nodes)

length of the time horizon is calculated as

$$t_f = np(t_{op} + t_{me}).$$ (5.11)

where np is the number of periods. If a mechanical action is to be performed in a given period, it will start at the beginning of element 2 and finish at the end of element 3 (end of period). Similarly, a chemical action will be performed during element 3. If no cleaning action is decided for a period the unit is considered to operate without any disruptions through elements 2 and 3.

The solution of the differential equations and the integral in each element are approximated by 3rd order polynomials. To facilitate discussion, the use of orthogonal collocation is briefly reviewed.

Let us consider the following ordinary differential equation:

$$\frac{dv}{dt} = f(v(t), t), \quad v(0) = v_0.$$ (5.12)

The time profile of variable $v(t)$ is to be approximated using a 3rd order Lagrange interpolation polynomial over the finite element shown in Figure 5.4, where τ_0, τ_1, τ_2 and τ_3 are the collocation nodes and h the length of the element. Using Radau collocation: $\tau_0 = 0$, $\tau_1 = 0.155051$, $\tau_2 = 0.644949$ and $\tau_3 = 1$. The first collocation node at τ_0 corresponds to the initial condition

$$v(t_0) = v_0.$$ (5.13)
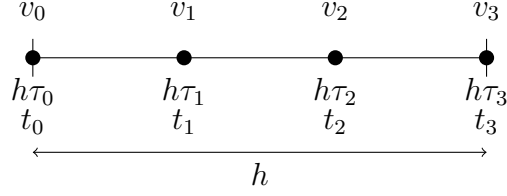
Figure 5.4: Orthogonal (Radau) collocation over finite element

Also,

$$v(t_i) = v_i; \quad i = 1, 2, 3 \tag{5.14}$$

where

$$t_i = t_0 + h\tau_i; \quad i = 1, 2, 3. \tag{5.15}$$

In Radau collocation the final element times are used as nodes, thus avoiding the need for extrapolation. The variables v_i for $i = 1, 2, 3$ are obtained by solving the following system of algebraic equations:

$$\sum_{i=0}^{3} v_i \frac{dq_i(\tau_k)}{d\tau} = hf(v_k, t_k); \quad k = 1, 2, 3 \tag{5.16}$$

where

$$q_i(\tau) = \prod_{\substack{j=0 \\ j \neq i}} \frac{\tau - \tau_j}{\tau_i - \tau_j}. \tag{5.17}$$

and

$$\frac{dq_i(\tau)}{d\tau} = \sum_{j=0}^{3} \prod_{\substack{m=0 \\ m \neq i,j}}^{3} (\tau - \tau_m) / \prod_{\substack{n=0 \\ n \neq i}}^{3} (\tau_i - \tau_n). \tag{5.18}$$

The use of orthogonal collocation for the purposes of this work is described in the section that follows. The next section introduces the proposed mathematical programming formulation for the scheduling problem.

5.4 Mathematical programming formulation

The task is to identify the optimal cleaning schedule for a heat exchanger network subject to chemical reaction fouling. Let us assume that $U' = \{1, 2, \ldots, nu\}$ is

the set of units, $P = \{1, 2, \ldots, np\}$ the set of discrete periods and $M = \{ch : \text{chemical}, me : \text{mechanical}\}$ the set of available cleaning modes.

The binary variables y^{ijm}, for $i \in U'$; $j \in P$; $m \in M$, are such that:

$$y^{ijm} = \begin{cases} 1, & \text{if cleaning mode } m \text{ is chosen for unit } i \text{ at period } j \\ 0, & \text{if cleaning mode } m \text{ is not chosen for unit } i \text{ at period } j \end{cases} \tag{5.19}$$

The following set of constraints:

$$\sum_{m \in M} y^{ijm} \leq 1; \quad i = 1, 2, \ldots, nu; \ j = 1, 2, \ldots, np \tag{5.20}$$

is necessary to ensure that at most one cleaning mode is selected for unit i at period j.

5.4.1 Constraints

The scheduling formulation includes two groups of constraints. The first group corresponds to the simulation of the network's operation, while the second group refers to process constraints.

5.4.1.1 Simulation constraints

All simulation constraints are equality constraints. The efficiency of the heat exchanger network decays in time due to the growth of gel layer and coke layer on the heat transfer surface of the units. The thickness of gel and coke layers and the temperature profile of each unit are calculated at the collocation nodes of the time elements.

Let us define the set of time elements $E = \{1, 2, 3\}$ and the set of collocation nodes $O = \{0, 1, 2, 3\}$. Moreover, let us assume that:

a) the heat exchangers are completely clean (fouling-free) at the beginning of the examined time horizon;

b) the gel formation rate is always greater than the ageing rate: $k_g > k_c$.

During the cleaning sub-periods the gel formation and ageing formation rates need to be controlled: if a unit is chosen to be cleaned, with either method, then the rates must be fixed to zero to stop the growth of the layers. For that purpose, the variable gel formation rate r_g^{ijkl} and the variable coke formation rate r_c^{ijkl} are introduced, together with the following set of constraints:

Element 1: operation

$$r_g^{ij,1,l} = k_g \tag{5.21}$$

$$r_c^{ij,1,l} = k_c \tag{5.22}$$

Element 2: potential mechanical cleaning

$$r_g^{ij,2,l} = k_g(1 - y^{ij,me}) \tag{5.23}$$

$$r_c^{ij,2,l} = k_c(1 - y^{ij,me}) \tag{5.24}$$

Element 3: potential mechanical or chemical cleaning

$$r_g^{ij,3,l} = k_g(1 - \sum_{m \in M} y^{ijm}) \tag{5.25}$$

$$r_c^{ij,3,l} = k_c(1 - \sum_{m \in M} y^{ijm}) \tag{5.26}$$

$$i = 1, 2, \ldots, nu; \ \ j = 1, 2, \ldots, np; \ \ l = 0, 1, 2, 3$$

Constraints (5.23) – (5.24) set the rates to zero during element 2 if a mechanical action is chosen, while constraints (5.25) – (5.26) fix the value of the rates at zero during element 3 if either of the cleaning actions is selected.

Applying orthogonal collocation, the thickness of the gel layer, δ_g^{ijkl}, and the thickness of the coke layer, δ_c^{ijkl}, for $i \in U'$; $j \in P$; $k \in E$; $l \in O$, are defined by

$$\sum_{l=0}^{3} \delta_g^{ijkl} \frac{dq_l(\tau^n)}{d\tau} = h^k(r_g^{ijkn} - r_c^{ijkn}) \tag{5.27}$$

$$\sum_{l=0}^{3} \delta_c^{ijkl} \frac{dq_l(\tau^n)}{d\tau} = h^k r_c^{ijkn} \tag{5.28}$$

$$i = 1, 2, \ldots, nu; \ \ j = 1, 2, \ldots, np; \ \ k = 1, 2, 3; \ \ n = 0, 1, 2, 3$$

where h^n is the length of element n: $h^1 = t_{op}$, $h^2 = t_{me} - t_{ch}$ and $h^3 = t_{ch}$. Recall, the term $\dfrac{dq_l(\tau^n)}{d\tau}$, for $n = 0, 1, 2, 3$, is a constant.

The units are free of fouling at the beginning of the time horizon. The initial condition for the thickness of each layer for the first element of the first period is:

$$\delta_g^{i,1,1,0} = 0 \tag{5.29}$$

$$\delta_c^{i,1,1,0} = 0 \tag{5.30}$$

$$i = 1, 2, \ldots, nu.$$

The initial conditions for the first element of every other period must set the thickness of the layers to be equal to that at the end of the previous period. Hence:

$$\delta_g^{ij,1,0} = \delta_g^{i,j-1,3,3} \tag{5.31}$$

$$\delta_c^{ij,1,0} = \delta_c^{i,j-1,3,3} \tag{5.32}$$

$$i = 1, 2, \ldots, nu; \; j = 2, 3, \ldots, np.$$

For the second element of the periods, the initial conditions depend on whether a mechanical action is performed or not, as follows:

$$\delta_g^{ij,2,0} = \delta_g^{ij,1,3}(1 - y^{ij,me}) \tag{5.33}$$

$$\delta_c^{ij,2,0} = \delta_c^{ij,1,3}(1 - y^{ij,me}) \tag{5.34}$$

$$i = 1, 2, \ldots, nu; \; j = 1, 2, \ldots, np.$$

If a mechanical action is performed, then the thickness of both layers, δ_g and δ_c, is set to zero by constraints (5.33) – (5.34). Otherwise, it is forced to be equal to the thickness of the layers at the end of element 1.

Finally, for the third element the initial conditions are crafted to account for a mechanical or chemical action, *viz.*

$$\delta_g^{ij,3,0} = \delta_g^{ij,2,3}\left(1 - \sum_{m \in M} y^{ijm}\right) \tag{5.35}$$

$$\delta_c^{ij,3,0} = \delta_c^{ij,2,3}(1 - y^{ij,me}) \tag{5.36}$$

$$i = 1, 2, \ldots, nu; \; j = 1, 2, \ldots, np.$$

Constraint (5.35) is used to set the thickness of the gel layer, δ_g, to zero if either of the cleaning actions is performed, while constraint (5.36) sets the thickness of the coke layer, δ_c, to zero only if mechanical cleaning is selected. If chemical cleaning is selected, then the value of δ_c is fixed to be equal to the thickness of the coke layer at the last node of element 2. Equations (5.33) – (5.36) define nonlinear constraints due to bilinearities of continuous/binary variables.

The negative effect of fouling on the heat transfer process is quantified through equation (5.4). Replacing U from equation (5.9) and discretising, this becomes

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \exp\Big(\frac{A^i C^i}{\frac{1}{U_0^i} + \frac{\delta_g^{ijkl}}{\lambda_g} + \frac{\delta_c^{ijkl}}{\lambda_c}} \Big) \tag{5.37}$$

$$i = 1, 2, \ldots, nu; \; j = 1, 2, \ldots, np; \; k = 1; \; l = 0, 1, 2, 3$$

for the first element of the time periods. For the second and third elements the nonlinear expression of the temperatures must be altered to account for any cleaning actions. While a unit is cleaned the outlet temperature of both streams must be set to be equal to the inlet temperature of the streams, *i.e.* the stream is bypassed to the next unit. Therefore, equation (5.37) is modified to

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl})$$
$$\left[(1 - y^{ij,me}) \exp\Big(\frac{A^i C^i}{\frac{1}{U_0^i} + \frac{\delta_g^{ijkl}}{\lambda_g} + \frac{\delta_c^{ijkl}}{\lambda_c}} \Big) + y^{ij,me} \right] \tag{5.38}$$

$$i = 1, 2, \ldots, nu; \; j = 1, 2, \ldots, np; \; k = 2; \; l = 0, 1, 2, 3$$

and

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl})$$
$$\left[(1 - \sum_{m \in M} y^{ijm}) \exp\Big(\frac{A^i C^i}{\frac{1}{U_0^i} + \frac{\delta_g^{ijkl}}{\lambda_g} + \frac{\delta_c^{ijkl}}{\lambda_c}} \Big) + \sum_{m \in M} y^{ijm} \right] \tag{5.39}$$

$$i = 1, 2, \ldots, nu; \; j = 1, 2, \ldots, np; \; k = 3; \; l = 0, 1, 2, 3$$

for elements 2 and 3, respectively. Equations (5.37) – (5.39) define nonlinear equality constraints.

The discrete energy balance for the units is given by

$$\dot{m}_c^i C_{p,c}^i (T_{c,o}^{ijkl} - T_{c,in}^{ijkl}) = \dot{m}_h^i C_{p,h}^i (T_{h,o}^{ijkl} - T_{h,in}^{ijkl}) \tag{5.40}$$
$$i = 1, 2, \ldots, nu; \ j = 1, 2, \ldots, np; \ k = 1, 2, 3; \ l = 0, 1, 2, 3.$$

5.4.1.2 Process constraints

The process constraints are set by the configuration of the units of the network. For heat exchangers in series such as the ones shown in Figure 5.5, the constraints refer to the inlet and outlet temperatures of the connected devices as follows:

$$T_{c,o}^{ijkl} = T_{c,in}^{i+1,jkl} \tag{5.41}$$
$$T_{h,o}^{ijkl} = T_{h,in}^{i+1,jkl} \tag{5.42}$$
$$j = 1, 2, \ldots, \ k = 1, 2, 3; \ l = 0, 1, 2, 3.$$

Constraint (5.41) corresponds to Figure 5.5(a) where the cold stream connects units i and j, while constraint (5.42) refers to Figure 5.5(b) where the hot stream connects the two exchangers.

(a) cold stream connection   (b) hot stream connection
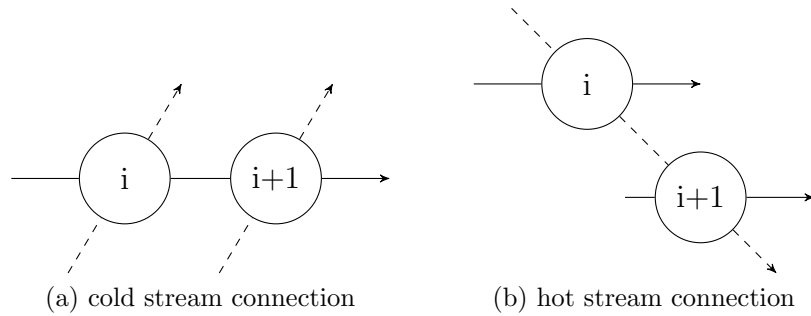
Figure 5.5: Units in serial configuration (solid line: cold stream; dashed line: hot stream)

For two heat exchangers in parallel configuration, as shown in Figure 5.6, the

following constraint

$$\sum_{m \in M} y^{ijm} + \sum_{m \in M} y^{i+1,jm} \leq 1; \quad j = 1, 2, \ldots np \tag{5.43}$$

ensures that only one of the units is selected for cleaning at a given period.
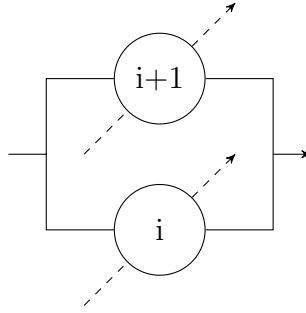
Figure 5.6: Units in parallel configuration (solid line: cold stream; dashed line: hot stream)

5.4.2 Objective function

The general form of the objective function of the scheduling problem is given by equation (4.7) in Section 4.2.4 and it involves the process costs (energy losses due to fouling and lost-production opportunity due to cleaning), $p(t)$, integrated over the examined time horizon, t_f, plus the maintenance costs, $m(y)$. Recall that:

$$z = \int_0^{t_f} p(t)\mathrm{d}t \ + \ m(y). \tag{4.7}$$

The current work focuses on a class of heat exchanger networks called preheat trains. A preheat train is used when a cold stream needs to be heated to a certain temperature before entering some other process. Figure 5.7 shows such a heat exchanger network.

The cold stream is required to be at a target temperature, T_{target}, before entering the process following the preheat train. The initially fouling-free heat exchanger network achieves the temperature target. However, the accumulation of foulant in the units will cause the final temperature, T_f, of the cold stream to
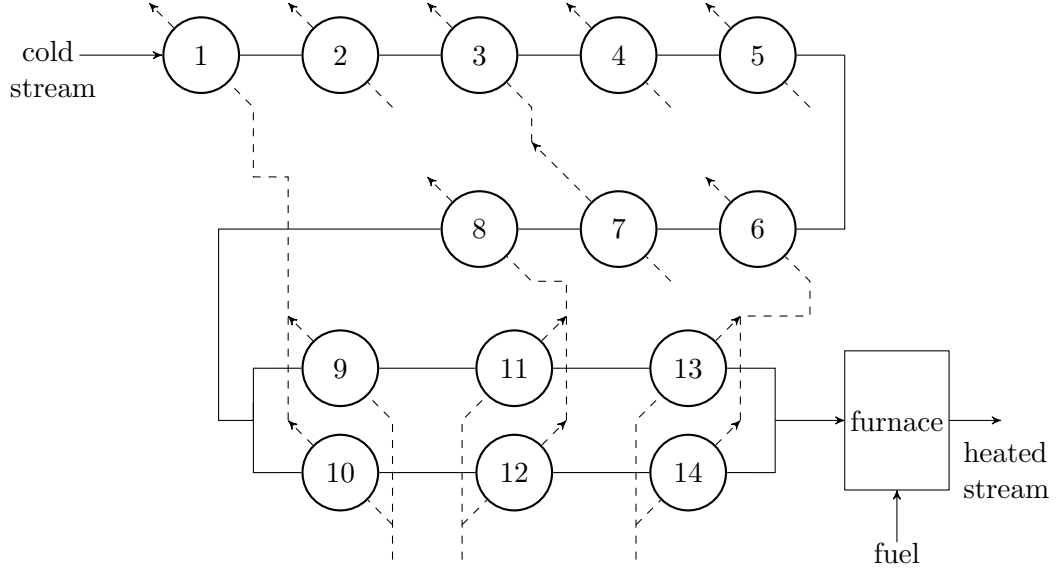
Figure 5.7: Example of a preheat train (solid line: cold stream; dashed lines: hot streams

deviate from the temperature target, T_{target}. For that purpose, it is assumed that a furnace is used to provide the lost energy to the cold stream.

Following the above, the integrated process costs for the network are given by

$$\int_0^{t_f} p(t)\mathrm{d}t = \underbrace{\sum_{i=1}^{nu} f_e \int_0^{t_f} (Q_0^i - Q^i(t))\mathrm{d}t}_{\substack{\text{energy losses +} \\ \text{lost-production opportunity}}}$$

$$= \sum_{i=1}^{nu} f_e \left[t_f Q_0^i - \int_0^{t_f} Q^i(t)\mathrm{d}t \right] \quad (5.44)$$

where Q_0 is the heat duty for a fouling-free exchanger and f_e the cost of energy.

The integral terms in equation (5.44) are calculated using orthogonal collocation as follows:

$$I_1 = \int_0^{t_f} Q(t)\mathrm{d}t \quad (5.45)$$

$$\sum_{l=0}^{3} I_1^{ijkl} \frac{dq_l(\tau^n)}{d\tau} = h^k \dot{m}_c^i C_{p,c}^i (T_{c,o}^{ijkn} - T_{c,in}^{ijkn}) \quad (5.46)$$

$$i = 1, 2, \ldots, nu; \; j = 1, 2, \ldots, np; \; k = 1, 2, 3; \; n = 0, 1, 2, 3$$

The initial conditions are the following:

$$I_1^{ij,1,1} = 0; \quad i = 1, 2, \ldots, nu; \; j = 1, 2, \ldots, np \tag{5.47}$$

$$I_1^{ijk,0} = I_1^{ij,k-1,3}; \quad i = 1, 2, \ldots, nu; \; j = 1, 2, \ldots, np; \; k = 2, 3 \tag{5.48}$$

Due to the discontinuities introduced to the model by the binary variables, the process costs are estimated separately for each period. For that purpose the value of the integrals is fixed to zero at the beginning of each period.

