Multi–scale Modelling of Refinery Pre–heat Trains Undergoing Fouling for Improved Energy Efficiency

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To my parents, Flavio and Rosa...
“Facesti come quei che va di notte, che porta il lume dietro e sé non giova, ma dopo sé fa le persone dotte.”

Thou didst as he who walketh in the night, Who bears his light behind, which helps him not, But wary makes the persons after him.

Dante Alighieri
Divina Commedia (Pur. XXII, 67-69)
Preface

The work described in this dissertation was carried out in the Department of Chemical Engineering at Imperial College London between October 2006 and June 2010. Except where specifically acknowledged, the material is the original work of the author and includes nothing which is the outcome of work in collaboration. No part of this material has been submitted for a degree in any other university.

Francesco Coletti
Abstract

Fouling in pre–heat trains of refinery crude distillation units causes major energy inefficiencies, resulting in increased costs, greenhouse gas emissions, maintenance efforts and health and safety hazards.

Although chemical and physical phenomena underlying fouling deposition are extremely complex and several details remain unknown, the understanding of the fouling process has progressed significantly in the past 40 years. However, this knowledge has so far not been exploited to effectively improve heat exchanger and heat exchanger network design and operation. As a result, old methodologies that neglect the local effects and dynamics of fouling, in favor of lumped, steady–state, heuristic models (e.g. using TEMA fouling factors) are still used.

In this thesis a novel mathematical model for pre–heat trains undergoing crude oil fouling was developed, validated with plant data and used to propose mitigation strategies. The model is dynamic, distributed and considers simultaneously several scales of investigation. Key phenomena are captured at the tube level as a function of local conditions. These include the dependence of fouling rate on temperature and velocity, the variation of physical properties, the structural changes of the deposits over time (ageing) and the dynamics of surface roughness.

The single tube model was then extended to describe a unit–scale heat exchanger geometry. This has been validated against plant data from four units in two refineries operated by major oil companies. The predicted outlet temperatures over extended periods (i.e. 4-16 months) are accurate within ±1% for the tube–side and ±2% for the shell–side. Model simulations were then used to assist the retrofit of one particular unit for which it was possible to save ca. 22% of the energy losses (not including pumping power) produced by fouling over ca. a year of operation.

Finally, the interconnection of single heat exchangers in a network allowed the simulation of the fouling behavior of two existing pre–heat trains. To systematically assess the impact of fouling on refinery economics, a set of key performance indicators (KPIs) was proposed. Network–level simulations were used in conjunction with the KPIs to unveil complex interactions and propose network retrofit arrangements that improve energy recovery over time whilst reducing fouling.

It is concluded that the model can be used with confidence to predict fouling and assist monitoring, design and retrofit of refinery heat exchangers and heat exchanger networks. The results shown indicate that the approach proposed can lead to substantial benefits.
Acknowledgements

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During the course of this work, several interactions with the researchers involved in the CROF project allowed me to deepen my knowledge of different research areas. I would like to thank especially Prof. Geoffrey Hewitt and Prof. Omar Matar for their leadership in making this collaboration exciting and successful. I would also like to thank the Cambridge team: Dr. Ian Wilson, Dr. Bill Paterson and Edward Ishiyama, for the fruitful collaboration on the development of the ageing model and Dr. Graham Polley for the cooperation on the network retrofit study.

This project has relied heavily upon the input and data from several industrial partners of the IHS ESDU Oil Industry Fouling Working Party led by Simon Pugh, whose invaluable insights into the oil business are gratefully acknowledged. The industrial perspectives given by Glen Brons and Dr. Amar Wanni of ExxonMobil, Tin Yin Lam and Dr. Christopher Bennett of Chevron and Himanshu Joshi of Shell have been precious in the development of this thesis.

I would also like to thank Susi Underwood and Rayner Simpson for supporting me with inexhaustible patience throughout my postgraduate career.

A big thank you goes to those who always gave me a good reason to go to college with a smile on my face. Uttam, for sharing with me the highs and lows of the MSc, the PhD and life in London; May for the many, endless laughs we had together; Murthy, on whom I can always count; Felicia (“chop chop”), Shirin (“shame!”), Jay (“lisssen brother”) and Silvia (“cioccolatina?”) for being great friends. Thanks also to all my flatmates in Durrels House, in particular to Elizabeth, Pall and Alexis. It was great living with you.

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Nomenclature

\( A \)  Cross-sectional area \( \, \text{m}^2 \)

\( a_1, a_2 \)  Fouling model constants

\( B_c \)  Baffle cut \( \, \% \)

\( C \)  Cost \( \, \text{US} $ \)

\( c \)  Concentration \( \, \text{kg} \, \text{m}^{-3} \)

\( C_C \)  Carbon content of fuel \( \, \text{kgC} \, \text{kg}^{-1} \text{fuel} \)

\( C_f \)  Fanning friction factor

\( \text{CII} \)  Colloidal instability index

\( c_p \)  Specific heat capacity \( \, \text{J} \, \text{kg}^{-1} \, \text{K}^{-1} \)

\( \mathcal{D} \)  Mass diffusivity \( \, \text{m}^2 \, \text{s}^{-1} \)

\( D_{otl} \)  Tube bundle diameter \( \, \text{m} \)

\( E \)  Energy \( \, \text{J} \)

\( e \)  Equivalent sand roughness \( \, \text{m} \)

\( E_a \)  Ageing activation energy \( \, \text{J} \, \text{mol}^{-1} \)

\( E_f \)  Fouling reaction activation energy \( \, \text{J} \, \text{mol}^{-1} \)

\( F_E \)  Energy content of fuel \( \, \text{J} \, \text{kg fuel}^{-1} \)

\( f_i \)  Correction factor for LMTD

\( K \)  Mass transfer coefficient \( \, \text{m} \, \text{s}^{-1} \)

\( k \)  Reaction rate \( \, \text{m} \, \text{s}^{-1} \)

\( k_a \)  Parameter in roughness model


\( k_p \) Parameter in roughness model \( s^{-1} \)

\( k_i \) Parameter in roughness model \( s^{-1} \)

\( L_{bc} \) Central baffle spacing \( m \)

\( L_{bo} \) Outlet baffle spacing \( m \)

\( L_{bi} \) Inlet baffle spacing \( m \)

\( L_{tp} \) Tube pitch \( m \)

\( M \) Mass \( kg \)

\( \dot{m} \) Mass flowrate \( kg \ s^{-1} \)

\( m_{CO2} \) carbon emission per joule of energy produced \( kg \ J^{-1} \)

\( \dot{m}_d \) Mass rate of fouling deposition \( kg \ s^{-1} \)

\( \text{MeABP} \) Mean average boiling point \( K \)

\( m_f \) Net mass of foulant \( kg \)

\( \dot{m}_r \) Mass rate of fouling removal \( kg \ s^{-1} \)

\( \text{MW} \) Molecular weight \( kg \ mol^{-1} \)

\( N \) Mass flux \( kg \ s^{-1} \ m^{-2} \)

\( N_b \) Number of baffles \( – \)

\( N_c \) Number of retrofit configurations \( – \)

\( N_D \) Cleaning frequency \( s^{-1} \)

\( N_p \) Number of tube–side passes \( – \)

\( N_s \) Number of shells per unit \( – \)

\( N_{ss} \) Number of sealing strip pairs \( – \)

\( N_t \) Total number of tubes \( – \)

\( N_u \) Number of units in the network \( – \)

\( P \) Pressure \( Pa \)