To facilitate understanding, the calculation of the energy losses plus the lost-production opportunity for unit i in period j in which a mechanical cleaning action is performed is illustrated. Figure 5.8 shows the time profile of the heat duty for unit i at period j. Area 1 represents the heat exchanged, area 2 the energy
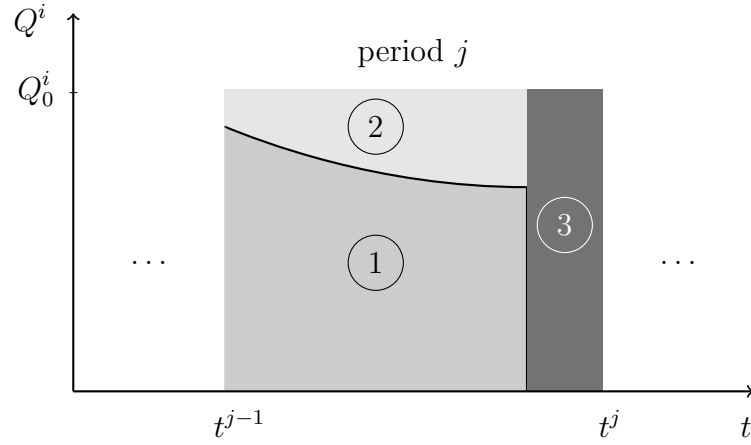
Figure 5.8: Variation of heat duty with time for unit i in time period j (1: heat exchanged, 2: energy losses and 3: lost-production opportunity)

losses and area 3 the lost-production opportunity in period j, respectively. Area 1 is calculated by $I_1^{ij,3,3}$. The sum of areas 2 and 3 is given by

$$A_2 + A_3 = (t^j - t^{j-1})Q_0^i - I_1^{ij,3,3} \tag{5.49}$$

where $t^{j-1} = (j-1)\sum_{k=1}^{3} h^k$ and $t^j = j\sum_{k=1}^{3} h^k$.

The maintenance costs depend only on the number of mechanical and chemical actions performed as it is assumed that the duration of cleaning is independent of the amount of foulant. The cost of each cleaning mode is fixed and it is given by the cost vector $C = \{c^m : m \in M\}$.

The objective function for the discrete scheduling model is given by

$$z = \sum_{i=1}^{nu} \sum_{j=1}^{np} f_e \big(Q_0^i \sum_{k=1}^{3} h^k - I_1^{ij,3,3} \big) + \sum_{i=1}^{nu} \sum_{j=1}^{np} \sum_{m \in M} y^{ijm} c^m. \qquad (5.50)$$

5.4.3 Characteristics of the proposed scheduling formulation

The mathematical programming formulation can be implemented for other types of heat exchanger networks without modifying the set of constraints. Only the objective function has to be altered since it refers to a class of heat exchanger networks known as preheat trains.

The scheduling formulation detailed above is a non-convex MINLP problem due to the nonlinear equality constraints defined by equations (5.37) – (5.39). These constraints include products of continuous variables with nonlinear functions of continuous variables. The equality constraints defined by equations (5.33) – (5.36) are also nonlinear as they consist of bilinear products of binary and continuous variables. However, these can be replaced by linear constraints if necessary by introducing additional variables. This is not required here since the decomposition algorithm suggested for the solution of the problem (see Section 5.5.2) can treat such bilinear products explicitly [Floudas, 1995]. Due to the non-convex nature of the scheduling formulation a number of sub-optimal points will exist. The number of local optima is expected to increase as the number of units and/or periods increases.

The non-convex MINLP scheduling problem includes $\mathcal{O}(120 \times nu \times np)$ continuous variables and $\mathcal{O}(2 \times nu \times np)$ binary variables. Also, it is comprised of $\mathcal{O}(72 \times nu \times np)$ equality constraints and $\mathcal{O}(nu \times np)$ inequality constraints which involve only binary variables. The decision variables (degrees of freedom) for the scheduling problem are the binary variables only.

5.4.4   The MILP formulation of Lavaja & Bagajewicz

For the scheduling problem with only one available cleaning method, a successful linearisation framework was presented by Lavaja and Bagajewicz [2004] based on the idea of parametrising the heat transfer coefficient of the units with the aid of the binary variables of the formulation.

In the initial formulation of Lavaja and Bagajewicz [2004], the non-linearity arose only by products of continuous variables with binary variables and products of binary variables. The authors used standard transformations (see [Williams, 1990]) to rewrite the constraints including these products in exact equivalent linear form. The transformations require the use of additional continuous variables and constraints. However, the number of variables and constraints to be added grows rapidly as the number of periods and the number of units increases, making the solution of the resulting MILP problems computationally unaffordable.

To overcome this drawback, Lavaja and Bagajewicz [2004] suggested a decomposition method based on the assumption that the cleaning schedule of an individual unit is not affected by the cleaning decisions for the rest of the units. Using this decomposition technique the computational effort for obtaining a solution is reduced significantly. Nonetheless, such an assumption is not valid for large networks with strong couplings between heat exchangers arising from hot streams passing through units in series.

To the author's understanding, the linearisation framework proposed by Lavaja and Bagajewicz [2004] is very difficult to adapt to the scheduling problem studied in this work. The presence of two layers on the heat transfer surface renders the parametrisation of the heat transfer coefficient to be extremely difficult. Moreover, even if one succeeds in adapting such a formulation to the case under study, the resulting models will require a prohibitively large computational effort to solve.

5.5   Solution methods

The non-convex MINLP scheduling problem is of the general form:

$$
\begin{aligned}
\min_{y} \quad & z = f(x,y) \\
\text{s.t.} \quad & g(x,y) = 0 \qquad\qquad\qquad\qquad \text{(SP)} \\
& h(x) = 0 \\
& w(y) \leq 0 \\
& x \in X \subseteq \Re^{n_x} \\
& y \in Y = \{0,1\}^{n_y}
\end{aligned}
$$

where x is the vector of continuous variables, y is the vector of binary variables, n_x the dimension of vector x and n_y the dimension of vector y.

The practical goal when dealing with non-convex problems is to obtain 'good' local optima. In that respect, solution algorithms addressing convex MINLP problems can be used to solve the scheduling problem (SP) even if such an approach is considered to be heuristic, in the sense that there is no guarantee that the global solution will be obtained. This line of approach is adopted in this work.

A number of well-known solution algorithms for MINLP problems employ a decomposition strategy. Such are the Generalised Benders Decomposition (GBD) [Benders, 1962; Geoffrion, 1972] and the Outer Approximation (OA) [Duran and Grossmann, 1986]/ Equality Relaxation (ER) [Kocis and Grossmann, 1987] algorithms. The iterative structure of the decomposition algorithms is illustrated in Figure 5.9. The MINLP problem is decomposed into a Nonlinear Programming
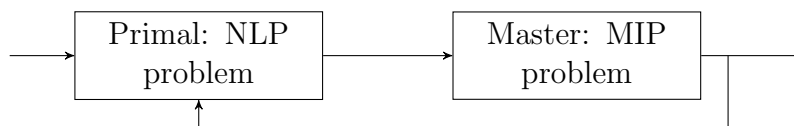
Figure 5.9: Iterative structure of decomposition algorithms

(NLP) problem, the Primal problem, where the binary variables y are fixed and one MIP problem, the Master problem. The Primal problem provides an upper

bound to the MINLP problem and the set of continuous variables to be used by the Master problem. Conversely, the Master problem provides a lower bound for the MINLP problem and the set of binary variables to be used by the Primal problem.

If the MINLP problem is convex, then at some iteration the upper bound provided by the Primal problem will become equal to the lower bound provided by the Master problem and the algorithm terminates having produced the global solution. For a non-convex MINLP problem the lower bound provided by the Master problem is not always valid: there is the danger of cutting off parts of the feasible region. Consequently, the global solution may be excluded from the search at some iteration. In such an event, the lower bound will exceed the upper bound at some iteration and the algorithm will terminate.

5.5.1   Outer approximation/Equality relaxation

One decomposition-based optimiser is DICOPT® [Kocis and Grossmann, 1989], included in the GAMS™ [Brooke *et al.*, 1992] modelling system. The DICOPT® solver is based on the OA/ER decomposition algorithm.

There are two drawbacks [Floudas, 1995] when applying the OA/ER algorithm to the non-convex MINLP scheduling problem (SP). Briefly, these are:

a) the formulation of the master problem at each iteration involves the linearisation of the objective function and the nonlinear constraints around the primal solution. Linear approximations for non-convex functions are often invalid.

b) A large number of constraints is added to the master problem at each iteration. Therefore, the computational effort for solving the corresponding MIP Master problem increases significantly after a few iterations.

Thus, the OA/ER algorithm is not a suitable candidate for the solution of large instances of the MINLP scheduling problem (SP), the main reason being that the size of the Master problem will grow rapidly as the number of units and the number of time periods increases. As a result, the algorithm will require prohibitively long computational times to converge.

5.5.2 Generalised Benders Decomposition algorithm

A more appropriate solution algorithm for the problem of interest to this work is Generalised Benders Decomposition [Benders, 1962; Geoffrion, 1972]. The key feature of GBD, that is of interest to this work, is that only one constraint is added to the Master problem at each iteration. As a result, the size of the corresponding MIP Master problem remains small even after a large number of iterations. On the other hand, one may argue that the Master problem in GBD provides looser lower bounds than the Master problem in OA/ER [Grossmann and Kravanja, 1995] and thus potentially requires many more iterations. However, for this application this may work to our benefit since the MINLP problem is non-convex and the danger of cutting off parts of the feasible region decreases.

There are three Nonlinear Programming (NLP) sub-problems to be derived from problem (SP) with respect to GBD [Floudas, 1995]:

a) NLP relaxation: the binary requirements for variables y are lifted. Here, variables y are continuous and constrained within the interval $[0, 1]$. The NLP sub-problem is the following:

$$
\begin{aligned}
\min_{y} \quad & z_R = f(x, y) \\
\text{s.t.} \quad & g(x, y) = 0 \qquad\qquad \text{(NLP-R)} \\
& h(x) = 0 \\
& w(y) \leq 0 \\
& x \in X \subseteq \Re^{n_x} \\
& y \in Y = [0, 1]^{n_y}.
\end{aligned}
$$

which yields a lower bound z_R to problem (SP) if it has a feasible solution [Grossmann and Kravanja, 1995].

b) NLP sub-problem for fixed binary variables y^k: this is the Primal problem and it is defined as follows:

$$
\begin{aligned}
\min \quad & z_{Pr}^{k} = f(x, y^k) \\
\text{s.t.} \quad & g(x, y^k) = 0 \qquad\qquad \text{(NLP-Pr)}
\end{aligned}
$$

$$h(x) = 0$$

$$x \in X \subseteq \Re^{n_x}.$$

The Primal problem yields an upper bound z_f^k to (SP) provided it has a feasible solution [Grossmann and Kravanja, 1995]. The index $k \in K$ corresponds to the iteration counter for the decomposition algorithm (K is the set of iterations).

In fact, there are no decision variables in the problem (NLP-Pr): once all the binary variables are fixed the behaviour of the system is fully determined. Thus, the solution of the Primal problem corresponds to the solution of a square matrix of equations (simulation of the network's operation). Hence, it is guaranteed that it will always have a feasible solution. The set of constraints $w(y)$ need not be included in the problem since the binary variables y are fixed.

c) NLP feasibility sub-problem for fixed y^k. The task here is to minimise the infinity-norm, l_∞, (among other appropriate norms) measuring the infeasibility of the corresponding (NLP-Pr) sub-problem. Since the Primal problem is never infeasible, the NLP feasibility sub-problem can be omitted.

The Master problem corresponding to (SP) is the following MILP problem:

$$\min_{y,\theta} \quad \theta$$

$$\text{s.t.} \quad \theta \geq L(x^k, y, \lambda_g^k, \lambda_h^k); \quad k \in K \qquad \text{(MILP-M)}$$

$$w(y) \leq 0$$

$$\sum_{i \in B^k} y_i - \sum_{l \in C^k} y_l \leq |B^k| - 1; \quad k \in K$$

$$y \in Y = \{0,1\}^{n_y}$$

$$B^k = \{i : y_i^k = 1\}, \; C^k = \{l : y_l^k = 0\}; \quad k \in K$$

where $|B^k|$ is the cardinality of set B^k and

$$L(x^k, y, \lambda_g^k, \lambda_h^k) = f(x^k, y) + \lambda_g^{k^T} g(x^k, y) + \lambda_h^{k^T} h(x^k); \quad k \in K \qquad (5.51)$$

is the Lagrange function evaluated at the solution of the Primal problem at each iteration. The parameters $\lambda_g^{k^T}$ and $\lambda_h^{k^T}$ are the Lagrange multipliers at the solution of the k-th Primal problem. The set of integer cuts given by

$$\sum_{i \in B^k} y_i - \sum_{l \in C^k} y_l \leq |B^k| - 1; \quad k \in K \tag{5.52}$$

$$B^k = \{i : y_i^k = 1\}, \ C^k = \{l : y_l^k = 0\}; \quad k \in K$$

eliminates binary combinations already found at previous iterations.

The inequality constraints defined by

$$\theta^k \geq L(x^k, y, \lambda_g^k, \lambda_h^k); \quad k \in K \tag{5.53}$$

are known as *Benders cuts* and they produce a non-decreasing sequence of lower bounds [Floudas, 1995]. *Benders cuts* represent local underestimators of the MINLP problem (SP). These underestimators are valid when the MINLP problem is convex and, particularly, when Slater's condition for strong duality [Boyd and Vandenberghe, 2004] holds. This is not true for problem (SP). As a result, there exists the possibility that some *Benders cuts* will not be valid and the global solution will be excluded from the search procedure. Figure 5.10 depicts the situation where an invalid underestimator cuts off a part of the feasible region that includes the global solution (point A).

Sahinidis and Grossmann [1991] and Bagajewicz and Manousiouthakis [1991] have shown that the GBD algorithm may terminate at a local optimum or even worse at a non-stationary point for non-convex problems. Furthermore, they have shown that if the starting point is a local minimum then the algorithm will terminate at this point. This result can be used as a second termination criterion for the GBD algorithm to guarantee that it will always converge at a local minimum: the algorithm is restarted at the last solution point obtained until it terminates at that same point. Algorithm 5.1 gives an overview of the GBD algorithm implemented in this work.
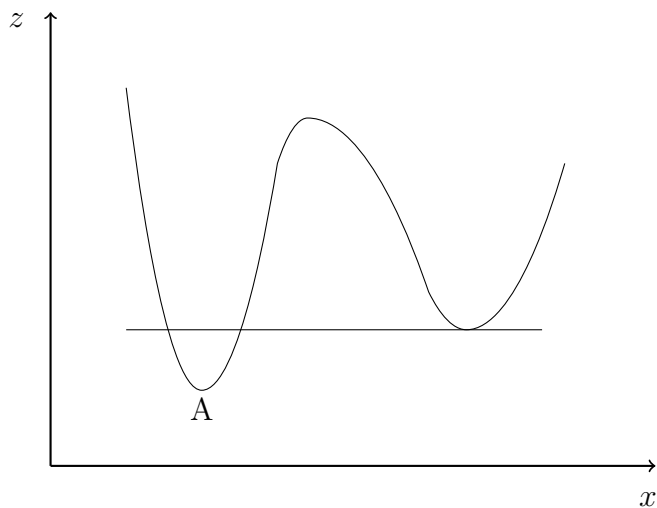
Figure 5.10: Invalid *Benders cut* (underestimator)

5.5.3 Receding Horizon heuristic

A heuristic solution procedure inspired by Control Theory, due to the dynamic nature of the scheduling problem, and particularly Model Predictive Control (MPC) is also used to solve the MINLP problem (SP). The basic steps in the MPC method [Camacho and Bordons, 2004] are the following:

a) calculate a control sequence after minimising an apt objective function over a fixed time horizon;

b) recede the horizon and repeat minimisation after applying the first signal of the control sequence.

The MPC approach can be adapted to attack the scheduling problem of cleaning heat exchanger networks subject to fouling. Here, the control sequence refers to the cleaning schedule and the first signal corresponds to the cleaning decisions for the first period of the examined number of periods, n_{RH} ($n_{\mathrm{RH}} < n_p$). Algorithm 5.2 describes the applied Receding Horizon (RH) heuristic solution procedure.

Note that the number of periods n_{RH} decreases as the iteration counter j approaches the value of n'_p. The solution procedure stops when $j = n_p$. Therefore,

---

Algorithm 5.1: Generalized Benders Decomposition

 1: **Begin**
 2: Set number of periods n_P
 3: Solve (NLP-R) ! obtain y_R to use as starting point
 4: $y^1 = 1 \; \forall \; y_R > 0.5$! R: Relaxed
 5: $y^1 = 0 \; \forall \; y_R \leq 0.5$
 6: termination = False
 7: **while** (termination = False) **do**
 8: $UB = +\infty, \; LB = -\infty$! UB: upper bound, LB: lower bound
 9: criterion = True
10: $k = 0$
11: **while** (criterion = True) **do**
12:   $k = k + 1$
13:   Solve (NLP-Pr) for given y^k
14:   Store $x^k = x, \; \lambda^k = \lambda, \; z_{Pr}^k$
15:   **if** $(UB \geq z_{Pr}^k)$ **then**
16:    $UB = z_{Pr}^k$
17:    $x^* = x^k$! x^*: optimal x vector
18:    $y^* = y^k$! y^*: optimal y vector
19:   **end if**
20:   Solve (MILP-M) for x^k
21:   Store $y^{k+1} = y, \; LB = \theta^k$
22:   **if** $(LB \geq UB)$ **then**
23:    criterion = False
24:   **end if**
25: **end while**
26: **if** $(k = 1)$ **then**
27:   termination = True
28: **end if**
29: **end while**
30: Solution: $x^*, \; y^*, \; UB$
31: **End**

---

the obtained cleaning schedule is for n_p periods and it is comparable to the cleaning schedules obtained using the GBD algorithm.

The merit of using the RH heuristic to solve the scheduling problem (SP) lies in the size of the sub-problems solved at each iteration: the sub-problems are relatively small and can be solved with relatively small computational effort. As the number of units, n_u, and/or the number of periods, n_p, increases it is ex-

---

Algorithm 5.2: Receding Horizon heuristic

 1: **Begin**
 2:      Set number of periods n_P
 3:      Set initial number of periods n_{RH}
 4:      $j = 0$! j indicates current period (iteration counter)
 5:      **while** $(n_{\mathrm{RH}} \geq 1)$ **do**
 6:          $j = j + 1$! recede horizon
 7:          **if** $(n_{RH} + j > n_P)$ **then**
 8:              $n_{\mathrm{RH}} = n_{\mathrm{RH}} - 1$
 9:          **end if**
10:          Solve (SP) for n_{RH} periods using Algorithm 5.1 (GBD)
11:          Apply cleaning actions for first period (current period j)
12:      **end while**
13: **End**

---

pected that the computational cost for applying the GBD algorithm will increase significantly. In such cases, the RH heuristic solution procedure may be more suitable to use.

5.6   Conclusions

A new mathematical programming formulation was presented in this chapter for the scheduling problem of cleaning heat exchanger networks subject to chemical reaction fouling. The scheduling problem takes into account the effects of ageing on fouling and cleaning dynamics. Moreover, it includes the selection between two cleaning methods, one mechanical and one chemical, which differ in their ability to remove the aged deposit.

A two-layer fouling model is used to track the effect of fouling on heat recovery and on cleaning effectiveness. It is assumed that the growth rate of both the gel layer (fresh deposit) and the coke layer (aged deposit) is constant and independent of any other parameters. The aged layer is considered to be more conductive than the fresh deposit and also not susceptible to removal by the chemical cleaning method.