\( P \) Price \( \text{US}\$ \ Wh^{-1} \)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_S$</td>
<td>Shell–side wetted perimeter</td>
<td>m</td>
</tr>
<tr>
<td>$P_t$</td>
<td>Tube–side inner perimeter</td>
<td>m</td>
</tr>
<tr>
<td>$P_x$</td>
<td>Pitch ratio</td>
<td>–</td>
</tr>
<tr>
<td>$Q$</td>
<td>Heat duty</td>
<td>W</td>
</tr>
<tr>
<td>$q''$</td>
<td>Heat flux</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$q'''$</td>
<td>Heat source</td>
<td>W m$^{-3}$</td>
</tr>
<tr>
<td>$q_{to}$</td>
<td>Heat flux value imposed at outer tube surface</td>
<td>W m$^{-2}$</td>
</tr>
<tr>
<td>$R$</td>
<td>Radius</td>
<td>m</td>
</tr>
<tr>
<td>$R_b$</td>
<td>Deposit bond resistance</td>
<td>Pa</td>
</tr>
<tr>
<td>$R_f$</td>
<td>Fouling resistance</td>
<td>m$^2$ K W$^{-1}$</td>
</tr>
<tr>
<td>$R_g$</td>
<td>Ideal gas constant</td>
<td>J K$^{-1}$ mol$^{-1}$</td>
</tr>
<tr>
<td>$R^*$</td>
<td>Asymptotic value of the fouling thermal resistance</td>
<td>m$^2$ K W$^{-1}$</td>
</tr>
<tr>
<td>$r$</td>
<td>Reaction</td>
<td>–</td>
</tr>
<tr>
<td>$r$</td>
<td>Radial coordinate</td>
<td>m</td>
</tr>
<tr>
<td>$\tilde{r}$</td>
<td>Dimensionless radial coordinate</td>
<td>–</td>
</tr>
<tr>
<td>$S$</td>
<td>Surface area</td>
<td>m$^2$</td>
</tr>
<tr>
<td>$Sc$</td>
<td>Schmidt number</td>
<td>–</td>
</tr>
<tr>
<td>$S_m$</td>
<td>Logarithmic mean area</td>
<td>–</td>
</tr>
<tr>
<td>$S_p$</td>
<td>Flow split</td>
<td>%</td>
</tr>
<tr>
<td>$Sv$</td>
<td>Savings</td>
<td>US$</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>K</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
<td>s</td>
</tr>
<tr>
<td>$\hat{T}_f$</td>
<td>Modified film temperature</td>
<td>K</td>
</tr>
<tr>
<td>$t_l$</td>
<td>Lag time</td>
<td>s</td>
</tr>
<tr>
<td>$T_o$</td>
<td>Temperature imposed at outer tube surface</td>
<td>K</td>
</tr>
<tr>
<td>Symbol</td>
<td>Definition</td>
<td>Unit</td>
</tr>
<tr>
<td>--------</td>
<td>------------</td>
<td>------</td>
</tr>
<tr>
<td>$T_w$</td>
<td>Wall temperature</td>
<td>K</td>
</tr>
<tr>
<td>$T'$</td>
<td>Reference temperature</td>
<td>K</td>
</tr>
<tr>
<td>$u$</td>
<td>Velocity</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$\dot{V}$</td>
<td>Volumetric flowrate</td>
<td>m$^3$ s$^{-1}$</td>
</tr>
<tr>
<td>$W$</td>
<td>Pumping Power</td>
<td>W</td>
</tr>
<tr>
<td>$y$</td>
<td>Youth variable</td>
<td>–</td>
</tr>
<tr>
<td>$z$</td>
<td>Axial coordinate</td>
<td>m</td>
</tr>
</tbody>
</table>

**Greek Symbols**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>Fouling model deposition constant</td>
<td>K m$^2$ W$^{-1}$ s$^{-1}$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Fouling model constant</td>
<td>–</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>Fouling suppression term constant</td>
<td>m$^4$ N K W$^{-1}$ s$^{-1}$</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Fouling layer thickness</td>
<td>m</td>
</tr>
<tr>
<td>$\Delta P_c$</td>
<td>Cross–flow pressure drop between baffle tips</td>
<td>Pa</td>
</tr>
<tr>
<td>$\Delta P_e$</td>
<td>Pressure drops in the inlet and outlet baffles</td>
<td>Pa</td>
</tr>
<tr>
<td>$\Delta P_s$</td>
<td>Shell–side pressure drop</td>
<td>Pa</td>
</tr>
<tr>
<td>$\Delta P_w$</td>
<td>Pressure drop in the baffle window</td>
<td>Pa</td>
</tr>
<tr>
<td>$\Delta T_{pp}$</td>
<td>Pinch point</td>
<td>K</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Efficiency</td>
<td>–</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Angular coordinate</td>
<td>rad</td>
</tr>
<tr>
<td>$\theta_{tp}$</td>
<td>Tube pitch angle</td>
<td>deg</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Thermal conductivity</td>
<td>W m$^{-1}$ K$^{-1}$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic viscosity</td>
<td>Pa s</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Kinematic viscosity</td>
<td>m$^2$ s$^{-1}$</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
<td>m$^3$ kg$^{-1}$</td>
</tr>
</tbody>
</table>
\( \sigma \) Variable defined by Equation 3.9
\( \tau \) Wall shear stress Pa
\( \phi_{cr} \) Fouling rate decrease by conversion of tarry layer to coke m² K W⁻¹ s⁻¹
\( \phi_d \) Fouling deposition term m² K W⁻¹ s⁻¹
\( \phi_r \) Fouling removal term m² K W⁻¹ s⁻¹
\( \phi_{tr} \) Fouling rate decrease by mass transfer of tars to the bulk of the fluid m² K W⁻¹ s⁻¹
\( \Omega \) Domain name –
\( \omega \) Physical property –

**Subscripts**

\( a \) Ageing
\( b \) Bulk
\( c \) Cold
\( elec \) Electricity
\( emiss \) CO₂ emission
\( f \) Fouling/foulant
\( fur \) Furnace
\( h \) Hot
\( i \) Inner or fluid/deposit interface
\( l \) Fouling layer
\( m \) Logarithmic mean
\( o \) Outer
\( pr \) Precursor
\( prod \) Production
\( Qloss \) Heat loss

XVII
$r$ Reacting species

$s$ Shell–side

$t$ Tube–side

$t_c$ Conversion tarry layer to coke

$tr$ Transfer of tars to bulk

$w$ Wall

**Superscripts**

0 Initial state

$\infty$ Final state

$in$ Inlet

$out$ Outlet

* Fouled conditions

**Abbreviations**

ANN Artificial neural network

CDU Crude Distillation Unit

CFD Computational fluid dynamics

CIP Coil Inlet Pressure

CIT Coil Inlet Temperature

COT Coil Outlet Temperature

CROF CRude Oil Fouling project

ETS Emissions Trading Scheme

FFL Furnace firing limit

GA Genetic algorithm
GHG  Greenhouse gas
HEN  Heat exchanger network
HEX  Heat exchanger
LMTD  Log mean temperature difference
MILP  Mixed integer linear programming
MINLP  Mixed integer non linear programming
ODE  Ordinary differential equations
PDAE  Partial Differential and Algebraic Equations
PHT  Pre–heat train
PT  Pinch Technology
SARA  Saturates, aromatics, resins and asphaltenes
TEMA  Tubular Exchangers Manufacturers Association
UHF  Uniform heat flux
UWT  Uniform wall temperature

Dimensionless numbers

\[ Bi_f = \frac{h_0 \delta}{\lambda_f} \]
\[ Pr = \frac{c_\rho \mu}{\lambda} \]
\[ Re = \frac{v \rho}{\mu} \]
\[ Sc = \frac{\mu}{\rho \mathcal{D}} \]
Chapter 1

Introduction

Stringent environmental policies and tightening refining margins in a highly competitive market are forcing oil companies worldwide to increase their focus on the efficient utilisation of energy. Refinery efficiency is so critical that it has been reported to be capable of moving the share price of major oil and gas companies (personal communication). In this perspective, the efficiency of heat exchange equipment and heat exchange networks is of paramount importance. Fouling, the deposition of unwanted material on heat transfer surfaces, is a major cause of inefficiencies with severe effects on refinery economics, operability, health & safety and environmental impact.

Fouling is a long-standing problem in the process and energy industry\(^1\) and has been described both as “the major unresolved problem in heat transfer” (Taborek et al., 1972) and “a nearly universal problem in heat exchanger equipment design and operation” (Watkinson, 1988). Indeed fouling is ubiquitous in oil refineries. The feed/effluent heat exchangers in naphtha hydrotreaters, the slurry exchangers and steam generators in fluid catalytic cracking units and the visbreaker’s furnace are all known to be affected by severe fouling problems. However, because of the large throughput and energy involved, the largest share (about 50%, Van Nostrand et al., 1981) of the total fouling–related costs for the whole refinery originate in the pre–heat train (PHT) of the atmospheric distillation unit (here referred to as crude distillation unit or CDU).

The PHT is an extensive network of heat exchangers used to reduce energy requirements in the CDU which is where primary fractionation of all the crude processed in the refinery is performed. If the PHT is not working efficiently, more fuel must be burnt at the downstream furnace that heats the crude to the required temperature for the distillation. The average energy

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\(^1\)Taborek (1997) tracked the origin of the first industrial concern about fouling back in the 1880’s USA power industry and the first mention of fouling in the open literature is in a paper by Orrok (1910).
involved with this process has been estimated to be over 190 TWh yr\(^{-1}\) \((6.86 \times 10^{17} \text{ J yr}^{-1})\) [DOE 2006], which makes the CDU the largest energy utiliser process in the refinery and one of the largest in the whole process industry. To put these figures into perspective it can be argued that the equivalent of ca. 6% of the total crude throughput is consumed as energy to sustain the refining process itself [ESDU 2000]. With a global crude production of ca. 85M bbl yr\(^{-1}\), this is roughly equivalent to the entire production of one ExxonMobil or Shell just to operate the world’s 720 refineries.

Although difficult to estimate precisely, there is little doubt that fouling has an enormous impact on the refinery. Economic costs of fouling in PHTs were estimated to add up to over US$1.2 billion yr\(^{-1}\) in the United States alone [ESDU 2000] at a time when the cost of the crude barrel was significantly lower. Last year, one 210,000 bbl day\(^{-1}\) UK refinery reported an average cost of US$2.5M over a 4 years run due to fouling in their PHT and estimated that each 1°C temperature drop in the crude from the preheat train cost them ca. £250,000 yr\(^{-1}\) in extra fuel alone (personal communication).

The environmental impact is even more staggering with fouling in refineries estimated to be responsible for 88 million t of CO\(_2\), or 2.5% of total worldwide anthropogenic emissions in 2009 [Müller-Steinhagen et al. 2009a].

How much of this inefficiency can be eliminated, and at what cost, is the key question. Fouling mitigation can provide increased capacity and reduced GHG emission without significant capital expenditure. A 2006 study for the US Department of Energy indicates that potential fuel savings of up to 55% can be achieved in oil refineries by improving operating practices and capital equipment [DOE 2006]. Amongst the suggested improvements it was found that fouling mitigation in the PHT and fired heater in atmospheric distillation units could lead to a 15% fuel saving (1/3 from existing technology, 2/3 from technology currently in R&D stage). As fuel consumption in the atmospheric furnace represents around 4% of the total refinery throughput [Yeap et al. 2004], a potential saving of 15% equates to a sizable 500,000 bbl day\(^{-1}\) potential savings worldwide, equivalent to the daily production of a large refinery, or (for oil at US$80 bbl\(^{-1}\)) a value of US$14.6bn yr\(^{-1}\).

However, much needs to be done to be able to tap into the potential savings offered by fouling mitigation starting with the way heat exchangers are designed.

Over the years, several projects have been coordinated to study the complex and interacting
phenomena involved in different types of fouling (Pilavachi and Isdale [1993]; Pritchard [1988a]).

For crude oil fouling, many experimental and theoretical studies have been produced by the University of British Columbia and the Argonne National Laboratory (Watkinson [1988], Panchal and Watkinson [1994], Kuru et al. [1997]), the University of Bath (Crittenden et al. [1987a,b]), the HTRI’s Crude Oil Fouling Task Force (Bennett et al. [2006, 2009]), IHS ESDU’s Oil Industry Fouling Working Party (ESDU [2000]) and a few others. More recently, the UK Engineering and Physical Sciences Research Council (EPSRC), has funded the £2.1M Crude Oil Fouling (CROF) Project (EP/D503051/1). This is the latest and largest effort made so far to tackle the fouling problem in crude distillation units (Macchietto et al. [2009]). Overall, the CROF project aims to provide a platform to investigate fundamental parameters leading to deposition, so as to predict fouling, avoid it by design and formulate methods for mitigation. The research effort, involving both experimental and modelling work, is coordinated across three universities, (University of Bath, University of Cambridge, Imperial College London) in 8 sub–projects which examine the fouling problem across all scales, from the molecular to the process unit to the overall heat exchanger network (Figure 1.1). To make the outcomes of the project relevant and transferable to industry, the research team has been working closely with experts from many leading oil companies (accounting for 70% of the world’s refining capacity) in the IHS ESDU Oil Industry Fouling Working Party.

Within the CROF framework (as a part of Sub–Project G), this thesis aims at developing a mathematical model for shell–and–tube heat exchangers undergoing crude oil fouling.
1.1 Motivations and Objectives

Although chemical and physical phenomena underlying the fouling process are extremely complex and several details remain unknown, understanding has improved significantly in the past 40 years (Macchietto et al., 2009). For example, it is now known that fouling in the hot–end of the PHT is originated by a series of chemical reactions triggered by the high temperatures. There is also experimental evidence that critical velocities exist above which fouling does not occur due to deposit removal by shear forces from the flow (Ebert and Panchal, 1997). However, all this knowledge has so far not been fully exploited and translated into tangible benefits for refinery operators. The improvement of traditional design methodologies to find fouling–resilient arrangements that allow undisrupted operations with minimal loss of efficiency is highly desirable.

Traditional design methodologies largely rely on highly empirical, fixed, TEMA ‘fouling factors’ (TEMA, 1941). These are basically “safety factors” which result in an over–designed heat transfer area that, in theory, should compensate for reduced thermal efficiency caused by fouling. Ultimately, however, this approach turns out to exacerbate fouling rather than mitigating it as a consequence of producing higher temperatures at start–up and lower fluid velocities than those for which the unit was designed.

The fundamental limitation of the fouling factor approach is that it does not capture in any detail actual fouling dynamics and its strong dependence on exchanger design and process conditions. The ability to capture at the design stage the dependence of fouling on process conditions and time becomes therefore pivotal to achieve fouling–resilient designs and retrofits of heat exchangers and networks, and to better support operating decisions. Butterworth (2004) in his process heat transfer outlook for 2010 noted that:

“The next major attack on fouling will be as a result of a better design process. For some key applications, such as crude–oil, preheat chain, we have equations which predict (though not very accurately) the way fouling develops and the effect of temperature and velocity on this. What we need therefore to do is to get these equations into our design software and to become skilled in using this to design for minimum fouling.”

Some tools that integrate fouling models with design software (ESDU, 2000; Butterworth).
do exist. However, their systematic application to the design of industrial units and networks is scarce and they cannot be used, for example, to simulate heat exchanger or network dynamic behaviour as a function of process conditions or be integrated in control systems. To effectively use the equations (or thermal fouling models) mentioned by Butterworth in the design of industrial units it is necessary to improve the accuracy of existing fouling models which, even when fitted (i.e. not in predictive mode) to calculated fouling resistances, usually give over 50% average relative error; in the best case 9% error. Such an improvement would give confidence to the designer in using a new, better performing approach rather than the well–established, traditionally perceived as safe but less effective TEMA approach.

The desired improvement in predictive capabilities can be achieved only by removing some of the several limitations that existing models suffer from. In particular, the underlying thermal model, the hydraulic model and the description of the thermo–physical properties of the oil are often simplistic. Models are typically lumped (i.e. are calculated for the unit as a whole, without accounting for changes in temperature profiles, velocities and properties across the unit), the heat transfer coefficient is assumed to be constant and include many other approximations (such as the “thin slab”, valid only for a fouling deposit thickness less than 10% of the tube diameter) which severely limit their overall accuracy and hence applicability.

Current network design methodologies (e.g. pinch technology) also suffer from several limitations as they aim at maximising energy recovery in clean conditions without accounting for the variation of performance over time produced by fouling. Only the use of a dynamic simulation which includes fouling as a function of process conditions, heat exchangers geometry and network topology would allow maximising energy recovery over extended periods.

A lack of models capable of accurately predicting fouling and, at the same time, easy to use and reliable has so far represented a barrier to the effective application of new tools in demanding industrial settings. Thus designers still rely on 70 year old TEMA fouling factors for the design of heat exchangers and 40 year old pinch technology methodology for the synthesis of networks. Prediction of fouling for monitoring purposes in refineries remain merely based on analysing current trends with managerial decisions assisted only by simple calculations and past experience.

This thesis aims at developing a novel mathematical model that overcomes the limitations of existing ones by integrating a dynamic fouling model with a detailed thermo–hydraulic model of
refinery heat exchangers and implement it in a user–friendly manner that allows an easy set–up of unit and network simulations. Specific objectives of this work are:

1. Develop a high fidelity model for shell–and–tube heat exchangers that accounts for thermo–hydraulic effects of tube–side fouling and validate it against plant data from different refinery sites to verify its predictive capabilities and robustness.
2. Develop a set of key performance indicators, which, when combined with model simulations, allows systematic quantification of energy losses, greenhouse gas emissions, reduction in throughput and economics due to fouling in PHTs.
3. The use of 1 and 2 to retrofit/design heat exchangers and heat exchanger networks that mitigate fouling.

The development of the model will follow a multi–scale logic as detailed in the next section.

1.2 Thesis Structure

In Chapter 2 background information regarding crude distillation units and a detailed analysis of the impact of fouling in pre–heat trains is reported. An overview of the basic science of fouling, which includes a description of the fouling mechanisms and the effects of different process variables on fouling rates, is presented. Basic models of chemical reaction fouling, relevant to crude oil, are also reviewed.

In Chapter 3 common methodology for design of heat exchangers and heat exchanger networks are presented and their limitations exposed. A survey of existing thermo–hydraulic models of shell–and–tube heat exchangers available in the literature is also presented with particular emphasis on those that include fouling as a dynamic process. Finally, gaps in the literature are identified and summarised, paving the way for the following development of a multi–scale model of shell–and–tube heat exchanger networks undergoing crude oil fouling.