The proposed formulation is reliant on the availability of the parameters of the two-layer fouling model. It is very likely that the resulting scheduling problems

will be highly sensitive to these parameters and reliable estimation of their values is going to be crucial in the application of the described scheduling formulation.

The scheduling problem is formulated for networks of single pass shell-and-tube exchangers operating in counter-current mode. It can be easily extended for other types of heat exchangers and different flow configurations. It is assumed that deposition of foulant occurs only in the tubes of the units where the cold stream flows.

The need to simulate the operation of heat exchanger networks in order to calculate the process costs due to fouling favours a discrete representation of time. An orthogonal collocation scheme is included in the problem formulation and is used to obtain numerical solutions for the differential equations, albeit these are of zero order (the future direction of the work is to replace the simple two-layer model with a more detailed one, *e.g.* the first order model described by Ishiyama *et al.* [2011a]), and to estimate the integral of the process costs over the examined time horizon.

The mathematical programming formulation of the scheduling task corresponds to a non-convex MINLP problem. Due to the non-convex characteristics of the problem it is very difficult to guarantee that a local solution is the globally optimal point. The non-convexity of the problem arises from the sets of equality constraints (5.37) – (5.39) and from the constraints defined by (5.23) – (5.26) (can be replaced by linear constraints if required / can be treated explicitly by Generalised Benders Decomposition).

The objective function of the scheduling problem is formulated for a special class of heat exchanger networks called preheat trains. Nonetheless, the scheduling problem may be extended to other types of heat exchanger networks after minor modifications. A preheat train is used to raise the temperature of a cold stream to a certain value before it enters some other process. Alas this target temperature is not achieved due to fouling. The objective function includes the energy losses due to fouling, the lost-production opportunity during the cleaning intervals and the maintenance costs.

The standard Outer Approximation/Equality Relaxation decomposition algorithm is deemed as unsuitable to attack large instances of the non-convex scheduling problem. In that regard, two alternative solution methods are proposed.

The first algorithm applies Generalised Benders Decomposition, a well-known exact solution method for convex MIP problems. For non-convex problems such as the one studied here there is a high probability that the global solution will be excluded by the search procedure at some iteration. Nonetheless, bearing in mind the unavoidable difficulties associated with non-convex problems, the goal here is to obtain 'good' local solutions with moderate computational cost. For that purpose, the use of Generalised Benders Decomposition is favourable.

The second solution approach is inspired by Model Predictive Control. The advantage of this heuristic solution procedure lies in the fact that the scheduling problem is solved over a short time horizon (instead of the whole time horizon) at each iteration. Thus, it is expected that a cleaning schedule can be obtained with relatively small computational effort even for large instances of the scheduling problem.

Chapter 6

Chemical reaction fouling: computational studies

In Chapter 5, a new MINLP formulation was presented for the problem of scheduling the cleaning actions for heat exchanger networks subject to chemical reaction fouling and ageing. The proposed formulation is evaluated in the current chapter through a series of computational studies. At first, the scheduling formulation is implemented for an isolated heat exchanger and the resulting model is solved using the Outer Approximation/Equality Relaxation algorithm. Subsequently, cleaning schedules are obtained for two heat exchanger networks of different size using the Generalized Benders Decomposition algorithm and the Receding Horizon heuristic procedure. An assessment is presented at the end of the chapter regarding the produced results and the computational performance of the different solution procedures.

6.1   Introductory remarks

For the computational studies, the scheduling problems are modelled in GAMS[TM] [Brooke *et al.*, 1992] installed on an ASUS[TM] Chassis computer with 2.21 GHz CPU. The DICOPT[®] solver (OA/ER algorithm) [Kocis and Grossmann, 1989], the GBD algorithm and the RH heuristic require the use of an MILP solver and an NLP solver. The MILP solver is CPLEX[®] 10.1.1 [GAMS, 2010] which is a

branch-and-cut algorithm. The NLP solver is CONOPT3® [GAMS, 2010], which applies the Generalised Reduced Gradient method [Abadie and Carpentier, 1969; Drud, 1994].

The different scheduling problems studied below are solved for multiple starting points in an attempt to compensate for the difficulty in obtaining the global solution imposed by the non-convex constraints. To facilitate the exposition of results, the best-obtained solution out of all starting points is referred to as the "optimal solution" (even if it is not the global solution).

The cleaning parameters are common for all scheduling tasks examined in this chapter. Table 6.1 gives the duration and cost for both cleaning actions. Other common parameters for all case studies are: the thermal conductivity of

Table 6.1: Cleaning parameters

Mode	Cost (£)	duration (days)
ch	5000	1
me	10000	5

the gel layer, $\lambda_g = 2 \times 10^{-3}$ kW/m.K, the thermal conductivity of the coke layer, $\lambda_c = 8 \times 10^{-3}$ kW/m.K, and the energy cost, $f_e = 0.5$ £/kW.day.

6.2 Isolated heat exchanger

At first, the proposed formulation is used to obtain cleaning schedules for an isolated heat exchanger. Two cases are studied for different coke formation rates, while the gel formation rate and all other parameters remain unchanged.

The operating parameters for the unit are given in Table 6.2. The heat transfer area, A, of the exchanger is 43.3 m^2 and the heat transfer coefficient in the clean state, U_0, is 400 W/m^2.K. The head load of the unit at a clean state is $Q_0 = 11$ MW. Table 6.3 gives the fouling parameters for the two case studies. The duration of the operating sub-period, t_{op}, is 10 days, hence, the length of a time period is 15 days.

For both case studies, the scheduling model is solved for 100 different starting points using the DICOPT® (OA/ER algorithm) solver. The starting points are random feasible combinations of the binary variables. The cleaning actions are

Table 6.2: Operating parameters: isolated heat exchanger

$T_{c,in}$ (^{o}C)	$T_{h,in}$ (^{o}C)	$\dot{m}_c$ (kg/s)	$\dot{m}_h$ (kg/s)	$C_{p,c}$ (kJ/kg.K)	$C_{p,h}$ (kJ/kg.K)
27	227	135	128	3.1	2.2

Table 6.3: Fouling parameters: isolated heat exchanger

Case study	k_g (m/day)	k_c (m/day)	k_g/k_c
A	1.6×10^{-6}	8×10^{-8}	20
B	1.6×10^{-6}	8×10^{-7}	2

scheduled over 24 periods corresponding to a time horizon of one year. The optimal schedule (best out of the 100) for both case studies is shown in Table 6.4. Moreover, the optimal value of the cost function, z^*, for each case study, is given in Table 6.5 and compared to the anticipated cost when no cleaning is performed, z_{no}.

Table 6.4: Optimal cleaning schedule: isolated heat exchanger (open circles: chemical actions; filled circles: mechanical action)

Case study	Period																								Mode

Case study	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	*ch*	*me*
A			○				○			○				○			○			○					6	
B			○				○					●			○				○						4	1

Table 6.5: Objective value for the optimal schedule and for the no-cleaning situation: isolated heat exchanger

Case study	$z_{no} \times 10^5$ (£)	$z^* \times 10^5$ (£)	Savings
A	6.8	2.5	63 %
B	5.1	2.6	49 %

The results presented in Tables 6.4 and 6.5 are in compliance with the assumption that the aged material is more conductive than the gel layer. For case study B, where the coke formation rate is ten times higher than that of case study A, the objective function value for the no-cleaning situation is considerably smaller: the objective value reflects the amount of heat losses due to fouling. Furthermore,

for case study A, where the coke formation rate is slow, the optimal schedule does not include any mechanical cleaning. In contrast, for case study B, a mechanical action is selected at period 12 as shown in Table 6.4.

The cleaning schedule for case study B suggests that an optimal mixed cleaning campaign can be identified, which can be repeated in time. This mixed cleaning heat exchanger cycle is termed the cleaning super-cycle and it includes a number of chemical actions to be followed by a mechanical cleaning, which will reset the unit to the clean state. The advantage of such a mixed cleaning strategy is that the operating time before lengthy cleaning shut-downs is extended by performing short-length chemical actions.

For case study B the cleaning super-cycle has a length of 12 periods (120 days) as seen in Table 6.4 and it includes 2 chemical actions. The mechanical cleaning performed at the end of period 12 restores fully the efficiency of the unit. Subsequently, the same cleaning pattern is observed, albeit, no mechanical action is performed at period 24 since there is no potential gain in cleaning the unit at the end of the examined time horizon. For case study A, where the coke formation rate is slower, a longer time horizon must be considered in order to obtain a cleaning super-cycle.

Figures 6.1(a) and 6.1(b) show the variation of the gel and coke thickness in time for case studies A and B, respectively. The timing of the cleaning actions is

(a) Case study A　　　　　　　(b) Case study B
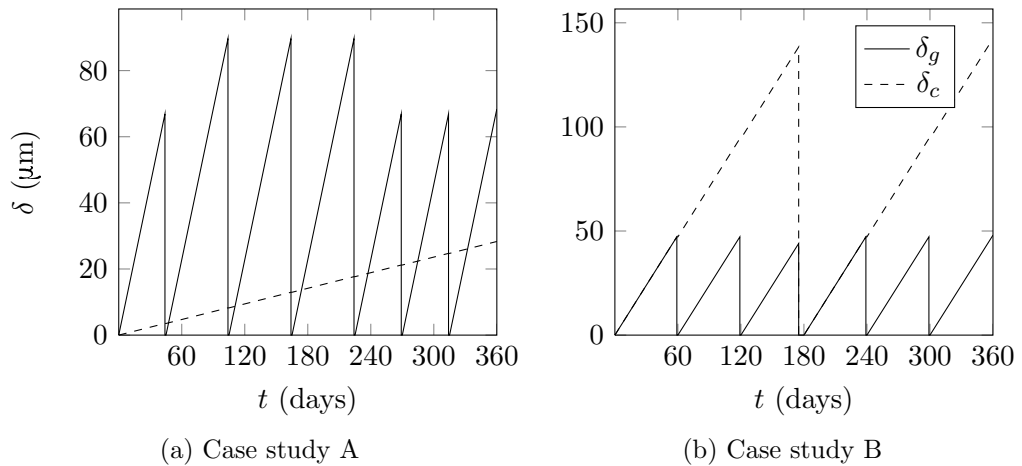
Figure 6.1: Time profile of gel and coke thickness: isolated heat exchanger

apparent on both graphs. For case study B, Figure 6.1(b) shows the mechanical cleaning occurring after 175 days, during which the thickness of both layers is set to zero. The thickness of the coke layer in case study A increases throughout the examined time horizon, as shown in Figure 6.1(a), since no mechanical action is performed.

6.3 Heat exchanger networks

The MINLP scheduling formulation is applied to the two heat exchanger networks reported by Smaïli *et al.* [2002]. The first network (referred to as heat exchanger network I) involves 14 units and introduces some of the complexities found in refinery networks caused by interconnecting hot streams [Smaïli *et al.*, 2002]. The second network (referred to as heat exchanger network II) consists of 25 units and bears a resemblance to a real network where several units are used in order to lessen the loss of production due to cleaning. Graphical representations of the smaller network and the more realistic network are shown in Figures 6.2 and 6.4, respectively.

The two networks are altered in this work: the flash drum included by Smaïli *et al.* [2002] is omitted. On the other hand, the desalter is included and therefore an extra set of constraints needs to be incorporated in the scheduling formulation. It is assumed that a drop of 10 °C occurs in the desalter. For heat exchanger network I where unit 5 precedes and unit 6 follows the desalter, the following set of constraints is added to the scheduling model:

$$T_{c,in}^{6,jkl} = T_{c,o}^{5,jkl} - 10; \quad j = 1, 2, \dots, np; \ k = 1, 2, 3; \ l = 0, 1, 2, 3. \qquad (6.1)$$

For heat exchanger network II the constraints are the following:

$$T_{c,in}^{8,jkl} = \frac{\dot{m}_c^6 T_{c,o}^{6,jkl} + \dot{m}_c^7 T_{c,o}^{7,jkl}}{\dot{m}_c^6 + \dot{m}_c^7} - 10 \qquad (6.2)$$

$$T_{c,in}^{9,jkl} = \frac{\dot{m}_c^6 T_{c,o}^{6,jkl} + \dot{m}_c^7 T_{c,o}^{7,jkl}}{\dot{m}_c^6 + \dot{m}_c^7} - 10 \qquad (6.3)$$

$$j = 1, 2, \dots, np; \ k = 1, 2, 3; \ l = 0, 1, 2, 3.$$

There are no constraints in the scheduling model of either network limiting the number of cleaning actions to be selected during the optimisation time horizon or in any of the periods. Furthermore, no firing limit is considered for the furnace, *i.e.* no lower limit is imposed on the value of the final temperature of the cold stream, T_f. Also, it is assumed that while a unit is being cleaned, the cold and hot streams are bypassed to the next unit.

For each network, two cases are studied with different coke formation rates. The coke formation rate is selected to be 25 times slower than the gel formation rate in case studies A_I and A_{II}, and 2.5 times slower in case studies B_I and B_{II}. All other parameters remain the same for all four case studies.

The duration of the operating sub-period is chosen to be 25 days, yielding discrete time periods of 30 days (1 month) in length. The cleaning actions for each case study are scheduled over 24 periods corresponding to a time horizon, t_f, of two years.

Two cleaning schedules are reported for each case study, one obtained using the GBD algorithm and the other using the RH heuristic procedure. The GBD algorithm is applied for 50 starting points which are random feasible combinations of the binary variables, and the best solution (cleaning schedule with the lowest objective function value) is presented. For the RH heuristic procedure, the length of the receding horizon for the MINLP sub-problems is selected to be 6 months ($n_{RH} = 6$ in Algorithm 5.2). Recall, the value of n_{RH} decreases as the value of j approaches that of n_p (in Algorithm 5.2), *e.g.* for $j = 20 \rightarrow n_{RH} = 5$.

The DICOPT$^{\circledR}$ MINLP solver was applied to all four case studies with no success: the OA/ER algorithm failed to converge after a reasonable amount of time. The algorithm remains trapped for a large amount of time at the first major iteration and specifically at the second step while trying to solve the MILP master problem. The failure of DICOPT$^{\circledR}$ to attack the MINLP models resulting from the proposed scheduling formulation was anticipated in Chapter 5: a large number of constraints is added to the master problem at each iteration, creating an MILP problem whose solution requires intense computational effort.

Sections 6.3.1 and 6.3.2 summarise the results for heat exchanger networks I and II, respectively, with no reference to the computational performance of the GBD algorithm or the RH heuristic procedure. The evaluation of the two solvers

is reserved for Section 6.3.3, where some solution statistics are also presented.

6.3.1 Heat exchanger network I

A schematic representation of heat exchanger network I is shown in Figure 6.2. Table 6.6 gives the operating and design parameters for the network along with the gel formation rate for each unit. Recall, the coke formation rate for case study A_I is $k_c = 0.04k_g$ and for case study B_I is $k_c = 0.4k_g$. The heat transfer coefficient at the initial clean state is equal for all units: $U_0^i = 0.5$ kW/m^2.K, for $i = 1, 2, \ldots, 14$. The mass flow rate of the cold stream is $\dot{m}_c^i = 95$ kg/s for units $i = 1, 2, \ldots, 8$ and $\dot{m}_c^i = 47.5$ kg/s for units $i = 9, 10, \ldots, 14$ in the split section. The cold stream enters the first unit of the network at a temperature of 26 °C.
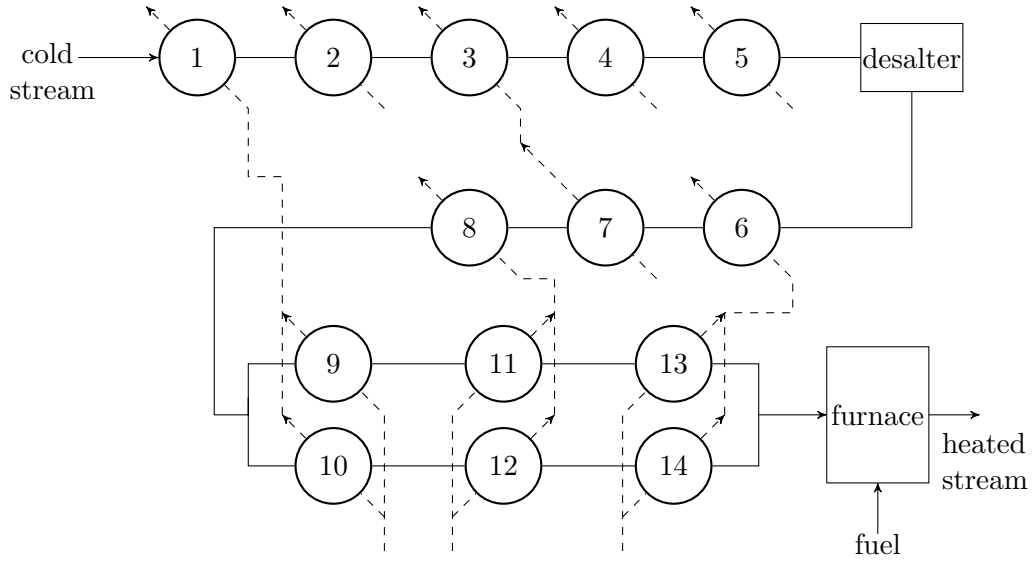
Figure 6.2: Heat exchanger network I

Tables 6.7(a) and 6.7(b) give the cleaning schedules for case study A_I obtained using the GBD algorithm and the RH heuristic procedure, respectively. Operating the network for 24 months without performing any cleaning actions results in an objective function value of $z_{no} = 9.7 \times 10^5$£. The optimal objective value for the GBD algorithm is $z_{GBD}^* = 5.9 \times 10^5$£, corresponding to 39% savings compared to when no cleaning actions are performed. Applying the RH cleaning schedule renders savings of 36% with an objective value of $z_{RH} = 6.2 \times 10^5$£. The solutions

Table 6.6: Problem parameters for heat exchanger network I

Unit	$T_{h,in}$ (°C)	$\dot{m}_h$ (kg/s)	$C_{p,h}$ (kJ/kg.K)	$C_{p,c}$ (kJ/kg.K)	A (m^2)	Q_0 (MW)	$k_g \times 10^{-7}$ (m/day)
1	-	19.1	2.8	1.92	56.6	3.5	1.2
2	296	3.3	2.9	1.92	8.9	0.9	1.8
3	-	55.8	2.6	1.92	208.3	9.3	1.2
4	170	49.7	2.6	1.92	112.9	2.8	1.6
5	237	49.7	2.6	1.92	121.6	5.2	1.6
6	-	34.8	2.8	2.3	110.1	5.8	3
7	205	55.8	2.6	2.3	67.2	1.2	2.2
8	-	45.5	2.9	2.3	67.1	2.4	3
9	249	9.5	2.8	2.4	91	1.5	3.2
10	249	9.5	2.8	2.4	91	1.5	3.2
11	286	22.8	2.9	2.4	61.3	2.1	3.6
12	286	22.8	2.9	2.4	61.3	2.1	3.6
13	334	17.4	2.8	2.4	55.6	2.4	3.8
14	334	17.4	2.8	2.4	55.6	2.4	3.8

obtained using the two methods feature similar objective function values and comparable cleaning schedules.