Chapter 4 deals with the development from first principles of the fundamental equations for a single tube undergoing crude oil fouling. The model proposed captures fouling as a function of local conditions and time. Two operating modes are investigated, namely uniform heat flux and uniform wall temperature, for which the impact of ageing (the structural change of deposits over time) on the thermal fouling resistance is analysed. A mathematical model that captures the
effects on the heat transfer coefficient given by the increase in roughness over time due to the fouling deposition is also proposed.

In Chapter 5, the model for the distributed tube developed in Chapter 4 is extended for use in a shell–and–tube heat exchanger. In this chapter the equations used for the shell–side thermal balance and calculation of heat transfer coefficient are reported. A formal validation of the heat exchanger model is performed against plant data from two refineries belonging to major oil companies, namely ExxonMobil and Shell. Procedures for the elimination of gross errors from plant data and estimation of model parameters are also reported.

In Chapter 6, it is shown that the detailed heat exchanger model can be used to simulate the thermal–hydraulic performance of a network of exchangers in a PHT. Moreover, a set of key performance indicators to systematically assess the impact of fouling on the economics of the refinery is devised. Finally, the capability of the model to unveil complex interactions, assess operating costs and effectively propose network retrofits that minimise fouling are demonstrated with two case studies based on existing PHTs.

Chapter 7 concludes the thesis and makes useful recommendations for future extensions of the present study.

Finally, the Appendices report the sensitivity analysis of the fouling model used in the thesis, an overview on the use of computational fluid dynamics in fouling research and a brief survey of commercially available software for the design of heat exchangers.
Chapter 2

Fouling in crude distillation units: basic science and economics

Synopsis

In this chapter the necessary background information to the fouling process with focus on crude fouling in refineries is presented. After a short description of a typical crude distillation unit and its main components (Section 2.2), the impact of fouling on economics, operability, environment and health and safety are considered in Section 2.3. The basic science and principles of the fouling process are examined in Section 2.4 whilst models that attempt to describe the dynamics of the fouling process are reviewed in Section 2.5.
2.1 Introduction

Fouling in heat exchangers is a complex problem that involves several phenomena which interact at different length and time scales. Moreover, fouling in various forms affects not only oil refineries but, at different level of severity, the whole process industry. The focus of this literature review is to present the necessary background information on the industrial and research problem addressed in this thesis: fouling in refinery pre–heat trains.

Many useful books (Bott, 1990, 1995; Müller-Steinhagen, 2000), review articles (De Deus, 1980; O’Callaghan, 1980; Collier, 1980; Epstein, 1981b; Somerscales, 1981; Bohnet, 1987; Bott, 1988b; Watkinson, 1988; Somerscales, 1990; Knudsen, 2002) and technical reports (ESDU, 1989) exist on the topic of fouling in heat exchangers. These provide a broad overview on the several issues related to fouling. A more in–depth analysis of chemical reaction fouling, which, as it will be shown later in more detail, is the mechanism most relevant to crude fouling in PHTs, has been reviewed by Crittenden (1988a,b); Watkinson (1988, 1992); Crittenden et al. (1999); Panchal (2001); Watkinson and Wilson (1997). Moreover, an ESDU Data Item provides background information, insights on technologies and practical guidelines on crude oil fouling mitigation in refinery pre–heat trains (ESDU, 2000).

The reader is referred to the publications above for more details on specific aspects not covered in this overview.

2.2 Crude distillation unit in oil refineries

The crude distillation unit (CDU) is the first of several units that the crude oil encounters in any refinery. A typical CDU (Figure 2.1) consists of a desalter, a pre–flash drum, a furnace, an atmospheric tower (where petroleum is fractionated in several products), three side strippers, a debutanizer/splitter (Hory, 2000) and the pre–heat train. Typical CDU capacity, which determines the total capacity of the refinery, ranges between 100,000–200,000 barrels per day (bbl day$^{-1}$). Large refineries that can process more than 500,000 bbl day$^{-1}$ may have more than one crude distillation unit.

The use of the pre–flash in CDUs was originally proposed by Brugma (1941) and discussed in a number of publications (Feintuch et al., 1985; Yahyaabadi, 2005; Errico et al., 2009). Nowadays almost all major refineries use it as a convenient way of de–bottlenecking the CDU.
and reducing the risk of two phase flow in the hot section of the train. From the pre–flash, the
gas phase is sent to the distillation column, whereas the liquid phase is further pre–heated in the
PHT hot–end before entering the furnace.

The atmospheric distillation column has typically 30 to 50 trays installed depending on
the degree of fractionation required and the number of side streams. Hot distillate products
(kerosene, light and heavy gasoil) are withdrawn from different sections of the tower, steam
stripped and sent to storage. Naphtha and LPG are removed from the column head. The final
products, characterised by their boiling ranges, are reported in Table 2.1.

**Table 2.1:** Typical atmospheric distillation product boiling ranges (Jones, 1995).

<table>
<thead>
<tr>
<th>Stream</th>
<th>Product name</th>
<th>Boiling range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Off gas</td>
<td>LPG</td>
<td>up to 30°C</td>
</tr>
<tr>
<td>Overhead distillate</td>
<td>Full–range naphtha</td>
<td>30°C–190°C</td>
</tr>
<tr>
<td>1\textsuperscript{st} side–stream</td>
<td>Kerosene</td>
<td>190°C–250°C</td>
</tr>
<tr>
<td>2\textsuperscript{nd} side–stream</td>
<td>Light gasoil</td>
<td>250°C–320°C</td>
</tr>
<tr>
<td>3\textsuperscript{rd} side–stream</td>
<td>Heavy gasoil</td>
<td>320°C–365°C</td>
</tr>
<tr>
<td>Residue</td>
<td>Fuel oil</td>
<td>365°C–500°C</td>
</tr>
<tr>
<td>Residue</td>
<td>Bitumen</td>
<td>&gt;500 °C</td>
</tr>
</tbody>
</table>
In US refineries the average CDU’s energy consumption has been evaluated in 31.9 kWh (114.9 GJ) per barrel processed \( \text{DOE} \; 2006 \) of which roughly 98% is due to fuel consumption at the furnace and the remaining 2% due to electricity (including also the energy used for desalting). Although this is relatively low compared to other conversion processes downstream (Figure \ref{fig:energy_use}(a)), because it processes all incoming crude oil, with a US average refinery consumption estimated in 190 TWh yr\(^{-1} \) \((6.86 \times 10^{17} \text{ J yr}^{-1})\) the CDU is the largest energy user in the whole refinery (Figure \ref{fig:energy_use}(b)). Figure \ref{fig:energy_use} considers the theoretical minimum energy required under ideal conditions (TME), the practical minimum energy required in non–ideal conditions (PME) and the current average energy consumed under actual plant conditions (CAE). The difference between PME and CAE is a measure of potential gains that may be achieved, according to the \text{DOE} \; 2006 study, by improving current technologies, process design or operating practices. Unlocking this “energy bandwidth” could lead to large benefits for the whole refinery and the society in general.

Given the large quantity of energy involved, the design of crude distillation systems — and the potential saving associated — has attracted the interest from both industrial and academic communities. In late 70’s, early researchers focused on improving the distillation column design (e.g. internal geometries, use of pump arounds etc.). When in the early 80’s, the use of Pinch Technology (described in Section \ref{sec:pinch}) became widespread, the focus shifted on improving heat integration. However, it was only through the mathematical methodologies and tools developed in the 90’s that researchers were finally be able to design, retrofit and optimise systematically and simultaneously both a distillation column and its associated heat exchanger network as a

Figure 2.2: Average energy use per barrel of feed processed (a) and per year (b) basis in refinery units. TME=theoretical minimum energy required, PME=practical minimum energy, CAE=current average energy.
2.2 Crude distillation unit in oil refineries

complex and integrated system (Liebmann and Dhole 1995; Liebmann et al. 1998; Suphanit 1999; Bagajewicz and Soto 2000; Ji and Bagajewicz 2002a,b; Basak et al. 2002; Gadalla et al. 2003, 2005).

2.2.1 The pre–heat train

To reduce energy requirements at the furnace, the crude oil is pumped from storage and heated in a series of heat exchangers, the pre–heat train (PHT), against overhead, product and pump–around streams from which nearly 60-70% of the heat necessary for primary fractionation (Panchal and Huangfu 2000) is recovered. Although a few examples exist of refineries using compact plate and frame design (Andersson et al. 2009), a typical pre–heat train is made up of as many as 60 shell–and–tube heat exchangers (Panchal and Huangfu 2000) with the crude usually processed on the tube–side. However, if the heating fluid is a heavy residue stream with larger fouling propensity or if the velocity of the crude is too low, the crude may be allocated to the shell–side.

In the PHT the crude reaches the so called coil inlet temperature (CIT) at which it enters the furnace where it is brought to the highest temperature possible for single phase flow (the coil outlet temperature or COT). Typically CIT ranges between 240–270°C (BP 2006), at a coil inlet pressure (CIP) between 12–15 bar, whilst typical COT is around 365°C (Shell 2006).

Following the changes in crude temperature, the PHT is usually divided into sections referred to as cold (upstream of the desalter), intermediate (between the desalter and the pre–flash) and hot (downstream of the pre–flash).

2.2.2 The role of the desalter

Crude oil contains varying amounts of inorganic salts such as NaCl, CaCl₂, MgCl₂ (Bai and Wang 2007). The presence of such salts not only plays an important part in the fouling process but it also increases corrosion in the train and poisons the catalysts in processing units downstream of the CDU. Liu et al. 2003 discussed the importance of reducing the concentration of salts in the crude stream salts. This is typically done through a desalting process by diluting the salt content with fresh water added before entering a desalter at a temperature between 90 and 120°C with a recommended addition rate of 3.0–4.5% of crude flow (Choi 2005). Different types of desalters exist. In the most common desalters — which operate at a pressure around 5–10 bar and temperature in the range of 100–150°C — the gravity settling of salt–containing water droplets
is enhanced by electrostatic precipitation. The water phase is sent to a sour water stripper and disposed whereas the oil phase is routed to the intermediate section of the PHT.

It is important to note that desalter performance is strictly interlocked with thermal efficiency of the heat exchangers. Desalters usually operate within a restricted optimum temperature range. Improved heat exchangers operation (i.e. ensuring stable temperature outlets and less down–time for cleaning) affects in a positive way desalter control which in turn is paramount to avoid fouling.

2.3 Impact of fouling on crude distillation units

Discussion with plant operators highlighted that they are constantly faced with problems caused by fouling of heat exchangers in the PHT (Figure 2.3). These include:

1. Operating difficulties
2. Economic penalties
3. Environmental impact
4. Health and safety hazards

Fouling deposits on the heat transfer surfaces have a thermal conductivity — typically between 0.2 and 1 W m\(^{-1}\) K\(^{-1}\) (Watkinson, 1988) — up to two orders of magnitudes lower than that of the tube metal wall (ca. 38 W m\(^{-1}\) K\(^{-1}\), depending on the metal used and temperature). As a consequence, heat transfer is impaired and energy recovery reduced. This progressive decay in performance results in a typical loss of 8–11°C yr\(^{-1}\) in the CIT (BP, 2006). To keep a steady

![Figure 2.3: Photos of crude oil fouling at tube ends of refinery heat exchangers (a). In some case fouling can result in plugging of tubes (b). Pictures courtesy Prof. Barry Crittenden.](image-url)
2.3 Impact of fouling on crude distillation units

Figure 2.4: Impact of fouling on PHT and related costs for a typical oil refinery processing 100,000 bbl \( \text{day}^{-1} \) of crude oil. The figures, reported in US$, are adjusted for inflation to 2009 (data from various sources, reported in Table 2.2).

Operating difficulties

There is little doubt that fouling affects greatly CDUs’ energy efficiency. Estimations of the extra energy requirements caused by fouling deposition reported in literature ranges from no less than 10% (Szklo and Schaeffer, 2007) to over 30% (Van Nostrand et al., 1981). Based on their experience Sikos and Klemes (2010) recently evaluated the energy consumption being 10–20%
higher because of fouling in CDUs. Thermal efficiency of the PHT is therefore a major concern, and plants usually have targets for CIT (Shell 2006). For example, when PHT efficiency goes below 30% some refineries shut the heat exchangers down for cleaning (Zabiri et al. 2006).

Whilst it is more common for a PHT to be thermally limited, in some occasions, the hydraulics implications of fouling may be dominating. Usually refineries have a discrete hydraulic flexibility but problems can arise if the progressive reduction of the cross-sectional area available to the crude flow causes an excessive increase in pressure drops. If the throughput is to be kept constant, more pumping power must be spent until pump capacity is reached. In some extreme (but not rare) cases, plugging of tubes (Figure 2.3(b)) can occur, forcing a shut down of the unit for cleaning.

When economic penalties become excessive, cleaning actions which disrupt normal refining operations are required. Refinery personnel give particular importance to the planning of cleaning actions. Dismantling units for cleaning is in fact an hazardous and costly operation (see Section 2.3.4) for which planning is paramount. Several authors dealt with different aspects of the cleaning scheduling of heat exchanger networks in general (Markowski and Urbaniec 2005; Sanaye and Niroomand 2007) and PHTs in particular (Wilson et al. 2001; Smaili et al. 2001; Lavaja and Bagajewicz 2004, 2005a,b; Rodriguez and Smith 2007; Ishiyama et al. 2009a).

### 2.3.2 Economic penalties: the cost of fouling

It has already been highlighted that the CDU is the largest energy consumer in the refinery. Because of that, the largest share of the total fouling–related costs for the whole refinery originate in the PHT (Figure 2.5). Of the total costs (US$22.6M yr⁻¹, 2009 basis) almost 50% of fouling–related costs of a hypothetical 100,000 bbl day⁻¹ refinery (Van Nostrand et al. 1981) are attributable to fouling in the CDU. The major loss is due to the reduction in throughput (ca. 40%), followed by the energy costs (ca. 10%) and only a small fraction (<1%) is due to maintenance.

Table 2.2 summarises the fouling–related costs in CDUs reported in literature or collected as personal communications. In some cases the estimates are considerably old and, where appropriate, the original figures are reported together with the ones taking inflation into account¹. However, it should be borne in mind that estimating fouling costs is a complex activity, especially when antifoulants are used (Pritchard 1988b), and many estimates depend on the current price

¹Calculations performed using the Consumer Price Indexes by the US Bureau of Labor Statistics.
2.3 Impact of fouling on crude distillation units

of the crude barrel and market demand. In one of the most comprehensive — although dated — studies, Van Nostrand et al. (1981) estimated the total extra cost due to fouling as US$4.4 bn in oil refineries in western countries. Of this figure, US$2.9 bn (more than 67% of the total) were due to fouling in the crude distillation unit. Adjusting for inflation alone to 2009, these figures

![Figure 2.5: Hypothetical typical refinery fouling related expenses data from Table 2.2](image)

### Table 2.2: Summary of typical economic losses associated to fouling in CDUs.

<table>
<thead>
<tr>
<th>Loss</th>
<th>Refinery size [bbl day$^{-1}$]</th>
<th>Original figure</th>
<th>Source</th>
<th>Adjusted to 2009 US$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Whole refinery</td>
<td>100,000</td>
<td>9.87M US$ yr$^{-1}$</td>
<td>Van Nostrand et al. (1981)</td>
<td>22.6M yr$^{-1}$</td>
</tr>
<tr>
<td>PHT</td>
<td>100,000</td>
<td>4.78M US$ yr$^{-1}$</td>
<td>Van Nostrand et al. (1981)</td>
<td>11M yr$^{-1}$</td>
</tr>
<tr>
<td>One branch of the PHT</td>
<td>210,000</td>
<td>2.5M US$ yr$^{-1}$</td>
<td>(personal comm. (2009))</td>
<td>–</td>
</tr>
<tr>
<td>Throughput reduction</td>
<td>360,000</td>
<td>1.8M US$ yr$^{-1}$</td>
<td>Liporace and de Oliveira (2007)</td>
<td>–</td>
</tr>
<tr>
<td>Throughput reduction</td>
<td>160,000</td>
<td>1.5M US$ in 3 months</td>
<td>ESDU (2000)</td>
<td>1.81×10$^6$</td>
</tr>
<tr>
<td>Throughput reduction</td>
<td>100,000</td>
<td>3.73M yr$^{-1}$</td>
<td>Van Nostrand et al. (1981)</td>
<td>8.5M yr$^{-1}$</td>
</tr>
<tr>
<td>Throughput reduction</td>
<td>n.a.</td>
<td>2 US$ bbl$^{-1}$ (Texas)</td>
<td>Personal comm. (2009)</td>
<td>–</td>
</tr>
<tr>
<td>Throughput reduction</td>
<td>n.a.</td>
<td>10 US$ bbl$^{-1} (India)</td>
<td>Personal comm. (2009)</td>
<td>–</td>
</tr>
<tr>
<td>Extra fuel at furnace</td>
<td>100,000</td>
<td>1.02M US$ yr$^{-1}$</td>
<td>Van Nostrand et al. (1981)</td>
<td>2.3×10$^6$ yr$^{-1}$</td>
</tr>
<tr>
<td></td>
<td>400,000</td>
<td>500,000</td>
<td>Panchal and Huangfu (2000)</td>
<td>510,000 yr$^{-1}$</td>
</tr>
<tr>
<td></td>
<td>750 tCO$_2$ yr$^{-1}$</td>
<td>(22,500 € yr$^{-1}$)</td>
<td>Yeap (2003)</td>
<td>31,000 yr$^{-1}$</td>
</tr>
<tr>
<td>Drop of 1 °C in CIT</td>
<td>100,000</td>
<td>1 tCO$_2$ day$^{-1}$ = 100,000 US$ yr$^{-1}</td>
<td>Baudelet and Krueger (1998)</td>
<td>130,000 yr$^{-1}$</td>
</tr>
<tr>
<td>Drop of 1 °C in CIT</td>
<td>210,000</td>
<td>250,000 £ yr$^{-1}$</td>
<td>Personal comm. (2009)</td>
<td>380,000 yr$^{-1}$</td>
</tr>
<tr>
<td>Production loss taking a unit out of service</td>
<td>100,000</td>
<td>20,000 US$ day$^{-1}$ = 80,000 per clean.</td>
<td>Baudelet and Krueger (1998)</td>
<td>24,000 day$^{-1}$ = 100,000 per clean.</td>
</tr>
<tr>
<td>Cleaning of a single unit</td>
<td>–</td>
<td>Personal comm. BP (2006)</td>
<td>30–50,000 per unit</td>
<td></td>
</tr>
<tr>
<td>Antifoulants</td>
<td>100,000</td>
<td>155,000 US$ yr$^{-1}$</td>
<td>Van Nostrand et al. (1981)</td>
<td>350,000 yr$^{-1}$</td>
</tr>
</tbody>
</table>
would be, respectively, US$10 bn and 6.8 bn\(^2\).