The GBD schedule includes 20 chemical actions, while the cleaning programme generated by the RH heuristic includes 22 chemical actions. An equal number of cleaning actions is selected for all units except 6, 7, 11 and 12, by both solvers. The GBD schedule includes a chemical action for unit 7 which receives no cleaning in the RH schedule. Also, an extra cleaning is included in the RH schedule for units 6, 11 and 12 in comparison to the GBD cleaning programme.

No cleaning actions are selected by either solver after period 19. The absence of cleaning actions at the end of the time horizon is expected since there is inadequate time to recover enough heat to offset the maintenance cost and the loss in performance caused by cleaning. This is called the 'end-zone effect'.

Unit 6 has the second highest heat load, Q_0, in the network and a relatively fast gel formation rate. It is cleaned more frequently than any other exchanger, in both schedules. Units 8 and 11–14, where the gel formation rate is also relatively high, receive more than one chemical action. On the other hand, units 9 and 10 are cleaned just once because of their relatively low heat load. Furthermore, in

Table 6.7: Cleaning schedule for heat exchanger network I: case study A_I (open circles: chemical actions)

(a) GBD algorithm

Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	ch	me
1																										
2																										
3										○															1	
4																										
5													○												1	
6						○						○							○						3	
7								○																	1	
8									○							○									2	
9								○																	1	
10														○											1	
11							○							○											2	
12								○									○								2	
13						○							○					○							3	
14								○							○				○						3	
$z_{\mathrm{GBD}}^* = 5.9 \times 10^5$ £																							Total		20	

(b) RH heuristic

Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	ch	me
1																										
2																										
3																			○						1	
4																										
5														○											1	
6					○				○				○				○								4	
7																										
8								○							○										2	
9																			○						1	
10																		○							1	
11						○						○						○							3	
12							○						○						○						3	
13						○					○					○									3	
14					○					○					○										3	
$z_{\mathrm{RH}} = 6.2 \times 10^5$ £																							Total		22	

both cleaning programmes, only one clean is performed on unit 3 even though it has the largest heat load due to its relatively low gel formation rate.

The large number of chemical actions and the absence of mechanical actions is a consequence of the slow coke formation rate. The thickness of the gel layer which poses a high resistance to heat transfer is increasing relatively quickly and as a response the solvers select frequent chemical actions in order to compensate the energy losses.

The schedules generated by the two solvers exhibit similar selection patterns but in the RH schedule the distribution of cleaning actions is more structured. The RH cleaning programme displays periodicity: the chemical actions for units which are cleaned more than once are selected after equal time intervals. Units 11–14 are cleaned thrice. The chemical actions for units 11 and 14 are performed one period after units 12 and 13 are cleaned, respectively.

The cleaning schedules obtained for case study B_I are given in Tables 6.8(a) and 6.8(b). Operating the network without applying any cleaning actions renders an objective value of $z_{\mathrm{no}} = 7.2 \times 10^5 £$. The optimal objective value for the GBD algorithm is $z_{\mathrm{GBD}}^* = 6 \times 10^5 £$, while the objective function value for the RH heuristic procedure is $z_{\mathrm{RH}} = 5.9 \times 10^5 £$. The solution generated from the RH heuristic in this case study is slightly better than the GBD solution. The corresponding savings in comparison to zero cleaning actions are 18% for the RH heuristic and 17% for the GBD algorithm.

A relatively small number of cleaning actions is selected by both solvers. For this case study, the two schedules are very different. The GBD cleaning programme includes four mechanical actions and two chemical actions, while the RH schedule includes only one mechanical action and 6 chemical actions. Furthermore, the cleaning actions are congested between periods 9 to 12 in the GBD schedule, whereas the RH schedule is more sparse. There, four out of the seven actions are performed after the fifteenth period. Nevertheless, both schedules include the same intuitive choices: only units 6, 8 and 11–14 are cleaned, where the gel and coke formation rates are relatively high.

For case study B_I, fewer cleaning actions are selected by the solvers, including some mechanical ones, compared to case study A_I due to the increase of the coke formation rate by a factor of 10. The aged material is four times more conductive

Table 6.8: Cleaning schedule for heat exchanger network I: case study B_I (open circles: chemical actions; filled circles: mechanical actions)

(a) GBD algorithm

Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	*ch*	*me*
1																										
2																										
3																										
4																										
5																										
6										●																1
7																										
8									●																	1
9																										
10																										
11											○														1	
12										○															1	
13									●																	1
14												●														1
$z^*_{\text{GBD}} = 6 \times 10^5 \text{£}$																						Total			2	4

(b) RH heuristic

Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	*ch*	*me*
1																										
2																										
3																										
4																										
5																										
6							○										○								2	
7																										
8																○									1	
9																										
10																										
11																			●							1
12																				○					1	
13										○															1	
14												○													1	
$z_{\text{RH}} = 5.9 \times 10^5 \text{£}$																						Total			6	1

than the fresh deposit. The objective value for the no-cleaning situation for case study A_I is $z_{no} = 9.7 \times 10^5 \pounds$, whereas for case study B_I is $z_{no} = 7.2 \times 10^5 \pounds$. This corresponds to a decrease of 26%. The preceding facts show the importance of the thermal conductivities of the two layers, which are parameters in the fouling model. It should be noted that if the deposits are allowed to get relatively thick this will affect the hydraulic performance of the network: this aspect is not considered here.

The GBD and RH schedules include the same intuitive cleaning choices present in those of case study A_I: units 6, 8 and 11–14, which exhibit a high gel formation rate, are cleaned more than once.

Figures 6.3(a) and 6.3(b) show the variation of the final temperature of the cold stream, T_f, with time for case studies A_I and B_I, respectively. The three profiles displayed on the graphs correspond to the GBD solution, the RH solution and the zero cleaning actions situation.

For case study A_I, the temperature profiles for the two solution methods are very similar. At the end of the time horizon, both the GBD and RH cleaning schedules achieve a final temperature, T_f, which is approximately 15 ºC higher than the case where no cleaning actions are performed.

The analogous temperature difference for case study B_I is close to 7^oC as seen in Figure 6.3(b). The temperature profiles are very different for the two schedules. The T_f^{GBD} is superior to T_f^{RH} around the midpoint of the time horizon, but it becomes inferior during the last periods.

The selection of multiple units to be cleaned in the same period has a commensurate effect on the final temperature, T_f. Large spikes are observed in the time profile of T_f for both case studies. These large drops in T_f can be avoided if the permissible number of cleaning actions at each period is restricted. This can be achieved by the following constraint:

$$\sum_{i=1}^{nu} \sum_{m \in M} y^{ijm} \leq nc; \quad j = 1, 2, \ldots, np \tag{6.4}$$

where nc is the allowed number of cleaning actions for a period. The set of constraints (6.4) will only participate in the Master problem (MILP-M).
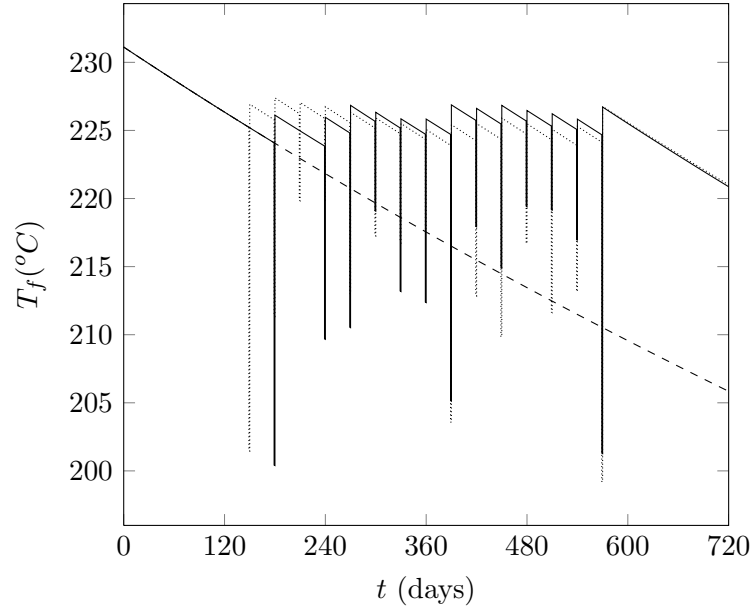
(a) Case study A$_I$
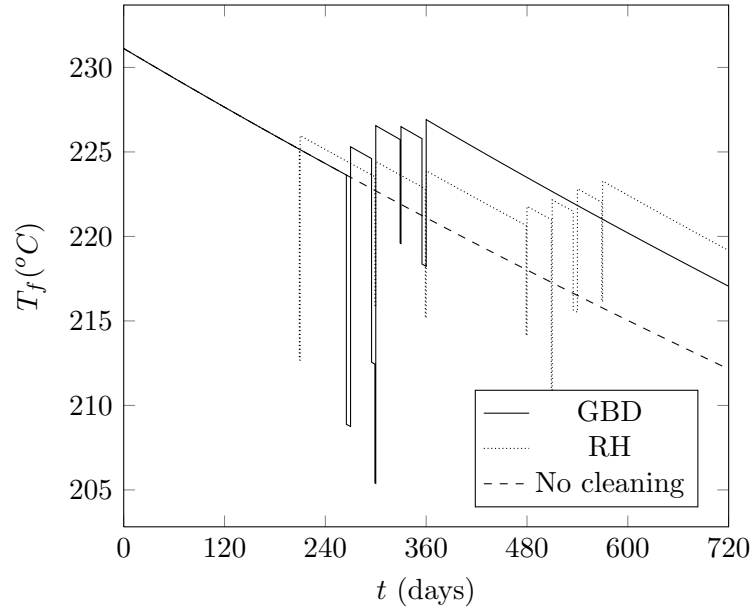
(b) Case study B$_I$

Figure 6.3: Time profile of T_f: heat exchanger network I

For industrial networks, the firing limits of the furnace will impose a lower bound on the value of T_f. In such a scenario, the following set of constraints needs to be included in the MINLP formulation:

$$T_f^{jkl} \geq T_f^{\text{limit}}; \quad j = 1, 2, \ldots, np; \; k = 1, 2, 3; \; l = 0, 1, 2, 3. \tag{6.5}$$

If not absolutely necessary, the addition of inequality constraints involving continuous variables to the formulation should be avoided. Constraints such as the ones given by equation (6.5) will cause the Primal Problem (NLP-Pr) to be infeasible for the given set of fixed binary values at some iterations of the GBD algorithm. Thus, the feasibility test step (see [Floudas, 1995]) omitted here from the algorithm will have to be included. In such a case, it is possible that the computational cost for generating a solution will increase. Even worse, due to the non-convex solution space of the problem the algorithm might terminate at an infeasible point.

6.3.2 Heat exchanger network II

A graphical representation of heat exchanger network II is given in Figure 6.4. The operating parameters, the area and the gel formation rate for each unit are summarised in Table 6.9 . The overall heat transfer coefficient in the fouling-free state is $U_0^i = 0.5$ kW/m^2.K for all units $i = 1, 2, \ldots, 25$. The inlet temperature of the cold stream at unit 1 is 26 ºC. The inlet cold stream mass flow rate is $\dot{m}_c^i = 95$ kg/s for units $i = 1, 2, \ldots, 5$, $\dot{m}_c^i = 47.5$ kg/s for units $i = 6, 7, \ldots, 13$ and $\dot{m}_c^i = 23.75$ kg/s for units $i = 14, 15, \ldots, 25$. The coke formation rate for case study A$_{\text{II}}$ is $k_c = 0.04 k_g$ and for case study B$_{\text{II}}$ is $k_c = 0.4 k_g$.

The optimal cleaning schedule for case study A$_{\text{II}}$, obtained using the GBD algorithm, is given in Table 6.10. The solver selects 19 chemical actions to be performed and the objective function value is $z_{\text{GBD}}^* = 6.7 \times 10^5$£. Applying the GBD schedule yields savings of 21%, with respect to the zero cleaning actions situation ($z_{\text{no}} = 8.7 \times 10^5$£).

Only chemical actions are performed, because of the slow coke formation rate, and only between periods 7 to 17. The absence of cleaning in the first six periods is due to the fact that the units are fouling-free at the beginning of the time horizon:
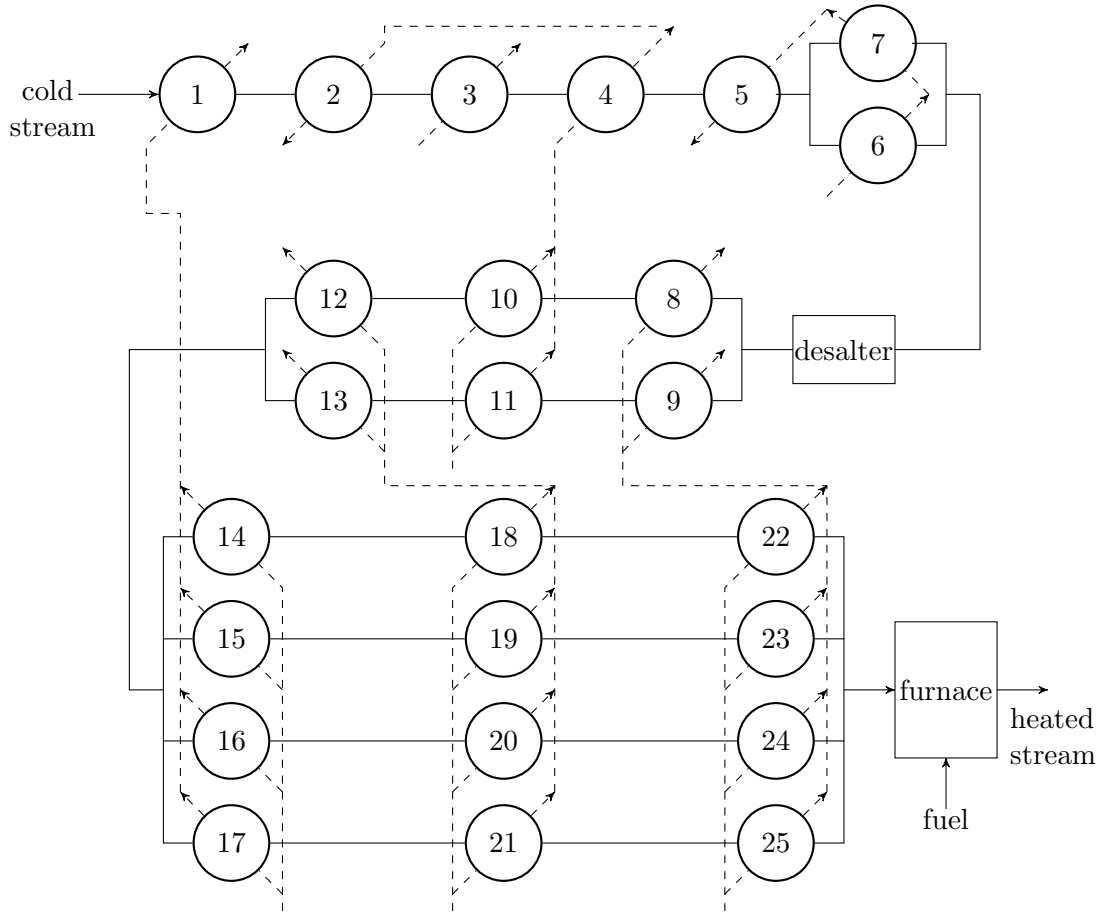
Figure 6.4: Heat exchanger network II

deposition has yet to cause significant loss of network performance. Moreover, the lack of cleaning after period 17 is due to the 'end-zone effect'. Out of the 25 units, eight (1, 3, 6-7, 14–19) do not receive any cleaning and 15 units are cleaned once. Units 8 and 9, which have a moderate heat load and a moderate gel formation rate compared to the other units, are cleaned twice.

At the hot end of the network, all heat exchangers of blocks 18-21 and 22-25 receive one cleaning. The units of block 14–17 have high gel formation rates but are not cleaned. The reason for this is because the heat load, Q_0, of these exchangers is relatively low (0.3 MW) and part of the energy lost due to fouling is recovered in the blocks downstream (18–21 and 22–25).

Table 6.11 shows the cleaning schedule produced by the RH heuristic proce-

Table 6.9: Problem parameters for heat exchanger network II

Unit	$T_{h,in}$ (°C)	$\dot{m}_h$ (kg/s)	$C_{p,h}$ (kJ/kg.K)	$C_{p,c}$ (kJ/kg.K)	A (m^2)	Q_0 (MW)	$k_g \times 10^{-7}$ (m/day)
1	-	19.2	2.8	1.92	56.6	4.1	1.2
2	-	55.8	2.6	1.92	96.6	6.5	1.8
3	296	3.3	2.9	1.92	8.5	0.7	1.2
4	-	55.8	2.6	1.92	109.6	7.7	1.8
5	-	49.6	2.6	1.92	129.2	3.4	1.6
6	-	50	2.6	1.92	80.3	2.1	1.6
7	237	50	2.6	1.92	60.8	2.1	1.6
8	-	34.8	2.6	2.3	79.1	3.3	2.2
9	-	34.8	2.9	2.3	79.1	3.3	2.2
10	293	56	2.9	2.3	29.2	1.2	3
11	293	56	2.8	2.3	29.2	1.2	3
12	-	45.6	2.8	2.3	35.4	0.8	3.2
13	-	45.6	2.6	2.3	35.4	0.8	3.2
14	249	19.2	2.8	2.4	31.4	0.3	3.2
15	249	19.2	2.8	2.4	31.4	0.3	3.2
16	249	19.2	2.8	2.4	31.4	0.3	3.2
17	249	19.2	2.8	2.4	41.4	0.3	3.2
18	286	45.6	2.9	2.4	29.7	0.7	3.6
19	286	45.6	2.9	2.4	29.7	0.7	3.6
20	286	45.6	2.9	2.4	29.7	0.7	3.6
21	286	45.6	2.9	2.4	29.7	0.7	3.6
22	334	34.8	2.8	2.4	21.3	0.8	3.8
23	334	34.8	2.8	2.4	21.3	0.8	3.8
24	334	34.8	2.8	2.4	21.3	0.8	3.8
25	334	34.8	2.8	2.4	21.3	0.8	3.8

dure. The corresponding objective function value is $z_{\mathrm{RH}} = 7.7 \times 10^5 \text{£}$ and the savings are 7% compared to the no-cleaning situation. The cleaning programme includes 7 chemical actions, which is noticeably fewer than the GBD schedule (19 chemical actions). No mechanical actions are selected. Out of the 25 units, 17 are not cleaned at all and among these are the units 14–25 at the hot end of the network. As in the GBD schedule, units 8 and 9 are cleaned twice and units 2 and 4, which have the highest heat load of all exchangers in the network, are cleaned once. Also, unit 12 receives a chemical action.

Table 6.10: Cleaning schedule for heat exchanger network II: GBD algorithm – case study A_{II} (open circles: chemical actions)

Units	Period																								Mode	
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	*ch*	*me*
1																										
2												○													1	
3																										
4															○										1	
5													○												1	
6																										
7																										
8								○								○									2	
9							○										○								2	
10										○															1	
11													○												1	
12												○													1	
13														○											1	
14																										
15																										
16																										
17																										
18															○										1	
19											○														1	
20												○													1	
21									○																1	
22														○											1	
23											○														1	
24													○												1	
25										○															1	
$z_{\mathrm{GBD}}^{*} = 6.7 \times 10^{5}$ £																						Total			19	

Table 6.11: Cleaning schedule for heat exchanger network II: RH heuristic – case study A$_{\text{II}}$ (open circles: chemical actions)

Units	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	*ch*	*me*
1																										
2																○									1	
3																										
4													○												1	
5																										
6																										
7																										
8									○										○						2	
9								○									○								2	
10																										
11																										
12																			○						1	
13																										
14																										
15																										
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17																										
18																										
19																										
20																										
21																										
22																										
23																										
24																										
25																										

$z_{\text{RH}} = 7.7 \times 10^5 \, \text{£}$ — Total: 7

For case study B_{II} the optimal objective value for the GBD algorithm is $z^*_{\text{GBD}} = 6 \times 10^5 \pounds$ and for the RH heuristic $z_{\text{RH}} = 6.2 \times 10^5 \pounds$, while the objective value for the no-cleaning situation is $z_{\text{no}} = 6.3 \times 10^5$. The resulting savings are 3% for the GBD solution and 2% for the RH solution.

The GBD and RH schedules include only two chemical actions. These are not presented here. The GBD algorithm selects the two actions close to the midpoint of the time horizon, with unit 8 being cleaned at period 14 and unit 9 being cleaned at period 15. In the RH cleaning schedule, unit 8 is cleaned at period 19 and unit 9 is cleaned at period 20.

The small number of cleaning actions in contrast to case study A_{II} is attributed to the high coke formation rate. The objective value for the no-cleaning situation is 26% less than that of case study A_{II}, where the coke formation rate is ten times lower. The decay in performance is relatively slow for the network and longer time horizons must be considered for possibly more cleaning actions to be selected.

The time profiles of the final temperature, T_f, for case studies A_{II} and B_{II} are shown in Figures 6.5(a) and 6.5(b), respectively.

For case study A_{II}, there is a 5 °C difference between the GBD and RH profiles at some instants, with T_f^{GBD} being always higher than T_f^{RH} after the seventh period. At the end of the time horizon the GBD algorithm achieves a final temperature which is 10 °C higher than that of the no-cleaning case. For the RH heuristic the temperature difference is close to 6 °C.

For case study B_{II} the temperature difference with respect to the no-cleaning situation is close to 1 °C for both solvers. As observed in Figure 6.5(b) the solvers allow a temperature drop of approximately 10 °C before selecting a cleaning action.
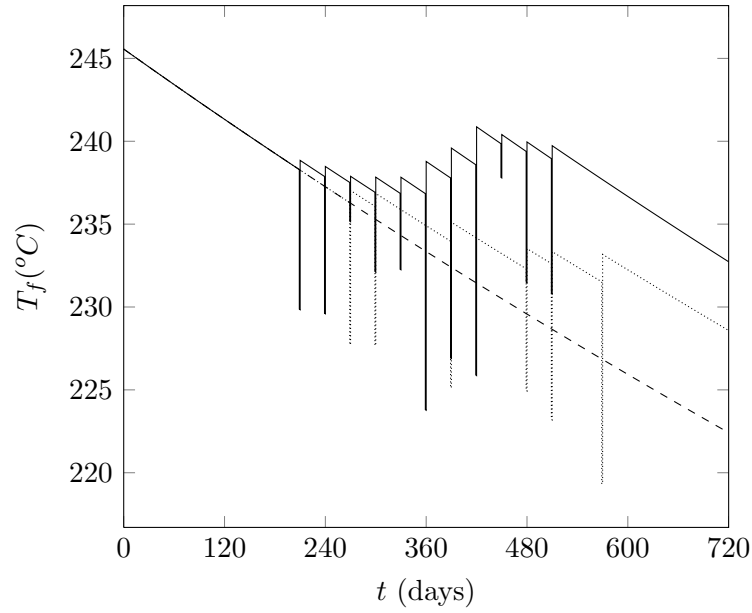
(a) Case study A$_{\mathrm{II}}$
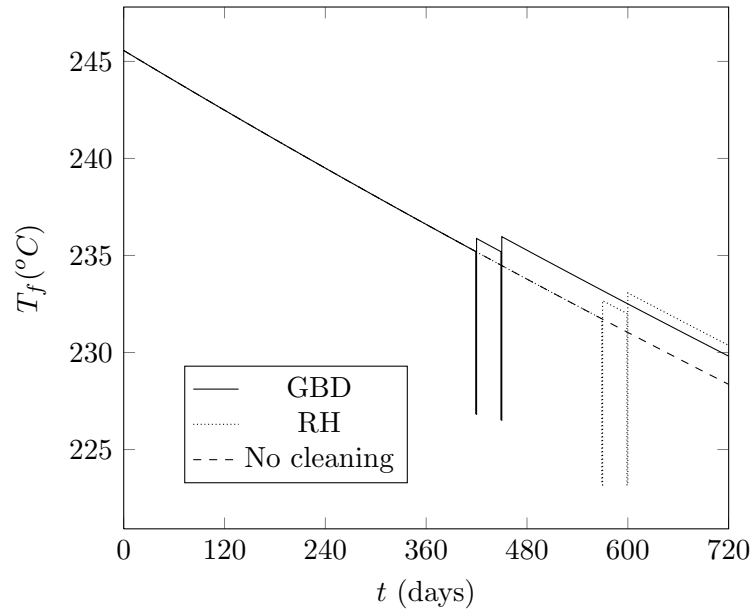
(b) Case study B$_{\mathrm{II}}$

Figure 6.5: Time profile of T_f: heat exchanger network II

6.3.3 Solution statistics

The size of the studied MINLP problems and some pertinent solution statistics are reported in this section in order to assist the evaluation of the results obtained. Table 6.12 shows the number of constraints and the number of continuous and binary variables for each case study. For the RH heuristic procedure, these numbers refer to the size of the MINLP sub-problems solved before the number of periods is reduced (19 out of the 24 sub-problems). Evidently, the size of the

Table 6.12: Size of studied scheduling problems

Solver	Continuous variables	Binary variables	Constraints
	heat exchanger network I		
GBD	40320	672	36000
RH	10080	168	9000
	heat exchanger network II		
GBD	72000	1200	65000
RH	18000	300	16250

MINLP problems under consideration is large and, together with a non-convex solution space, clearly poses a challenge to both solution procedures.

Table 6.13 gives the execution time for both solvers and for each scheduling task. The reported time for the GBD algorithm corresponds to the multiple starting point search. An average execution time can be calculated by dividing the value shown by 50 (the number of starting points). The ensuing average run

Table 6.13: Execution times

Case study	CPU time (min)	
	GBD	RH
A_I	132	4
B_I	223	5
A_{II}	554	11
B_{II}	526	13

time for the GBD algorithm is very similar to the execution time reported for the RH solution procedure for all case studies.

The execution times for the RH heuristic are relatively short, if one considers the size of the original MINLP problem. The execution time for the GBD
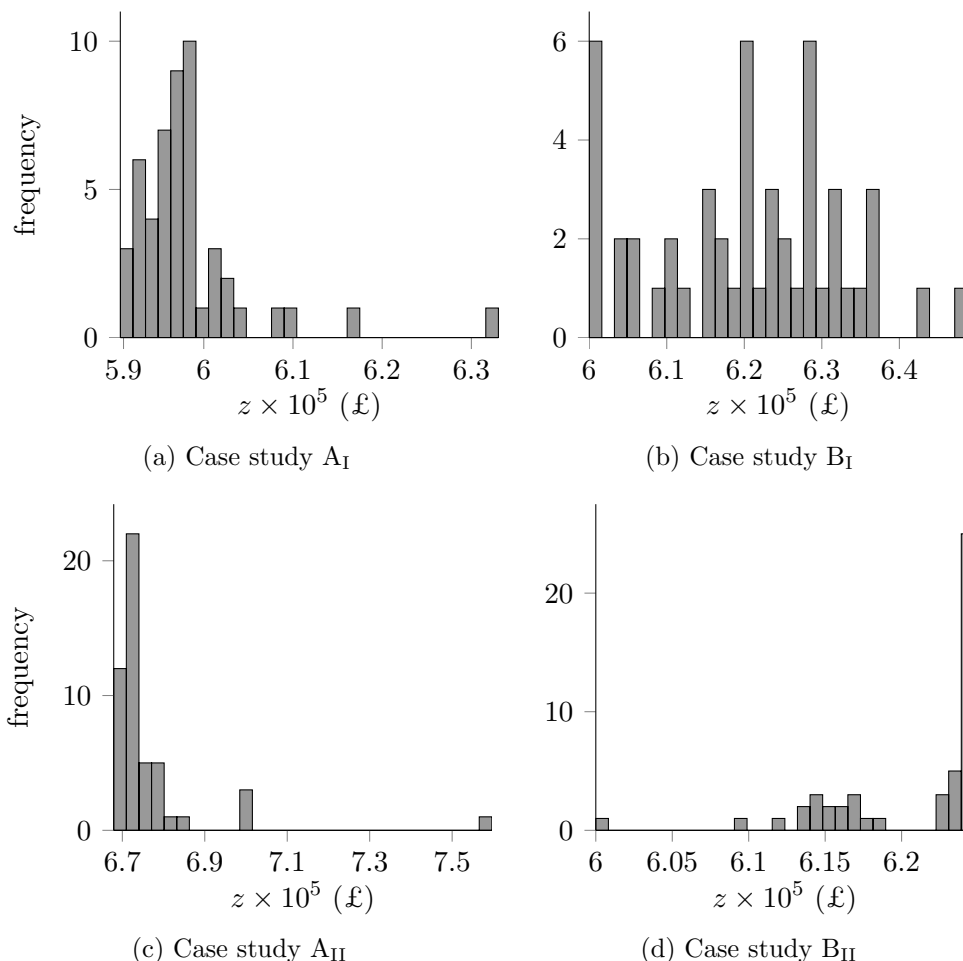
Figure 6.6: Distribution of solutions generated by the GBD algorithm for 50 random starting points

algorithm depends on the starting point which is chosen randomly here. The execution times for the bigger network are longer than those of network I. This is expected since the scheduling problem for heat exchanger network II is considerably larger.

Figure 6.6 shows the distributions of the locally optimal objective function values obtained by the GBD algorithm for the different starting points, for networks I and II. The non-convex nature of the scheduling formulation is evident from the presence of local solutions. The convergence of the GBD algorithm to a particular local optimum depends on the starting point. In all four case studies

the GBD algorithm converged to the reported optimal solution only once. It is, however, apparent from the dispersion of local solutions that a large number of local optima lies within a short range (with respect to the magnitude of the objective values reported). For case study A_I, the local points generated lie in a band of width 0.3×10^5 £, for case study B_I in a band of width 0.4×10^5 £ and for case study B_{II} in a band of width 0.2×10^5 £. The band is slightly bigger for case study A_{II}: 0.7×10^5.

6.4 Conclusions

The scheduling framework presented in Chapter 5 was used to obtain cleaning programmes for an isolated unit and two heat exchanger networks operating subject to chemical reaction fouling. Two cases were studied for each network and the isolated unit, one with a higher coke formation rate than the other.

The results presented for the single unit exhibited the merits for optimising the cleaning schedule: considerable savings are achieved compared to the no-cleaning situation. Furthermore, the results suggest that for an isolated unit, it is possible to identify an optimal mixed-cleaning campaign which can be repeated over time. This optimal heat exchanger cycle, called the cleaning super-cycle, includes a number of chemical actions before concluding with a mechanical action which resets the unit to a completely clean state. The advantage of adapting such a mixed-cleaning strategy is that the operating time before time-consuming mechanical actions is prolonged by performing short-length chemical actions.

The Outer Approximation/Equality Relaxation (OA/ER) algorithm was successfully used to obtain cleaning schedules for the isolated heat exchanger, but failed to generate a solution for the case studies concerning the two heat exchanger networks. In all cases, the DICOPT$^®$ solver remained trapped in the first iteration for a relatively long period of time, as it was not able to solve the first Master problem. The failure of the solver is due to the large size of the MINLP scheduling models.

The Generalised Benders Decomposition (GBD) algorithm and the Receding Horizon (RH) heuristic procedure described in Chapter 5 were used to optimise the cleaning schedules for a network of 14 units and a network of 25 units. The

performance of the GBD algorithm and the RH heuristic procedure are found to be satisfactory with respect to the computational effort required to generate a solution.

A multiple starting point search was used in order to increase the possibility of attaining a 'good' quality local solution: for each case study the scheduling problem was solved by the GBD algorithm for 50 random starting points. These starting points were feasible combinations of the binary variables. For the majority of the starting points the algorithm converged to a different local optimum, indicating the non-convex nature of the MINLP scheduling problem. The best solution found was reported. No multiple starting point scheme was implemented in conjunction with the RH heuristic.

The schedules generated by the two solution procedures are not always similar in terms of objective function value or cleaning choices. Also, the schedules obtained by the GBD algorithm are congested around the midpoint of the time horizon, while the schedules generated by the RH heuristic are more sparse.

It emerges from the results that when deciding which units to clean the solvers balance the choice between high heat load and high fouling rates. In that respect, the units with moderate to relatively high heat load and moderate to relatively fast fouling rates are selected for cleaning more frequently than units with just high heat load or just high fouling rates.

The cleaning schedules generated suggest the importance of the thermal conductivities of the two layers. The cleaning programmes for the cases with high coke formation rate are found to be very different than those with slow coke formation rate. The increase in the amount of aged material in the system and the proportional decrease in the amount of fresh deposit lead to a significant reduction of the energy losses.

Chapter 7

Biological fouling: formulations & computational studies

Chapters 5 and 6 discussed the problem of scheduling the cleaning actions for heat exchanger networks subject to chemical reaction fouling when two cleaning methods are available. The current chapter studies the scheduling problem for heat exchanger networks subject to biological fouling assuming that three cleaning options are available.

The biological fouling model used to describe the progression of the thermal fouling resistance is described first. Then, two mathematical programming formulations are proposed for the scheduling problem under investigation. Section 7.4 presents and discusses the results obtained from implementing one of the formulations for a small network of heat exchangers.

7.1   Introductory remarks

The problem of scheduling the cleaning actions for heat exchanger networks subject to biological fouling is formulated according to the methodology presented in Chapter 5 for networks operating under chemical reaction fouling. The heat transfer analysis, the time representation and the process constraints remain the same. The set of assumptions regarding heat transfer analysis is restated for the sake of lucidity. For a shell-and-tube unit in operation these are:

a) it is in counter-current mode. Therefore, the configuration correction factor, F, is equal to one;

b) the cold stream flows on the tube side and the hot stream on the shell side;

c) none of the streams changes phase;

d) the specific heat capacities of the streams are constant;

e) the mass flow rate of both streams remains constant.

The fouling analysis differs since here the accumulation of deposits is due to a different formation mechanism. Consequently this brings alterations to the simulation constraints. Moreover, there are now three available cleaning actions.

7.2 Fouling analysis

The accumulation of foulant is entirely due to the attachment and growth of micro-organisms on the heat transfer surface. It is assumed that a biofilm is formed only on the tube side of the exchanger while the shell side remains clean. The thermal fouling resistance, R_f, is considered to be zero for a period of time known as the initiation period, during which the heat transfer surface is colonised by micro-organisms [Bott, 2011]. After this induction period and the pre-conditioning of the surface, the progression of R_f follows an asymptotic curve such as the one shown in Figure 4.2.

The three cleaning methods available for the removal of the biofilm are the following: (i) a water flush which removes most of the biofilm but leaves the surface colonised and ready to restart growth when process operation resumes; (ii) chemical cleaning, which removes all biofilm and imposes a short initiation period; and (iii) chemical cleaning followed by disinfection (referred to as chemical disinfection for simplicity), which restores the efficiency of the heat exchanger back to its clean level and results in a longer induction period. The progression of the thermal fouling resistance after each cleaning action is shown in Figure 7.1(a).
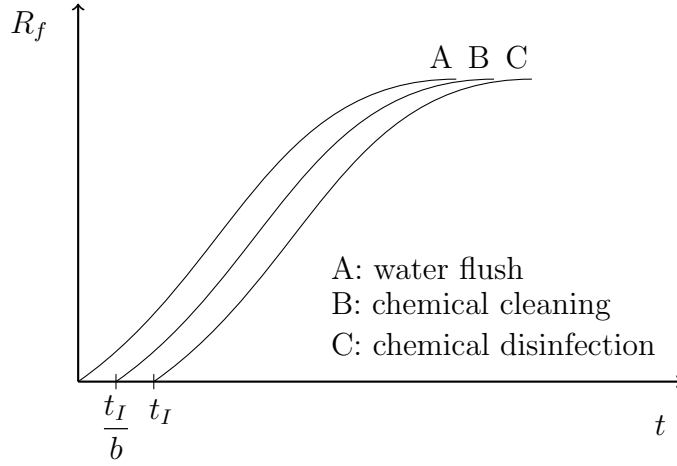
(a) Initiation period and asymptotic model
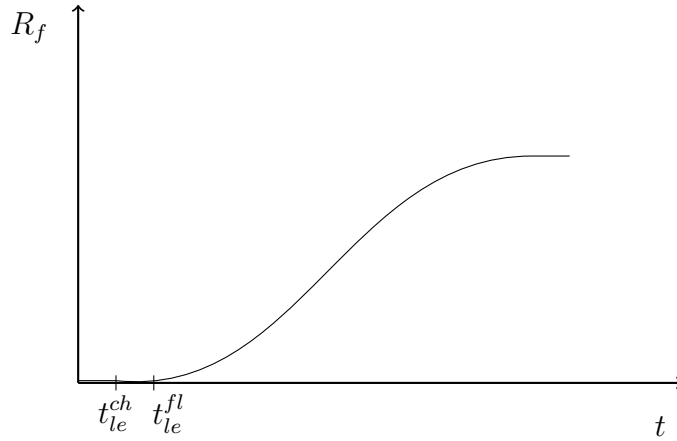
(b) Sigmoid model

Figure 7.1: Progression of thermal fouling resistance after cleaning

Curve A shows the evolution of R_f after a water flush cleaning is performed, where the surface is receptive to immediate biofilm growth. Curves B and C give the progression of R_f after a chemical cleaning, which imposes a short initiation period of length $\dfrac{t_I}{b}$ ($b > 1$) and after a chemical disinfection, which results in a longer induction time, t_I, respectively.

Following a cleaning action, it must be determined if an initiation period will occur and which of the three curves A, B and C will describe the progression of R_f. The model proposed by Kern and Seaton [1959] can be used to describe the asymptotic behaviour of R_f, but does not consider the initiation period. The

latter can be included explicitly in the scheduling formulation but this introduces additional complexity. Modifications need to be made to the time discretisation scheme presented in Section 5.3 since two extra elements must be added to each discrete period (at the beginning of the period) to account for the shorter or longer initiation time after a chemical action or a chemical disinfection, respectively.

Alternatively, the fouling model proposed by Nebot *et al.* [2007] can be used to describe the progression of thermal fouling resistance in time. The evolution of R_f follows a sigmoidal curve such as the one shown in Figure 7.1(b). The thermal fouling resistance is modelled as to be negligible for a period of time ($t \in [0, t_{le}^{fl}]$ on the graph) termed as the delay period. Thereafter, the biofilm undergoes an exponential growth before reaching a steady state, where the thermal fouling resistance attains the asymptotic value $R_{f\infty}$. The delay period during which the value of R_f is almost zero corresponds to the initiation period during which the value of R_f is zero.