Data for the UK assess the overall cost of PHTs fouling between £5–7M yr\(^{-1}\) (Pritchard, 1979), which, in 2009 US dollars is ca. 6.8–9.5 million and correlate well with the above US data. More recent figures (2009), however, indicate that fouling in the PHT costs a 210,000 bbl\(^{\text{day}}\)–1 UK refinery ca. US$2.5M yr\(^{-1}\) (personal communication, April 2009). If this cost is considered representative of all UK refineries, it can be roughly estimated, on the basis of cost of fouling per barrel processed\(^3\) that in 2009 fouling in PHTs cost the UK economy over US$20 million.

In the following paragraphs a breakdown analysis highlights the individual contribution to the losses due to fouling in the CDU.

### 2.3.2.1 Energy costs

Van Nostrand \textit{et al.} (1981) reported a typical decay rate in the coil inlet temperature due to fouling in the PHT of 4–10°F, month\(^{-1}\) (ca. 2–5 °C yr\(^{-1}\)). Experts from BP (2006) and ConocoPhillips (2006) in a personal communication were much less optimistic estimating this figure and reported, respectively, 8-11°C yr\(^{-1}\) in heavy fouling trains. The cost associated with the extra fuel burnt to counter this drop in CIT is very significant for the economics of the refinery. A 1°C drop in CIT has been reported to cost for a UK refinery (processing 210,000 bbl\(^{\text{day}}\)–1) ca. £250,000 yr\(^{-1}\) (ca. US$400,000 yr\(^{-1}\), personal communication, April 2009). Assuming an average 5°C drop over a year, this would cost to the refinery over US$2,000,000. Panchal and Huangfu (2000) estimated for a smaller refinery, processing 100,000 bbl\(^{\text{day}}\)–1, an economic loss of about US$510,000 yr\(^{-1}\). Recently Liporace and de Oliveira (2007) reported US$1.8M yr\(^{-1}\) losses in fuel alone due to fouling in one PHT branch of a 360,000 bbl\(^{\text{day}}\)–1 Brazilian refinery.

### 2.3.2.2 Reduction in throughput

Refinery operating strategy is normally that of maximum throughput. The reduction in thermal efficiency caused by fouling is paid not only at the furnace as extra energy and emissions (discussed in Section 2.3.3) but, most of all, as loss in production. A furnace has a maximum heat duty achievable, \(Q_{\text{fur}}^{\text{max}}\) (often referred to as furnace firing limit), which is constrained by the

\(^{2}\)It should be noted that the estimations were made at a time (1981) when environmental policies were not as strict as at present (e.g. Emission Trading Scheme), and the cost of a crude barrel was significantly lower (ca. US$30) and overall throughput was considerably lower, which would further increase the value of these figures.

\(^{3}\)Considering that the UK had 1.9 million bbl\(^{\text{day}}\)–1 of refining capacity in 2006 (according to OGJ) and refinery utilization of 90%, the refinery accounts for 12% of all the oil processed in the UK.
2.3 Impact of fouling on crude distillation units

maximum temperature of the flue gases in the chimney. The heat duty at the furnace, $Q_{fur}$ is:

$$Q_{fur} = \dot{m}c_p (COT - CIT)$$ (2.1)

where $\dot{m}$ is the crude mass flowrate in the furnace and $c_p$ its specific heat capacity. Given that the COT must be kept constant whilst the CIT decreases because of fouling, the heat duty increases (i.e. extra fuel must be burnt). With a large decline in CIT due to fouling, the furnace hits its firing limit, $Q^{max} = Q^{max}_{fur}$. At this point, the throughput must be reduced causing loss of production, which is responsible for the major share of the total costs related to fouling in the CDU.

Tackery (1979) suggested that loss in production is the most difficult loss to estimate since it depends on the current level of market products demand. Regional differences also affect the cost of loss in production; Polley et al. (2009a) reported that at the beginning of 2009, this cost was US$2 bbl$^{-1}$ in some USA refinery, over US$5 bbl$^{-1}$ in Asian refineries and over US$10 bbl$^{-1}$ in one Indian refinery. The importance of including throughput loss in scheduling and operability considerations has been highlighted by several authors (Lavaja and Bagajewicz, 2005a; Polley et al., 2009b). Overall, Van Nostrand et al. (1981) estimated the throughput loss in US$8.5M yr$^{-1}$ (2009 dollars) for the 100,000 bbl day$^{-1}$ refinery they considered.

2.3.2.3 Maintenance (cleaning)

If an unacceptable reduction of throughput occurs or if it is estimated by the operator that extra costs for energy are too high, selected units are usually taken off–line and cleaned. Worrell and Galitsky (2005) reported the results of an audit of the Equilon refinery in Martinez, California (now owned by Shell) where it was found that regular cleaning of heat exchangers and maintenance of insulation would result in estimated annual savings of over US$14M at a total expenditure of US$9.85M with a payback period of around 8 months (DOE, 2002). In this context, monitoring of fouling (discussed in Section 3.3) is a key activity to identify units that need maintenance. Cleaning is usually performed via dismantling a chosen unit and using water jets — typically at 1000 bars but in some special cases 2000 bars are required — to mechanically remove deposits from the heat transfer surfaces. The expense to clean a single unit via this methodology is between US$30,000 and 50,000 (ExxonMobil, 2006). To this figure it must be added the cost due to production loss estimated in US$24,000 per day in a 100,000 bbl day$^{-1}$ refinery (Baudelet and Krueger, 1998). Considering that to clean each unit requires up to a week
before it is in service again, the total cost due to maintenance of a single unit can add up to US$150,000–200,000.

An alternative to the expensive (in terms of time, safety and money) mechanical cleaning is chemical cleaning, performed by flowing a solvent chemical through the exchanger without the need for disassembly. The chemical action of the solvent dissolves some or all of the constituents of the solid foulant deposit. However, Joshi and Brons (2003) reported that attempts to chemically clean heat exchange equipment have been successful only in a limited number of cases, and even then, with benefits sustained for only a relatively short period compared to mechanical cleaning.

2.3.2.4 Antifoulants

Despite the optimism of Canapary who stated in 1961 that “a complete antifouling program will solve process side fouling in oil refineries”, a chemical solution capable of eliminating fouling seems to be still lacking. In the 100,000 bbl day$^{-1}$ refinery monitored by Van Nostrand et al. (1981) the decline rate of the PHT heat duty was 1.5 MW month$^{-1}$ when no chemicals were used whilst the decay rate was reduced to 0.56 MW month$^{-1}$ when antifoulants were added to the crude stream. They estimated the cost of chemicals at around US$355,000 yr$^{-1}$ (2009 basis) which was paid back by the 65% reduction in fouling and associated decrease in the number of cleaning required per year. However, the complexity of the crude compositions, their variability over time and the fact that fouling mechanisms are not yet fully understood (see Section 2.4) force suppliers to provide ad hoc solutions for each refinery, with the risk that the same treatment will not work for extended period of time. Moreover, the use of chemicals require dosing equipment to inject the antifoulants at the correct point in the crude stream that further increases the capital costs.