After a cleaning action is performed, the evolution of R_f will resume from a different time point (starting time), t_0, on the sigmoid curve:

$$
t_0 = \begin{cases} 0, & \text{if chemical disinfection has occured} \\ t_{le}^{ch}, & \text{if chemical cleaning has occured} \\ t_{le}^{fl}, & \text{if water flush cleaning has occured} \end{cases} \tag{7.1}
$$

The parameters t_{le}^{fl} and t_{le}^{ch} are the 'leap' times after a water flush action and a chemical action, respectively. The parameters derive their name from the fact that the evolution of R_f does not resume from zero but from a point forward in time (a jump in time takes place). Note that $t_{le}^{fl} = t_I$ and $t_{le}^{ch} = t_I/b$.

The merit of using the model suggested by Nebot *et al.* [2007] is due to the fact that it takes into account the existence of the induction period while still being continuous. It is relatively straightforward to incorporate this fouling model in the scheduling formulation since it does not require any changes in the time representation scheme. Hence, the complexity of the scheduling problem does not increase.

According to Nebot *et al.* [2007], the fouling rate is given by the following

second order kinetic expression:

$$\frac{dR_f}{dt} = k(R_{f\infty} - R_f)R_f.$$
(7.2)

where k is a constant representing the rate at which the asymptotic value $R_{f\infty}$ is attained. In this work, the rate is considered to be uniform across the tubes of the unit. By integration of equation (7.2) an algebraic expression is obtained which relates the thermal fouling resistance to time as follows:

$$R_f = \frac{R_{f\infty}}{1 + (\frac{R_{f\infty}}{R_{f0}} - 1)\exp(-kR_{f\infty}t)}$$
(7.3)

where R_{f0} represents the thermal fouling resistance during the delay period. Since R_f is negligible during the early stages when the heat transfer surface is colonised, the parameter R_{f0} has a very small value.

Equation (7.2) is a modified version of the generalised expression for asymptotic fouling proposed by Konak [1973] for any deposition mechanism, *viz.*

$$\frac{dR_f}{dt} = k(R_{f\infty} - R_f)^n$$
(7.4)

The term $(R_{f\infty} - R_f)$ was postulated by Konak [1973] to be the driving force for the accumulation of foulant. Integrating equation (7.4) for $n = 1$ yields the following expression:

$$-\ln(1 - \frac{R_f}{R_{f\infty}}) = kt$$
(7.5)

which is a form of equation (4.6) proposed by Kern and Seaton [1959].

The differential equation (7.2) used by Nebot *et al.* [2007] to describe the growth of the biofouling layer is not a new one. It coincides in form with the logistic function suggested by the French mathematician Pierre-François Verhulst in 1838 to describe the self-limiting growth of a biological population.

7.3 Mathematical programming formulations

The task is to identify the optimal cleaning schedule for a heat exchanger network subject to biological fouling. Let us assume that $U' = \{1, 2, \ldots, nu\}$ is the set of units, $P = \{1, 2, \ldots, np\}$ the set of discrete periods and $M = \{fl :$ water flush, $ch :$ chemical, $cd :$ chemical disinfection$\}$ the set of available cleaning modes. Two mathematical programming formulations are described below for the studied problem: one MILP and one non-convex MINLP.

The binary variables y^{ijm}, for $i \in U'$; $j \in P$; $m \in M$, are such that correspond to 'yes' or 'no' decisions (cleaning choices and timings) as follows:

$$y^{ijm} = \begin{cases} 1, & \text{if cleaning mode } m \text{ is chosen for unit } i \text{ at period } j \\ 0, & \text{if cleaning mode } m \text{ is not chosen for unit } i \text{ at period } j \end{cases} \tag{7.6}$$

Time is discretized as detailed in Section 5.3. Accordingly, orthogonal collocation is used in order to acquire numerical estimations for the integrals involved in the objective function of the scheduling problem. Furthermore, the duration of a chemical disinfection is equal to the added length of elements 2 and 3 (see Figure 5.3), while the duration of a chemical cleaning is equal to the length of element 3 alone. The duration of a water flush cleaning is negligible compared to the time scales involved in the problem and therefore it is assumed to be zero days.

To facilitate the description of the proposed formulations the following function of v is defined:

$$r_f(v) \equiv \frac{R_{f_\infty}}{1 + (\frac{R_{f_\infty}}{R_{f_0}} - 1)\exp(-kR_{f_\infty}v)} \ . \tag{7.7}$$

7.3.1 MINLP formulation

With the intention of avoiding confusion it is clarified that time, the dimension with the aid of which events are ordered as past, present or future and which is discretised here, does not coincide with the variable t^{ijkl} involved in some of the constraints given below. Here, the variable t^{ijkl} is used in order to keep track of the

thermal fouling resistance, R_f, for a unit after a cleaning action is performed. It is because of the discontinuities introduced in the system by the binary variables that t^{ijkl} does not represent the dimension of time. For the remainder of this chapter, the variable t^{ijkl} is referred to as sigmoid time.

Assume that all units are in a completely clean state at the beginning of the time horizon. The sigmoid time for each unit for the first element of the first period is given by

$$t^{i,1,1,l} = \tau^l h^1; \quad i = 1, 2, \ldots, nu; \ l = 0, 1, 2, 3 \tag{7.8}$$

where, recall, τ^l is the normalised position of the l-th Radau collocation node and h^1 the time-length of element 1. For any other period the sigmoid time during element 1 has to account for any cleaning action as follows:

$$t^{ij,1,l} = \tau^l h^1 + t^{i,j-1,3,3}\Big(1 - \sum_{m \in M} y^{i,j-1,m}\Big) + t_d^{i,ch} y^{i,j-1,ch} + t_{le}^{i,fl} y^{i,j-1,fl} \tag{7.9}$$

$$i = 1, 2, \ldots, nu; \ j = 2, 3, \ldots, np; \ l = 0, 1, 2, 3.$$

To understand the set of constraints (7.9) better, suppose that a chemical action is selected for unit i at period $j-1$, *i.e.* $y^{i,j-1,ch} = 1$. In that case, equation (7.9) yields the following set of equality constraints:

$$t^{ij,1,l} = \tau^l h^1 + t_{le}^{i,ch}; \quad l = 0, 1, 2, 3.$$

This correctly reflects the fact that the chemical cleaning action in period $j-1$ has effectively reset time, as far as the fouling resistance is concerned, to t_{le}^{ch}. The set of equality constraints that involve the temperatures of the streams is given by

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \exp\Big(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(t^{ijkl})}\Big) \tag{7.10}$$

$$i = 1, 2, \ldots, nu; \ j = 1, 2, \ldots, np; \ k = 1; \ l = 0, 1, 2, 3$$

for element 1.

The sigmoid time for each exchanger for elements 2 and 3 is given by

$$t^{i,j,k,l} = \tau^l h^k + t^{i,j,k-1,3} \tag{7.11}$$

$$i = 1, 2, \ldots; \ j = 1, 2, \ldots, np, \ k = 1, 2, 3; \ l = 0, 1, 2, 3.$$

There is no need to set the sigmoid time to zero while a unit is cleaned since it will be controlled to account for the cleaning at the beginning of the next period.

The temperature constraints for element 2 are given by

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \left[(1 - y^{ij,cd}) \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(t^{ijkl})} \right) + y^{ij,cd} \right] \tag{7.12}$$

$$i = 1, 2, \ldots, nu; \ j = 1, 2, \ldots, np; \ k = 2; \ l = 0, 1, 2, 3$$

and for element 3 by

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl})$$
$$\left[(1 - \sum_{\substack{m \in M \\ m \neq fl}} y^{ijm}) \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(t^{ijkl})} \right) + \sum_{\substack{m \in M \\ m \neq fl}} y^{ijm} \right] \tag{7.13}$$

$$i = 1, 2, \ldots, nu; \ j = 1, 2, \ldots, np; \ k = 3; \ l = 0, 1, 2, 3.$$

The MINLP formulation is non-convex due to equality constraints (7.9) (these are treated explicitly by the GBD algorithm), (7.10), (7.12) and (7.13). It includes $\mathcal{O}(72 \times nu \times np)$ continuous variables, $\mathcal{O}(3 \times nu \times np)$ binary variables and $\mathcal{O}(48 \times nu \times np)$ constraints (simulation constraints, process constraints, integral constraints and inequality constraints of binary variables).

7.3.2 MILP formulation

An alternative MILP scheduling formulation can be derived for the problem by parametrising the thermal fouling resistance along the lines proposed by Georgiadis *et al.* [2000] and Lavaja and Bagajewicz [2004] (for a linear fouling model). The parametrisation scheme for the asymptotic fouling model by Nebot *et al.* [2007] is described below.

Assume that the completely clean unit i will start operating at the beginning of period 1. The thermal fouling resistance during the first period is given by

$$R_f^{i,1,kl} = r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n); \quad k = 1, 2, 3; \ l = 0, 1, 2, 3. \tag{7.14}$$

For the second period the thermal fouling resistance takes into account any possible cleaning action performed in period 1 as follows:

$$R_f^{i,2,kl} = r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + t_{le}^{i,ch})y^{i,1,ch} + r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + t_{le}^{i,fl})y^{i,1,fl} \tag{7.15}$$

$$r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n)y^{i,1,cd} + r_f(t_p + \tau^l h^k + \sum_{n=1}^{k-1} h^n)(1 - \sum_{m \in M} y^{i,1,m})$$

$$k = 1, 2, 3; \ l = 0, 1, 2, 3.$$

where $t_p = \sum_{k=1}^{3} h^k$ is the time-length of a period. Accordingly, for the third period the thermal fouling resistance is given by

$$R_f^{i,3,kl} = \left[r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + t_{le}^{i,ch} + t_p)y^{i,1,ch} + r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + t_{le}^{i,fl} + t_p)y^{i,1,fl} \right.$$

$$\left. + r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + t_p)y^{i,1,cd} \right](1 - \sum_{m \in M} y^{i,2,m}) \tag{7.16}$$

$$+ r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + t_{le}^{i,ch})y^{i,2,ch} + r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + t_{le}^{i,fl})y^{i,2,fl}$$

$$+ r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n)y^{i,2,cd}$$

$$+ r_f(2t_p + \tau^l h^k + \sum_{n=1}^{k-1} h^n)\prod_{p=1}^{2}(1 - \sum_{m \in M} y^{ipm})$$

$$k = 1, 2, 3; \ l = 0, 1, 2, 3.$$

If a water flush cleaning is performed at period 1 ($y^{i,1,fl} = 1$) the above set of

constraints becomes

$$R_f^{i,3,kl} = r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + t_{le}^{i,fl} + t_p); \quad k = 1, 2, 3; \; l = 0, 1, 2, 3 \qquad (7.17)$$

and if a chemical disinfection is performed at period 2 ($y^{i,2,cd} = 1$) it becomes

$$R_f^{i,3,kl} = r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n); \quad k = 1, 2, 3; \; l = 0, 1, 2, 3. \qquad (7.18)$$

If no cleaning action is performed in neither periods 1 and 2 the equality constraints are the following:

$$R_f^{i,3,kl} = r_f(2t_p + \tau^l h^k + \sum_{n=1}^{k-1} h^n); \quad k = 1, 2, 3; \; l = 0, 1, 2, 3. \qquad (7.19)$$

Equations (7.15) – (7.16) include only parameters and binary variables and equation (7.14) only parameters. The above parametrisation scheme can be generalised for periods: $j = 2, 3, \ldots, np$. The general form of the thermal fouling resistance is as follows:

$$
\begin{aligned}
R_f^{ijkl} = \sum_{n=1}^{j-1} & \left[\left(r_f(t_{le}^{i,ch} + (j - n - 1)t_p + \tau^l h^k + \sum_{n=1}^{k-1} h^n) y^{in,ch} \right. \right. \\
& + r_f(t_{le}^{i,fl} + (j - n - 1)t_p + \tau^l h^k + \sum_{n=1}^{k-1} h^n) y^{in,fl} \qquad (7.20) \\
& \left. + r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + (j - n - 1)t_p) y^{in,cd} \right) \prod_{p=n+1}^{j-1} \left(1 - \sum_{m \in M} y^{ipm} \right) \right] \\
& + r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n + (j - 1)t_p) \prod_{n=1}^{j-1} (1 - \sum_{m \in M} y^{inm}) \\
i = 1, 2, & \ldots, nu; \; j = 2, 3, \ldots, np; \; k = 1, 2, 3; \; l = 0, 1, 2, 3.
\end{aligned}
$$

For the first period, there are three different sets of equality constraints relating the inlet – outlet temperatures of the streams, one for each element. For the

first element the set is as follows:

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(\tau^l h^k)}\right) \tag{7.21}$$

$$i = 1, 2, \ldots, nu; \ j = 1; \ k = 1; \ l = 0, 1, 2, 3.$$

For element 2 the constraints needs to account for a chemical disinfection, *viz.*

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl})$$
$$\left[(1 - y^{ij,cd}) \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n)}\right) + y^{ij,cd}\right] \tag{7.22}$$

$$i = 1, 2, \ldots, nu; \ j = 1; \ k = 2; \ l = 0, 1, 2, 3.$$

Moreover for element 3 the equality constraints are modified to take into account a chemical disinfection or chemical cleaning as follows:

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl})$$
$$\left[\left(1 - \sum_{\substack{m \in M \\ m \neq fl}} y^{ijm}\right) \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(\tau^l h^k + \sum_{n=1}^{k-1} h^n)}\right) + \sum_{\substack{m \in M \\ m \neq fl}} y^{ijm}\right] \tag{7.23}$$

$$i = 1, 2, \ldots, nu; \ j = 1; \ k = 3; \ l = 0, 1, 2, 3.$$

The constraints given by equation (7.21) are linear, while the constraints given by equations (7.22) – (7.23) include only products of binary variables with continuous variables which can be easily replaced by new linear constraints [Williams, 1990], with the addition of new continuous variables, as shown next.

The term xy, where x is a continuous variable and y a binary variable, can be replaced by a new continuous variable v by adding the following logical constraints:

$$v - By \leq 0 \tag{7.24}$$
$$v - x \leq 0 \tag{7.25}$$
$$x - v + By \leq B \tag{7.26}$$

where B is the upper bound for x.

The temperature constraints for the remaining periods, for element 1 are given by

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + R_f^{ijkl}}\right) \tag{7.27}$$

$$i = 1, 2, \ldots, nu; \ j = 2, 3, \ldots, np; \ k = 2; \ l = 0, 1, 2, 3.$$

Combining equations (7.20) and (7.27) yields

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + \sum_{n=1}^{j-1} \left[(T_{h,in}^{ijkl} - T_{c,o}^{ijkl})\left(B_1^{ijkl} y^{in,ch} + B_2^{ijkl} y^{in,fl} + B_3^{ijkl} y^{in,cd}\right) \right.$$
$$\left. \prod_{p=n+1}^{j-1}\left(1 - \sum_{m\in M} y^{ipm}\right) \right] + B_4^{ijkl}(T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \prod_{n=1}^{j-1}\left(1 - \sum_{m\in M} y^{inm}\right) \tag{7.28}$$

$$i = 1, 2, \ldots, nu; \ j = 2, 3, \ldots, np; \ k = 1; \ l = 0, 1, 2, 3$$

where

$$B_1^{ijkl} = \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(t^{i,ch} + t_p(j - n - 1) + \tau^l h^k + \sum_{n=1}^{k-1} h^n)}\right) \tag{7.29}$$

$$B_2^{ijkl} = \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(t^{i,fl} + t_p(j - n - 1) + \tau^l h^k + \sum_{n=1}^{k-1} h^n)}\right) \tag{7.30}$$

$$B_3^{ijkl} = \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(t_p(j - n - 1) + \tau^l h^k + \sum_{n=1}^{k-1} h^n)}\right) \tag{7.31}$$

$$B_4^{ijkl} = \exp\left(\frac{A^i C^i}{\frac{1}{U_0^i} + r_f(t_p(j - 1) + \tau^l h^k + \sum_{n=1}^{k-1} h^n)}\right) \tag{7.32}$$

Similarly, for element 2 the constraints are given by

$$T_{h,o}^{ijkl} = T_{c,in}^{ijkl} + \left\{ \sum_{n=1}^{j-1} \left[(T_{h,in}^{ijkl} - T_{c,o}^{ijkl})\left(B_1^{ijkl} y^{in,ch} + B_2^{ijkl} y^{in,fl} + B_3^{ijkl} y^{in,cd}\right) \right.\right.$$
$$\left.\left. \prod_{p=n+1}^{j-1}\left(1 - \sum_{m\in M} y^{ipm}\right) \right] + B_4^{ijkl}(T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \prod_{n=1}^{j-1}\left(1 - \sum_{m\in M} y^{inm}\right) \right\}$$

$$(1 - y^{ij,cd}) + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl})y^{ij,cd} \tag{7.33}$$

$$i = 1, 2, \ldots, nu; \; j = 2, 3, \ldots, np; \; k = 2; \; l = 0, 1, 2, 3$$

and for element 3 by

$$
\begin{aligned}
T_{h,o}^{ijkl} = & T_{c,in}^{ijkl} + \left\{ \sum_{n=1}^{j-1} \left[(T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \left(B_1^{ijkl} y^{in,ch} + B_2^{ijkl} y^{in,fl} + B_3^{ijkl} y^{in,cd} \right) \right. \right. \\
& \left. \prod_{p=n+1}^{j-1} (1 - \sum_{m \in M} y^{ipm}) \right] + B_4^{ijkl}(T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \prod_{n=1}^{j-1} (1 - \sum_{m \in M} y^{inm}) \right\} \\
& (1 - \sum_{\substack{m \in M \\ m \neq fl}} y^{ijm}) + (T_{h,in}^{ijkl} - T_{c,o}^{ijkl}) \sum_{\substack{m \in M \\ m \neq fl}} y^{ijm} \tag{7.34}
\end{aligned}
$$

$$i = 1, 2, \ldots, nu; \; j = 2, 3, \ldots, np; \; k = 3; \; l = 0, 1, 2, 3.$$

In equations (7.28), (7.33), (7.34) the binary variables and the binary products are moved out of the exponentials (terms B_1^{ijkl}, B_2^{ijkl}, B_3^{ijkl} and B_4^{ijkl}). This is due to the fact that one, and only one, of the corresponding terms can be different from zero.

The nonlinearities in the aforementioned sets of constraints consist of products of binary variables with continuous variables. These can be linearised by introducing new variables and additional constraints as shown above. However, by doing so the size of the resulting MILP models will grow rapidly as the number of periods and the number of units increases. Applying the MILP formulation for a heat exchanger network is impractical (as Lavaja and Bagajewicz [2004] reported for a similar formulation), even if the global minimum can be obtained, since the solution of the corresponding model will be computationally unaffordable.

7.3.3 Objective function

The objective function depends on the type of network under consideration and the performance targets imposed by the operator or other interacting processes. Here, for the computational studies undertaken and presented in the next section, the objective function needs to include only the energy losses due to fouling, the lost-production opportunity during cleaning intervals and the cost of the cleaning

actions, as follows:

$$z = \sum_{i=1}^{nu} \sum_{j=1}^{np} f_e \big(Q_0^i \sum_{k=1}^{3} h^k - I_1^{ij,3,3} \big) + \sum_{i=1}^{nu} \sum_{j=1}^{np} \sum_{m \in M} y^{ijm} c^m \tag{7.35}$$

where $C = \{c^m : m \in M\}$ is the cost vector. The variable I_1^{ijkl} (calculation of integral for process costs) is involved in the equality constraints (5.46) – (5.48) given in Chapter 5. These are re-introduced here:

$$\sum_{l=0}^{3} I_1^{ijkl} \frac{dq_l(\tau^n)}{d\tau} = h^n \dot{m}_c^n C_{p,c}^n (T_{c,o}^{ijkn} - T_{c,in}^{ijkn}) \tag{5.46}$$

$$i = 1, 2, \ldots, nu; \ j = 1, 2, \ldots, np; \ k = 1, 2, 3; \ n = 0, 1, 2, 3$$

$$I_1^{ij,1,1} = 0; \quad i = 1, 2, \ldots, nu; \ j = 1, 2, \ldots, np \tag{5.47}$$

$$I_1^{ijk,0} = I_1^{ij,k-1,3}; \quad i = 1, 2, \ldots, nu; \ j = 1, 2, \ldots, np; \ k = 2, 3. \tag{5.48}$$

7.4   Computational studies

The MINLP formulation is implemented in the computational studies presented next. The Generalised Bender's Decomposition algorithm, described in Chapter 5, is utilised to solve the resulting scheduling models. Cleaning schedules are obtained for the fictional heat exchanger network shown in Figure 7.2 for three case studies with different fouling parameters.
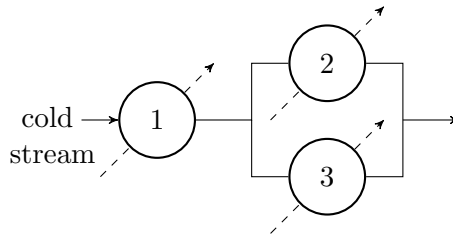

Figure 7.2: Heat exchanger network subject to biological fouling

Table 7.1 summarises the operating and design parameters for the three units of the network. The energy cost is $f_e = 0.5$ £/kW.day. Furthermore, the specific heat capacity is $C_{p,h} = 2.2$ kJ/kg.K and $C_{p,c} = 4.2$ kJ/kg.K for the hot streams

and cold stream, respectively. The inlet temperature of the cold stream at the first unit of the network is 25 °C.

Table 7.1: Operating and design parameters for heat exchanger network subject to biological fouling

Unit	$T_{h,in}$ (°C)	$\dot{m}_h$ (kg/s)	$\dot{m}_c$ (kg/s)	U_0 (kW/m^2.K)	A (m^2)	Q_0 (MW)
1	200	20.5	75	0.55	33	2.6
2	190	20	37.5	0.55	30	1.8
3	210	25.8	37.5	0.55	32.5	2.3

The parameters for the fouling model are given in Table 7.2. For case study A, the thermal fouling resistance, R_f, in each unit, approaches the relatively high asymptotic value, $R_{f\infty}$, with a relatively fast rate k. For case study B, the asymptotic value is decreased by a factor of two, while the rate for each exchanger remains the same compared to case study A. Finally, for case study C the asymptotic value is equal to that of case study A but the rate, k, is decreased by 33%. The changes in $R_{f\infty}$ cause also the parameters t_{le}^{fl} and t_{le}^{ch} to take different values.

Table 7.2: Parameters for biological fouling model

Unit	$R_{f\infty}$ (m^2.K/kW)	R_{f0} (m^2.K/kW)	k (kW/m^2.K.day)	t_{le}^{ch} (days)	t_{le}^{fl} (days)
		case study A			
1	0.8	1×10^{-4}	0.18	19	38
2	0.8	1×10^{-4}	0.22	15	30
3	0.8	1×10^{-4}	0.25	13	26
		case study B			
1	0.4	1×10^{-4}	0.18	31	62
2	0.4	1×10^{-4}	0.22	26	52
3	0.4	1×10^{-4}	0.25	23	46
		case study C			
1	0.8	1×10^{-4}	0.12	24	48
2	0.8	1×10^{-4}	0.15	19	38
3	0.8	1×10^{-4}	0.17	17	34

If left unmitigated, the biofilm causes the overall heat transfer coefficient, U,

to decrease from 0.55 kW/m^2.K at the clean state to 0.38 kW/m^2.K at the steady state (31% drop), for case studies A and C. For case study B, U drops to 0.45 kW/m^2.K, representing a 18% decrease compared to the fouling-free state.

The duration of the operating sub-period, $t_{op} = h^1$, is chosen to be 10 days, while the duration of a chemical disinfection, $t_{cd} = h^2 + h^3$, is 5 days. Hence, the length of a time period is 15 days. The duration of a chemical action is $t_{ch} = h^3 = 1$ day. Recall, the duration of a water flush cleaning is considered to be negligible. The cleaning schedule is optimised over 24 periods (360 days).

Table 7.3 summarises the cleaning parameters used in the case studies.

Table 7.3: Cleaning parameters

Mode	Cost (£)	duration (days)
fl	1000	0
ch	2500	1
cd	3500	5

A multiple starting point search is performed in order to increase the possibility of finding a 'good' local solution. Therefore, the MINLP problem for each case study is solved for 100 random starting points. These are feasible combinations of the binary variables. Table 7.4 reports the best cleaning schedule and the objective function value obtained for each of the case studies.

For case study A, operating the examined network without performing any cleaning action for 360 days corresponds to an objective function value $z_{no} = 2.4 \times 10^5$ £. Applying the best found cleaning schedule results in 46% savings. The schedule includes cleaning by all three modes and the units are cleaned frequently: nine cleaning actions are selected for units 1 and 3 and ten for unit 2. Unit 1 receives all the chemical actions and some water flush actions. Regular water flush cleaning is performed on units 2 and 3, which also receive one and two chemical disinfections, respectively. The cleaning actions span between periods 3 to 22.

For case study B, the savings for implementing the best schedule generated are 42% ($z_{no} = 1.2 \times 10^5$ £). Here, the cleaning actions are less frequent compared to case study A, where fouling is more severe. One chemical disinfection, six chemical actions and six water flushes are selected. Unit 1 receives only chemical

Table 7.4: Cleaning schedule for heat exchanger network subject to biological fouling (open circles: water flush; filled grey circles: chemical cleaning; filled black circles: chemical disinfection)

(a) Case study A

Units	Period																								Mode		
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	*fl*	*ch*	*cd*
1			◉			◉			○		○		◉		○		◉			○	◉				4	5	
2			○		○		○			○		○	○		○		○	○		●					9		1
3				○		○		○	○		●			○		●			○		○	○			8		1
	$z^* = 1.3 \times 10^5$£																						Total	21	5	2

(b) Case study B

Units	Period																								Mode		
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	*fl*	*ch*	*cd*
1							◉							◉					◉							3	
2					○		○					●					○			○					4		1
3				◉				◉					○			◉						○			2	3	
	$z^* = 0.7 \times 10^5$£																						Total	6	6	1

(c) Case study C

Units	Period																								Mode		
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	*fl*	*ch*	*cd*
1					○			●						◉		○			●						2	1	2
2					◉				○		○		●					●							2	1	2
3				○		○		○		◉				◉			○		◉			○			5	3	
	$z^* = 1 \times 10^5$£																						Total	9	5	4

actions, while unit 2 receives the chemical disinfection. All the cleaning actions are performed between periods 5 to 22.

The optimal (best found) objective value for case study C is $z^* = 1 \times 10^5 \pounds$ and it yields savings of 54% compared to the no-cleaning situation, where the objective value is $z_{\mathrm{no}} = 2.2 \times 10^5 \pounds$. The best found cleaning programme includes cleaning by all methods. A mixed cleaning campaign is performed on units 1 and 2, while unit 3 receives only chemical and water flush cleaning.

Figures 7.3, 7.4 and 7.5 show the progression of the thermal fouling resistance, R_f, in time for each unit, for case studies A, B and C, respectively. The time profile of R_f for the no-cleaning situation is also displayed on the graphs.

As observed in Figure 7.3(a) the thermal fouling resistance for unit 1, which has the highest heat load in the network, is maintained below 0.4 m^2.K/kW during the 360 days. For units 2 and 3, R_f reaches the asymptotic value, $R_{f\infty} = 0.8$ m^2.K/kW, once. When no cleaning is performed, R_f attains the value of $R_{f\infty}$ in 115 days, 96 days and 85 days in units 1, 2 and 3, respectively.

For case study B, the $R_f < 0.3$ m^2.K/kW throughout the 24 periods for unit 2, while it exceeds this value only once for unit 1 and twice for unit 3. The asymptotic value is attained after 209 days in unit 1 and after 171 days in units 2 and 3.

For case study C, the thermal fouling resistance of all three units is maintained at a lower level than that for case study A. The value $R_{f\infty}$ is reached after 171 days and 136 days for units 1 and 2, respectively. For unit 3, the growth reaches the steady state after 121 days have elapsed.

For the three case studies, comparing the times in which the asymptotic value is attained in each unit, it becomes apparent that the decay in network performance is faster for case study A than for case studies B and C. Also, it is faster for case study C than for case study B. This also becomes palpable when comparing the objective values for the no-cleaning situation. The aforesaid explains the relatively large number of cleaning actions selected for case study A (29 actions) compared to case studies B (13 actions) and C (18 actions).
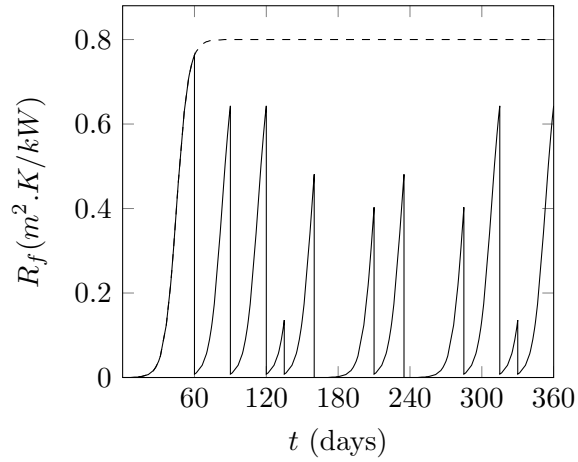
It emerges from the results that cleaning by water flush is favoured over the other two methods when the thermal fouling resistance increases relatively quickly for these cost parameters. Twenty-one water flush actions are selected for case
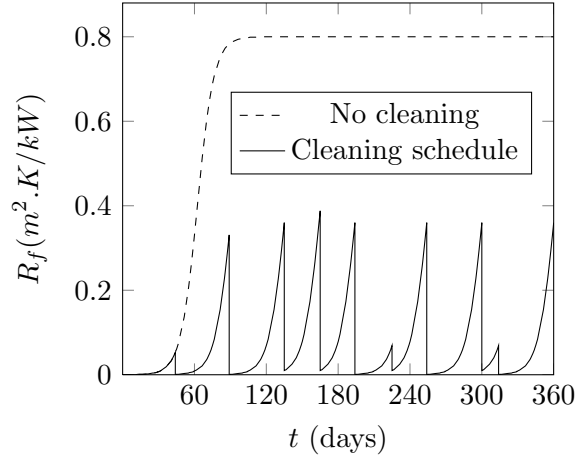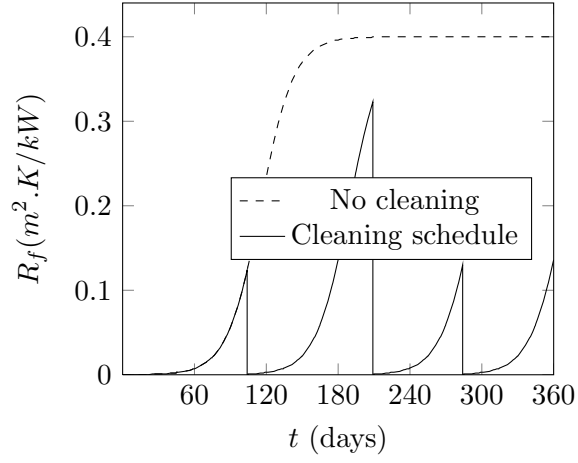
(a) unit 1
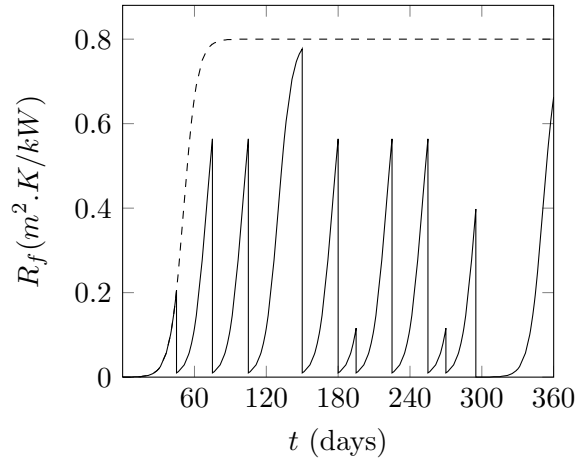
(b) unit 2
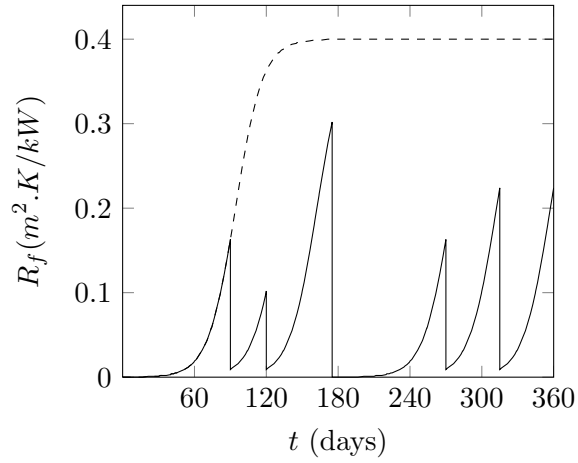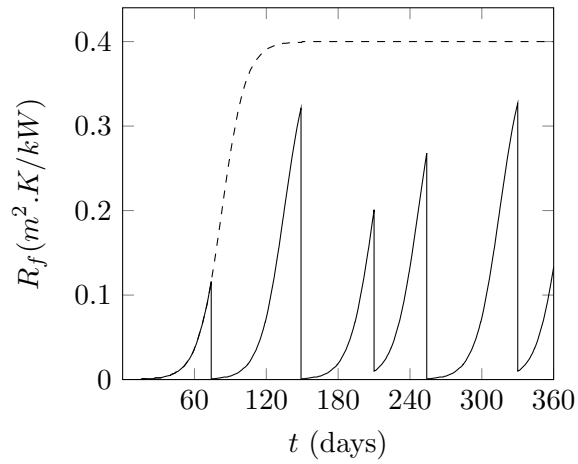

(c) unit 3

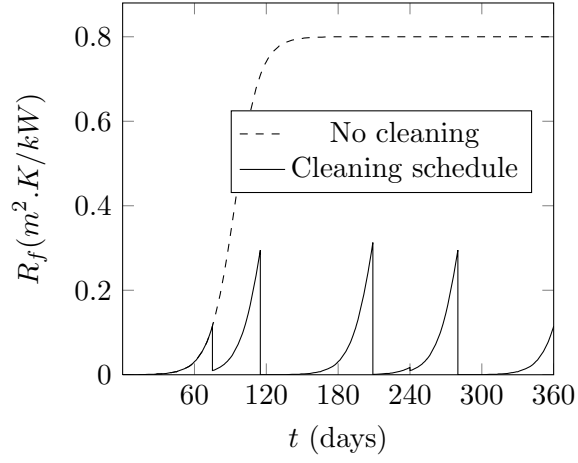Figure 7.3: Time profile of R_f: case study A
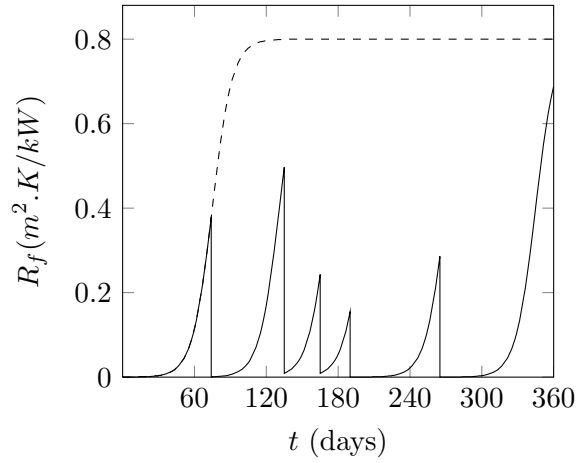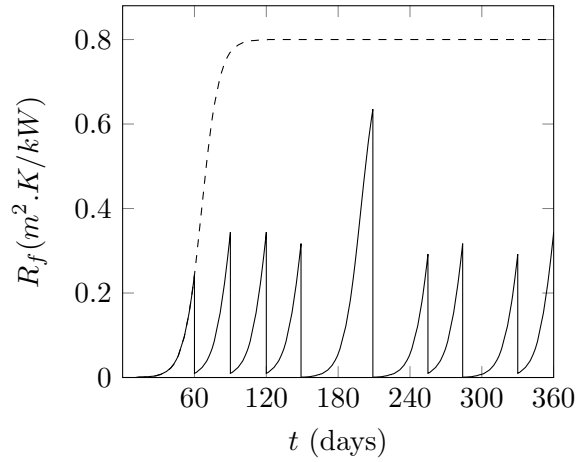
(a) unit 1

(b) unit 2

(c) unit 3

Figure 7.4: Time profile of R_f: case study B

133

(a) unit 1

(b) unit 2

(c) unit 3

Figure 7.5: Time profile of R_f: case study C

study A, where the decay in heat transfer efficiency is faster than the other two case studies. The solver prefers the cheapest, albeit less effective, water flush cleaning which has negligible duration and therefore does not result in loss of production, rather than the other two more time-consuming and expensive methods. For case studies B and C, where the rate of decay is slower compared to case study A, fewer water flush actions are selected.

7.4.1 Solution statistics

The MINLP problem solved for each case study involved 216 binary variables, 5100 continuous variables and 5400 constraints. The execution time for solving the scheduling problem for 100 different random points was 50 minutes for case study A and 38 minutes for cases B and C.

Figures 7.6(a) – 7.6(c) show the distribution of the local points obtained during the multiple starting point search, for case studies A, B and C, respectively. The local optima generated lie within a band of width $0.5 \times 10^5 \pounds$ for case study A, of width $0.2 \times 10^5 \pounds$ for case study B and of width $0.6 \times 10^5 \pounds$ for case study C.

7.5 Conclusions

A novel approach was presented in this chapter for the problem of scheduling the cleaning actions for heat exchanger networks operating subject to biological fouling. The proposed scheduling approach features the selection between three cleaning techniques and it explores the concept of selection between cleaning methods further.