2.3.2.5 Capital costs

Heat exchanger design methodologies deal with fouling by simply compensating for the reduced heat transfer efficiency with the addition of larger heat transfer surfaces. However, as it will be shown in detail in Section 3.2, this practice not only is far from being optimal but it also increases the total capital expenditure. The cost of a PHT heat exchanger, typically sized between 300 and 900 m$^2$, can be roughly estimated at US$67,000–150,000 using a cost per unit area in the
range of US$170–225 m\(^{-2}\) (ESDU, 1994). Considering that most heat exchangers are 30–50% oversized at the design stage (Shell, 2006) due to the fouling factors design approach, the capital costs associated to the extra area can be evaluated in the range of US$20,000–75,000 per unit. As already mentioned, a typical PHT can use 16 to 60 heat exchangers therefore the total extra capital cost ranges from US$320,000 to US$4.5M. If special material of construction is used to avoid corrosion, the figures calculated may grow substantially.

2.3.3 Environmental aspects

Environmental impact of fouling in refineries has been estimated as being responsible for 88M t of CO\(_2\), accounting for 2.5% of all worldwide anthropogenic emissions in 2009 (Müller-Steinhagen et al., 2009a). Cap–and–trade regulations such as the Emissions Trading Scheme (ETS) enforced in Europe gives a tag value to each t of CO\(_2\) emitted by the refinery adding to the total cost of fouling. According to ETS regulations, each installation is allocated allowances for emission of carbon dioxide. If the refinery exceeds the allocated allowances, it is necessary to buy extra ones on the market. The reverse is also true: if the allocated allowance is not reached, the excess allowance can be sold. Table 2.2 reports calculations made with a carbon tax rate at €30 t\(^{-1}\) which is the peak value reached in April 2006. Phase two of ETS started in January 2008 with a price fixed at €25 t\(^{-1}\) which dropped to €10 t\(^{-1}\). The importance of considering the impact of energy consumption on CO\(_2\) emissions in CDUs was highlighted by Gadalla et al. (2005).

Ecological aspects involve also the disposal of the carbonaceous deposits formed on the heat transfer surfaces which can be substantial. To illustrate the quantity of deposits that must be removed from the PHT of a refinery, Murphy and Campbell (1992) considered a refinery processing 27,000 t day\(^{-1}\) (ca. 200,000 bbl day\(^{-1}\)) of crude which contains 0.05% of what they call “sediments” and 10 ppm of salts. The potential deposits each year are 5000 t of sediments and 100 t of salts. More optimistically, Watkinson (2005) assumed that only one part per million by weight of the oil would deposit producing 15 t yr\(^{-1}\) (in a 300,000 bbl day\(^{-1}\) refinery) of solid carbonaceous material. These deposits can contain sulphur, nitrogen and metals and must be disposed in an adequate way.

\(^4\)Original figures, £60–80 m\(^{-2}\), have been adjusted for inflation and converted at 2009 exchange rates without including changes in capital cost for raw materials etc.

\(^5\)As a general rule, Müller-Steinhagen (2000) suggests that an excess area of 30%–40% may correspond to 25% additional capital costs without including increased shipping and installation expenses due to the larger dimensions.
2.3 Impact of fouling on crude distillation units

2.3.4 Health and safety hazards

An aspect often overlooked in literature is the health and safety hazards involved in dismantling a pressurised unit treating hydrocarbons for cleaning. During the cleaning process refinery procedures require a safety observer in 100% attendance to supervise the following risky activities:

1. Opening of the units. Although units are flushed with steam, flammable atmospheres and pyrophoric material are often present.
2. Extraction of the bundle with cranes (typically units are 6.1 m long and up to 1.5 m diameter) in confined spaces (Figure 2.6). Electrical hazards are also involved.
3. Transportation on trucks to storage.
4. Cleaning with 1000 bar water jets (although ultra–high pressure pumps can provide up to 2800 bar for heavily fouled tube–side surfaces) with associated noise and toxic material being thrown in the atmosphere.
5. Delivery and reinsertion of the bundle with crane and trucks movement.

Certainly, safety in the oil industry is a primary concern. Discussions with industry experts indicted that safety considerations, let alone the costs involved, can affect operating decisions and reducing the number of cleanings by reducing fouling would be highly beneficial.

Figure 2.6: Tube bundle has to be pulled out from shell for cleaning with cranes in confined spaces creating safety issues. Photo courtesy Prof. Barry Crittenden.
2.4 Basic science in the fouling process

To understand how fouling affects heat exchangers’ thermo–hydraulic behaviour and, ultimately, to be able to mitigate it, it is necessary to understand the mechanisms through which the accumulation of unwanted deposit on the heat transfer surfaces occurs. It should be noted immediately at this stage that, because of the complex interacting phenomena and the intrinsic difficulties in obtaining sound experimental data, several areas of the fouling process remain largely unknown. In one of the most cited articles in fouling research, Epstein (1983) summarised the level of understanding in different aspects of the fouling process in a matrix (Figure 2.7(a)) where the five columns are the different fouling mechanisms whilst the five rows are the sub–processes involved. The Epstein matrix has been updated to reflect current level of understanding in 1987 by Bohnet (Figure 2.7(b)) and, more recently, by researchers of different level of expertise in the field (Figure 2.7(c)) participating in the ‘Heat Exchanger Fouling and Cleaning’ conference held in Austria in June 2009 (Müller-Steinhagen et al., 2009b). Over the years, many gaps in research seem to be filling. In particular transport, which was already identified as the most studied sub–process in the original Epstein matrix, has gained a remarkable level of attention across all fouling mechanisms types. On the other end of the scale, ageing was identified as the topic having received least attention. The next sections investigate the fouling mechanisms and the sub–processes involved in fouling.

![Fouling matrix](image)

**Figure 2.7:** Original 5×5 fouling matrix (Epstein, 1983) (a), interpretation by Bohnet (1987) (b) and by researchers attending the 2009 Heat Exchanger Fouling and Cleaning conference in Austria (adapted from Müller-Steinhagen et al., 2009b). Light to dark shading indicates increase in research level.
2.4 Basic science in the fouling process

2.4.1 Fouling mechanisms

The columns in the Epstein matrix (Figure 2.7) represent the five major categories in which fouling has been divided accordingly to the mechanism that produces it (Epstein, 1983):

1. Crystallization fouling: precipitation and deposition of dissolved salts that, at process conditions, become supersaturated (Hasson, 1981; Bott, 1988a; Yiantios et al., 1997).

2. Particulate fouling: deposition of suspended particles on heat transfer surfaces. (Gudmundsson, 1981; Epstein, 1988b; Karabelas et al., 1997).

3. Chemical reaction fouling: deposits resulting from one or more chemical reactions between reactants contained in a flowing fluid accumulate on the heat transfer surface (Watkinson, 1988; Crittenden et al., 1999; Watkinson and Wilson, 1997).

4. Corrosion fouling: deposits are produced by a chemical reaction that involves a reactant on the metal surface. The increased roughness of the surface may also promote fouling due to other mechanisms (Somerscales, 1997, 1999; Lister, 1981).

5. Biological fouling: formation of organic films consisting of micro–organisms that promote attachment of macro–organisms (e.g. mussels, algae, etc.) (Kent, 1988; Melo, 1999).

Fouling in different sections of the PHT can happen via any of the above mechanisms and often it is a combination of mechanisms (mixed fouling) that leads to deposition. It is not unusual to find deposits due to bio–fouling at the cold end of the train whereas corrosion fouling afflicts the whole network (Canapary, 1961). Joshi (2001) showed the case of one heat exchanger processing crude at about 88°C where suspected salt deposition is responsible for fouling. However, field observations indicate that fouling is particularly severe in the hot end where there is evidence (ESDU, 2000) that chemical reactions, triggered by the high temperatures, generate foulant precursors that eventually led to deposition on the heat transfer surface. A first attempt to tackle the fouling problem in CDUs should therefore aim at investigating in more detail the nature of the chemical reaction involved and their possible routes.

2.4.2 Routes of chemical reaction fouling

Little is known regarding the chemical reactions that lead to deposition from crude oils at high temperatures. Better understanding of fouling mechanisms can be achieved through the characterization of the deposited species (Dickakian, 1989; Young et al., 2009; Venditti et al., 2009).
2.4 Basic science in the fouling process

From which conjectures can be made on the reactions that took place to produce a particular deposit composition.