The approach postulates that the receptiveness of the surface to immediate biofilm growth differs after each cleaning action. The first cleaning method is a simple water flush which removes most of the biofouling layer but leaves the heat transfer surface colonised and ready to resume growth as soon as the unit is back in operation. The second technique, a chemical cleaning, removes all the biofoulant and imposes a short induction period. The third and most effective cleaning option refers to chemical cleaning followed by disinfection, which resets the surface to the clean, non-colonised, state and results in a longer induction
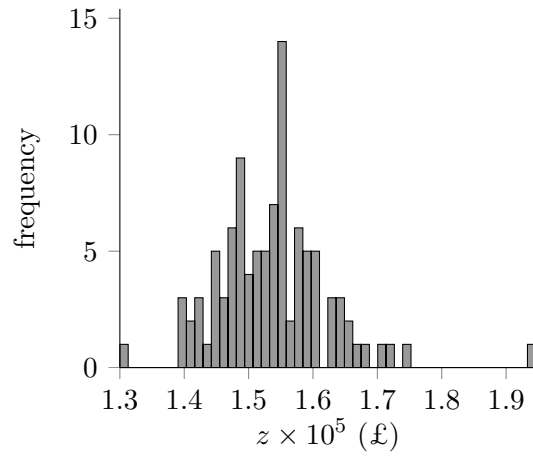
(a) Case study A
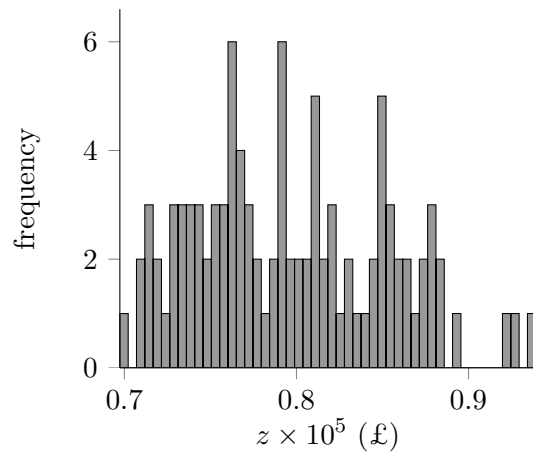
(b) Case study B
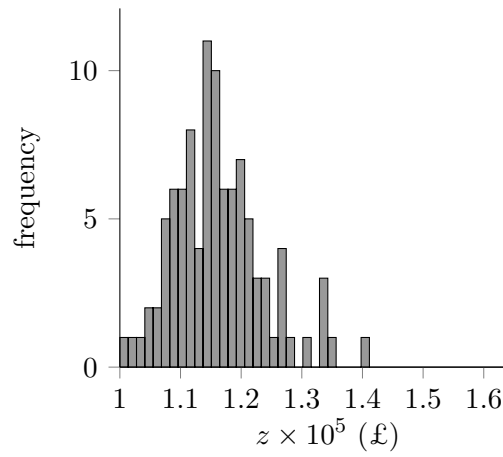
(c) Case study C

Figure 7.6: Distribution of solutions generated by the GBD algorithm for 100 random starting points

period. This distinct conditioning of the heat transfer surface by each cleaning method acts as the selection criterion.

The progression of the thermal fouling resistance in time is modelled according to the logistic model proposed by Nebot *et al.* [2007]. The benefit of using this fouling model arises from the fact that it takes into account the presence of the induction period during which the growth of biofoulant is sluggish. The evolution of thermal fouling resistance follows a sigmoidal curve. At first, the thermal resistance of the biofilm remains negligible for a time interval termed as the "delay period", which corresponds to the induction period. Afterwards, the thermal fouling resistance follows an exponential growth and asymptotic behaviour.

Two different mathematical programming formulations are introduced to describe the scheduling problem: a non-convex MINLP and an MILP. The former corresponds to scheduling problems that cannot be solved to global optimality but remain tractable as the number of units and time periods increases. On the other hand, the MILP formulation produces problems which can, in principle, be solved to attain the global optimum but are not tractable for heat exchanger networks involving more than a few units.

A series of computational studies was presented, demonstrating the implementation of the non-convex MINLP formulation for a small network of heat exchangers. The Generalised Bender's Decomposition (GBD) algorithm was used to obtain cleaning schedules in conjunction with a multiple starting point search. The best mixed cleaning campaigns generated resulted in significant savings compared to the no-cleaning case.

The results of the computational studies are sensitive to the parameters of the fouling model. Thus, reliable estimation of these parameters is crucial for the application of the proposed scheduling approach.

Chapter 8

Conclusions & Recommendations

The theme of the first part of this thesis has been the Travelling Salesman Problem (TSP). A novel way of describing the problem mathematically has been proposed, which resulted in reducing the binary degrees of freedom, for the first time, to $\mathcal{O}(n\lceil\log_2(n)\rceil)$. Three mathematical programming formulations have been introduced and a series of computational studies has been conducted in order to evaluate their computational performance in practice.

The second part of this dissertation reported the utilisation of Mixed-Integer Programming (MIP) for scheduling the cleaning actions for heat exchanger networks subject to fouling. It described the extension of a novel work presented for isolated units to networks of exchangers. The concept of choice between alternative cleaning methods was explored, with respect to the state of the deposit for networks subject to chemical reaction fouling and the conditioning of the heat transfer surface for networks subject to biological fouling.

8.1 Travelling Salesman Problem

The novel way of mathematically expressing the Travelling Salesman Problem originates from work in Binary Arithmetic. The problem is described as the repeated halving (partitioning) of the set of cities at each level of a *regular* and *full* binary tree to left and right directions. Eventually, the cities are placed sequentially on the leaves of the tree according to their position in the tour. In

that respect, the original problem can be viewed as a data storage problem on a binary tree structure.

The new contribution of this work is that it reduces the binary degrees of freedom for the Travelling Salesman Problem to $\mathcal{O}(n\lceil\log_2(n)\rceil)$. To the author's knowledge, up to date, no other mathematical description of the problem, among those found in the literature, succeeded in reducing the required number of binary variables below $\mathcal{O}(n^2)$. The current work takes an incremental step towards decreasing the formulation complexity of the Travelling Salesman Problem.

Two Mixed-Integer Linear Programming (MILP) formulations are developed for the general case of the Asymmetric Travelling Salesman Problem (ATSP), where the length of an arc connecting two cities depends on the direction in which it is travelled. These are the Tree-1 and Tree-2 formulations. Another MILP formulation is introduced for the special case where the distance between two cities is calculated on the basis of the rectilinear metric. This special case is referred to as the Manhattan Travelling Salesman Problem.

8.1.1 Asymmetric formulations

The two asymmetric formulations utilise a set of logical checks which force an arc to be present in the optimal tour if two cities are placed on neighbouring leaves of the binary tree. These adjacency constraints are the only difference between formulations Tree-1 and Tree-2. The set of adjacency constraints proposed by Millar and Cyrus [2000] is used in the Tree-1 formulation, while for Tree-2 the logical checks are derived by Theorem 3.1. The Tree-1 and Tree-2 formulations include $\mathcal{O}(n^3)$ and $\mathcal{O}(n^2\lceil\log_2(n)\rceil)$ adjacency constraints, respectively.

The proposed formulations were implemented for small instances of the Travelling Salesman Problem ($n \leq 12$). It emerged from the results that the Tree-1 formulation is superior in computational performance to the Tree-2 formulation. In particular, the branch-and-cut solver visits considerably fewer nodes of the solution tree for Tree-1 than for Tree-2. In fact, the exact algorithm failed to converge after one day of execution, when applying Tree-2 to a problem involving 12 cities. For the same problem, the optimal solution was obtained after 363 CPU seconds when Tree-1 was applied. The dissimilar computational performance is

due to the different adjacency constraints included in each formulation.

Nevertheless, neither Tree-2 nor Tree-1 were successful when applied to problems involving $12 < n \leq 20$ cities. In all cases the branch-and-cut algorithm failed to obtain the optimal solution after one day of execution. For all intents and purposes, the solution of such small problems should be trivial.

The computational efficiency of the two formulations was found to be worse than that of the well-known formulations proposed by Wong [1980] and Miller *et al.* [1960]. The basis for the comparison was the strength of the Linear Programming (LP) relaxation of each formulation. The formulation suggested by Miller *et al.* [1960] is proven to be one of the weakest in comparison to others existing in the literature [Öncan *et al.*, 2009]. Therefore, the Tree-1 and Tree-2 are also placed among the weakest formulations.

The key finding that emerged from the computational studies is that the Tree-1 and Tree-2 formulations are not tightly constrained, which means that the resulting mixed-integer models have a large feasible region. It is due to this that the proposed formulations can only be applied to very small instances of the Travelling Salesman Problem.

8.1.2 Manhattan formulation

The computational performance of the Manhattan formulation in practice is found to be worse that of Tree-1. For the solution of two small problems ($n = 8$ and $n = 10$), noticeably more computational effort is required when implementing the former rather than the latter formulation. Therefore, it is concluded that the Manhattan formulation is also loosely constrained.

8.1.3 Recommendations for future work

Future attempts for continuation of this work should focus on improving the Tree-1 formulation. It is strongly recommended that additional constraints are added to the formulation in order to reduce the size of the feasible region. Nonetheless, the search for appropriate tightening constraints is not a trivial task and it might not have fruitful results.

At the same time, future work should be directed towards developing pertinent heuristic procedures in order to exploit the hierarchical structure of the asymmetric formulations. Such a heuristic procedure might be successful in generating initial tours that are close to the optimal solution.

8.2 Scheduling cleaning actions for heat exchanger networks subject to fouling

In previous attempts to schedule the cleaning actions for heat exchangers subject to fouling it was postulated that the only form of cleaning available is one that restores the performance of the unit back to its clean level. A recent study presented by Ishiyama *et al.* [2011b] for an isolated evaporator included the economic competition between two cleaning methods: one less time-consuming and partially effective, the other requiring more resource but giving complete cleaning. The work reported in the second part of this thesis extends their approach to accommodate heat exchanger networks and explores the concept of selection of cleaning methods further.

The cleaning actions were scheduled for: (i) heat exchanger networks subject to chemical reaction fouling and (ii) heat exchanger networks subject to biological fouling. The goal was to minimise the process costs, including those associated with the energy losses due to fouling and with the loss of production during cleaning intervals, and the cleaning costs for an arbitrarily chosen time horizon.

8.2.1 Networks subject to chemical reaction fouling

The scheduling task for heat exchanger networks subject to chemical reaction fouling, as per the work by Ishiyama *et al.* [2011b], featured the selection between two methods that achieve a different degree of cleaning. Fouling was defined as the combination of deposition and ageing phenomena. Ageing was assumed to convert the initial fresh deposit into a harder and more conductive material removable only by time and cost intensive mechanical cleaning. A less expensive and faster chemical cleaning was assumed to remove only the soft deposit. A two

layer model was used to distinguish soft and aged deposits in order to track the cleaning effectiveness and the decay in heat transfer efficiency.

A non-convex Mixed-Integer Nonlinear Programming (MINLP) formulation was proposed to describe the scheduling problem. It was developed for networks of single-pass shell-and-tube heat exchangers operating in counter-current mode. The formulation can be altered to accommodate other types of units and flow configurations without difficulty.

The scheduling formulation was applied to a heat exchanger operating in isolation. A mixed cleaning cycle can be identified for a unit: a number of chemical actions that partially restore the performance precede a mechanical action that resets the exchanger to a clean state and restarts the cycle. This mixed cleaning campaign was named a super-cycle and succeeds in extending the operating time before lengthy mechanical cleaning by performing a number of short-length chemical actions.

Cleaning schedules were also obtained for two preheat train networks of 14 and 25 units. The results suggest the importance of the fouling parameters, namely the formation rates and the thermal conductivities of the two layers. The reliable estimation of these parameters is imperative for the application of the proposed scheduling formulation.

8.2.2 Networks subject to biological fouling

The new study of scheduling cleaning actions for heat exchanger networks subject to biological fouling involved the competition between three cleaning modes differing in cost, duration and effectiveness. The evolution of the biofilm was assumed to follow an exponential growth with asymptotic behaviour, after an induction period during which the heat transfer surface is colonised. Thermal fouling is modelled using the relation proposed by Nebot *et al.* [2007].

The three cleaning types considered are the following: (i) cheap water flush of negligible duration which removes the bulk of the biofoulant but leaves the surface colonised and ready to restart growth when process operation resumes; (ii) relatively expensive but short-length chemical cleaning which removes all biofilm and imposes a short induction period and (iii) expensive and time-consuming chem-

ical cleaning followed by disinfection, which resets the unit to its original clean state.

A non-convex MINLP formulation was developed to describe the scheduling problem. The formulation is applied to a small heat exchanger network in a series of computational studies. Again, the results of the studies are found to be sensitive to the parameters of the fouling model.

A MILP formulation can also be derived for the scheduling problem. For that purpose, it was sufficient to express the thermal fouling resistance (of a unit) at every node of a given time period as the function of the cleaning decisions of all previous periods. The resulting constraints include only products of binary variables with continuous variables, which can be replaced by linear terms using standard transformations [Williams, 1990]. However, the transformations require the addition of new continuous variables and extra constraints and cause the MILP problem to be non-tractable for networks involving more than a few units.

8.2.3   Numerical methods

A direct transcription approach was adopted for the dynamic scheduling problems. The time horizon under consideration was discretised into a finite number of periods, which in turn were represented by three elements in time. In each element the variable profiles were approximated by polynomials, and orthogonal collocation was used to calculate the values of the variables at selected points. In particular, Radau collocation was chosen because it allows large time steps for systems with slow time scales [Biegler, 2010].

The MINLP formulations presented for the two scenarios are non-convex. Therefore, the resulting scheduling models cannot be solved to global optimality. Despite the non-convex characteristics of the problems, it was decided to use a rigorous solution method developed for convex problems, in a heuristic attempt to obtain 'good' quality local optima.

The discretisation of time yielded relatively large scheduling problems. The problems included a prohibitively large number of nonlinear equality constraints with respect to the capabilities of the standard Outer Approximation/Equality Relaxation (OA/ER) decomposition algorithm, which failed to converge to a

solution (after a considerable amount of time) when applied in practice.

Generalised Benders Decomposition (GBD) was selected as a suitable alternative algorithm to handle the relatively large Mixed-Integer Nonlinear Programming problems. This algorithm was found to be superior to the OA/ER algorithm in terms of computational performance, for this particular case. The reason for this is that only one constraint is added to the Master Problem (see Section 5.5) at each iteration of the GBD procedure, whereas the OA/ER algorithm demands the addition of a relatively large number of constraints.

A heuristic solution procedure based on Model Predictive Control (MPC) was also used to generate cleaning schedules for the two heat exchanger networks subject to chemical reaction fouling. At each iteration of the heuristic procedure the GBD algorithm was utilised to solve the scheduling problem for a small number of periods. In that respect, the scheduling problem is solved repeatedly over a short time horizon rather than solved once for a long time horizon. The computational cost for both approaches proved to be similar.

Inequality constraints involving continuous variables, *e.g.* performance targets for a network, were not included in the scheduling formulation considered in this work. The addition of such inequality constraints would presumably increase the computational effort required by the GBD algorithm to obtain a local solution or, in a more pessimistic scenario, cause the solver to terminate at an infeasible point.

8.2.4   Recommendations for future work

The simple two-layer model included in the scheduling formulation proposed for heat exchanger networks subject to chemical reaction fouling assumes that the rates of gel and coke formation are constant throughout process operation. Future continuation of this work can consider more detailed two layer models, such as the ones presented by Ishiyama *et al.* [2011a], where the gel formation rate and coke formation rate depend on the gel/bulk-fluid interface temperature and the gel/coke interface temperature, respectively. A more detailed fouling analysis will lead to more valid estimates of the decay in heat transfer efficiency. However, these more realistic fouling models are highly nonlinear. As a result, the new

scheduling formulations might yield MINLP problems that are no longer tractable by the GBD algorithm employed in the current work. In such an event, other apt heuristic solution procedures will have to be considered.

Another direction for future study could be to consider the negative impact of fouling on the hydraulic performance of the heat exchangers. The formation of fouling in the channels of a unit causes a reduction in the flow area, with an associated increase in pressure drop. This results in loss of throughput if the pumping power is limited, and it affects the network profitability directly. This was ignored in the current work. The increase in pressure drops might influence the cleaning choices, especially for networks where the rate of formation of the more conductive aged material is relatively high.

The computational studies conducted for the purposes of this work did not consider any variations in the cost or the duration of the different cleaning methods. Future work can focus on analysing the sensitivity of the generated schedules to different combinations of these parameters.

In addition to heat transfer systems, fouling is a major operational problem in many mass transfer process [Tang *et al.*, 2011; Wang and Tang, 2011]. Membrane fouling results in loss of permeability and necessitates the cleaning or replacement of the fouled units. The problem of scheduling the cleaning actions for networks of membranes has been studied in the past [Lu *et al.*, 2006; See *et al.*, 1999]. It would be very interesting to revisit the problem and add novelty to the area by introducing the concept of choice of cleaning methods.

Appendix A

Table A.1: Cost matrix for ATSP case study: $n = 8$

	1	2	3	4	5	6	7	8
1	∞	29	28	11	2	8	17	6
2	21	∞	2	13	12	9	5	23
3	27	24	∞	8	7	8	38	3
4	28	23	26	∞	1	13	28	25
5	21	2	23	15	∞	16	17	41
6	12	18	33	25	3	∞	15	2
7	3	13	9	27	24	25	∞	19
8	27	8	40	8	27	13	2	∞

Table A.2: Cost matrix for ATSP case study: $n = 10$

	1	2	3	4	5	6	7	8	9	10
1	∞	21	27	22	6	35	33	33	24	41
2	78	∞	34	23	46	48	4	2	13	22
3	32	7	∞	10	7	11	6	47	10	10
4	21	13	3	∞	47	40	48	21	45	17
5	13	27	12	8	∞	16	32	5	18	15
6	25	6	10	34	35	∞	21	49	4	22
7	25	7	22	25	39	27	∞	12	16	10
8	22	28	30	26	28	23	31	∞	45	33
9	24	5	39	5	21	5	32	26	∞	16
10	29	3	7	31	21	4	26	35	30	∞

Table A.3: Cost matrix for ATSP case study: $n = 12$

	1	2	3	4	5	6	7	8	9	10	11	12
1	∞	633	257	91	412	150	80	134	259	505	353	324
2	633	∞	390	661	227	488	572	530	555	289	282	638
3	257	390	∞	228	169	112	196	154	372	262	110	437
4	91	661	228	∞	383	120	77	105	175	476	324	240
5	412	227	169	383	∞	267	351	309	338	196	61	421
6	150	488	112	120	267	∞	63	34	264	360	208	329
7	80	572	196	77	351	63	∞	29	232	444	292	297
8	134	530	154	105	309	34	29	∞	249	402	250	314
9	259	555	372	175	338	264	232	249	∞	495	352	95
10	505	289	262	476	196	360	444	402	495	∞	154	578
11	353	282	110	324	61	208	292	250	352	154	∞	435
12	324	638	437	240	421	329	297	314	95	578	435	∞

Table A.4: Coordinates for Manhattan-TSP case study: $n = 8$

x	y
-9.847410E+2	-8.154400E+2
-6.160710E+2	-5.708020E+2
-2.574970E+2	-5.779210E+2
-2.191710E+2	-7.294700E+2
-1.541140E+2	-2.258680E+2
89.83980000	-1.172060E+2
-9.062380E+2	160.76700000
-8.003230E+2	-4.185860E+2
-9.847410E+2	-8.154400E+2

Table A.5: Coordinates for Manhattan-TSP case study: $n = 10$

x	y
-79.29160000	-21.40330000
-72.07850000	0.18158100
-64.74730000	21.89820000
-50.48080000	7.37447000
-50.58590000	-21.58820000
-36.03660000	-21.61350000
-0.13581900	-28.72930000
-14.65770000	-43.38960000
-29.05850000	-43.21670000
-65.08660000	-36.06250000
-79.29160000	-21.40330000

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