Crittenden et al. (1992) sought to gain a better understanding by performing chemical analysis on the deposits of a refinery PHT and measuring the fouling layer thickness at a given position inside the tubes. Data collected showed the presence of high molecular carbonaceous matter but inorganic compounds were also found: iron (due to corrosion), high sulphur and sodium content. Whilst for some fluids it is clear which are the precursors of fouling (e.g. milk Beuf et al. (2003); Bansal and Chen (2006)), crude oil has a complex composition which makes it difficult to identify them. Even when the precursors have been identified, it is challenging to determine their exact role in the deposition process. Very often, analysis of the deposits only reveals the product of several reactions preventing the possibility to establish a link between precursors and deposits, thus making it virtually impossible to determine underlying fouling mechanisms.

So far, researchers have been only able to interpret experimental and field data to find indications of possible causes of fouling without finding conclusive theories on the actual deposition mechanisms. Therefore, only conjectures on possible reaction mechanisms exist for crude oil and hydrocarbon fouling (Panchal and Watkinson 1994; Watkinson and Wilson 1997). Eaton and Lux (1984) proposed the following series of degradation reactions as the crude oil fouling mechanism:

\[
\text{Saturated hydrocarbons} \xrightarrow{\text{Inorg. acids}} \text{Unsaturated hydrocarbons} \xrightarrow{O_2} \text{Organic acids} \xrightarrow{\Delta} \text{Metals} \xrightarrow{\Delta} \text{Resins & asphaltenes} \xrightarrow{\Delta} \text{Wall} \xrightarrow{\Delta} \text{Cokelike deposits}
\]

Besides the limitations of analytical techniques (e.g. instrument resolution, limited solubility of the samples), the number and complexity of the reactions involved make it very difficult to confirm the above mechanism and even harder to measure the individual reactions rates and their respective kinetic parameters. However, from all the experimental evidence reported in literature, there seems to be agreement on a generalised reaction fouling mechanism which comprises the following three steps:

\[
\text{Reactant A} \xrightarrow{f_1} \text{Precursor B} \xrightarrow{f_2} \text{Foulant C} \xrightarrow{f_3} \text{Aged deposit D} \quad (2.2)
\]

In the first step, the soluble precursors are formed via a reaction (or series of reactions) amongst species in the crude. In some cases, the formation of the precursors can happen before the crude enters the unit. Panchal and Watkinson (1994) found indications that these could have a more
significant effect than the precursors generated in the exchanger itself. In the second step, the precursors react giving insoluble foulant species that will then deposit on the surface. A third step involves chemical and physical changes of the deposits caused by the high wall temperatures. This last process goes under the name of ageing (see Section 2.4.3.5) and, as it will be shown in later chapters, it plays an important role in the overall heat exchanger performance.

According to Panchal and Watkinson [1994], reaction $r_1$ and $r_2$ can take place in the bulk, in the boundary layer or at the wall. Figure 2.8 summarises the three possible scenarios:

- **Case 1**: Precursor generation in the bulk. In Case 1a, reaction $r_2$ occurs on the wall surface whilst in Case 1b, reaction $r_2$ occurs in the bulk itself.
- **Case 2**: Precursor generation in the boundary layer. In Case 2a, reaction $r_2$ occurs on the wall surface whilst in Case 2b, reaction $r_2$ occurs in the boundary layer itself.
- **Case 3**: Precursor generation on the wall surface.
Panchal and Watkinson (1993, 1994) developed a mathematical model for fouling in a single tube (reviewed in Section 3.5.2) based on the reaction scheme shown in Equation 2.2. They compared model simulations in the different cases with experimental data finding a relatively good match to Case 1a and 2 suggesting that fouling may occur via reaction in the bulk or in the boundary layer. However, admittedly, they neglected reaction r3 (i.e. ageing) which may affect the accuracy of their final conclusions. Indeed, the question of where the reactions take place is still open. Ebert and Panchal (1997) and Srinivasan and Watkinson (2005), for example, suggested that the fouling reaction takes place in the bulk film and not at the wall surface, whereas Crittenden et al. (1992) argue that most of the deposits are generated in the highest temperature region, i.e. at (or near) the surface.

Paterson and Fryer (1988) showed using a reaction engineering approach that even if the reaction rate is well correlated in terms of the surface temperature, there is no reason to assume the surface reaction as the rate controlling step. They stated that chemical reactions occur throughout the region of the fluid which is hot enough to support significant reaction rates and found fouling rate being controlled by the size of the sublayer and the temperature and the fluid velocity therein. Whilst they used data for milk fouling to support their conclusions, the general approach can be applied to other systems involving chemical reaction fouling.

2.4.3 Sequential events in fouling

Fouling is a dynamic process. Figure 2.9 shows the idealised fouling curves at a specific point where the fouling layer thickness, δ, is plotted against time. A lag time, \( t_l \) is often seen before the layer starts growing on the initially clean heat transfer surface. This goes under the name of initiation or induction period which is the first of the 5 sub–processes identified by Epstein (1983) in the rows of his 5×5 matrix (Figure 2.7):

1. Initiation (Yang et al., 2009a)
2. Transport to surface (Panchal and Watkinson, 1994)
3. Attachment (Visser, 1988a,b)
4. Removal (Yiantsios and Karabelas, 1994; Bohnet et al., 1999)
5. Ageing (Wilson et al., 2009)

A brief discussion for each of those sub–processes is provided in the following sections.
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2.4.3.1 Initiation

The initiation — or induction — is the period of time in which no significant fouling is observed. Some authors believe that during the lag period the surface is conditioned via absorption processes. This can be related to surface properties such as roughness or surface energy (Watkinson 2008). Epstein (1983) noted that for all fouling mechanisms the induction period seems to reduce with increased surface roughness as the roughness projections provide sites for the deposits to nucleate while the grooves provide regions protected from the removal action of the shear stress. In chemical reaction fouling, the induction period seems to decrease with increasing wall temperature (Watkinson and Epstein 1969). Bott (1995) reports that typical induction periods may be in the range 50–400 h. As suggested by Yang et al. (2009a), understanding why the induction period happens could allow to extend this no–fouling period indefinitely. However, discussion with refiners indicate that for crude oil fouling in industrial units, the induction period is seen lasting only less than half a day. Therefore, the importance of the induction period should not be underestimated in the interpretation of experimental results whilst neglecting it in industrial applications seems to be reasonable.

2.4.3.2 Transport

Transport is governed by the principles of mass transfer and depends on the reaction zones where the foulant is formed. In Case 1a Figure 2.8 molecular transport of the soluble precursors,
2.4 Basic science in the fouling process

formed in the bulk, to the wall occurs whilst in Case 1b insoluble foulant species are generated in the bulk and transported to the wall. In Case 2 mass transfer occurs between the boundary layer where the soluble precursors are formed and then either transported to the wall (Case 2a) or generate insoluble foulants (Case 2b). In both Case 2a and 2b, back–diffusion of soluble precursors from the boundary layer to the bulk can take place. In Case 3 the reactants are transported to the surface where the formation of the precursors and foulant occurs.

2.4.3 Attachment

Attachment to the wall depends on the dominant forces that come into play when a foulant particle approaches the wall. These may include long range attractive forces such as the van der Waals force, magnetic attraction and electrostatic forces or short range forces such as chemical bonding and hydrogen bonds (Bott, 1995). An extensive review of adhesion (and removal) from a colloidal science point of view can be found in Visser (1988a,b). In crude oil fouling, attachment plays an important part especially if fouling occurs via the mechanisms shown in Case 1b and Case 2b in Figure 2.8.

2.4.3.4 Removal

Removal may — or may not — happen right after the foulant has been deposited on the wall surface. It is believed (Somerscales and Sanatgar, 1989) that removal can happen via dissolution (the concentration of the deposit the layer/fluid interface is in equilibrium concentration corresponding to the local solubility product), erosion (deposit is finely removed by mechanical action of the fluid on the deposit layer surface), spalling (deposit removed in large pieces either by changes in the solubility of the deposits at the layer/liquid interface or by thermal stresses). In crude oil fouling, given that the fouling species are insoluble in the bulk of the fluid, hydrodynamic forces play a pivotal role in the removal process. The shear stress acting on the fluid/deposit interface counteracts the deposition by impeding the foulant species to stick to the wall. The importance of shear stress will be further explored in the following Section 2.4.4.4.

2.4.3.5 Ageing

The exposure of the fouling layer to high wall temperatures over extended periods can trigger chemical and physical transformations which alter the structure and properties of the deposits.
Nelson (1939a,b) described initial deposition of crude oil fouling as involving a gel which changes its structure over time to a harder material similar to coke. These transformations not only alters the rheology of the deposit layer (Sileri et al., 2009) but also its thermal conductivity, and thus:

- The overall thermo–hydraulic behaviour of the exchanger.
- The nature of the material recovered for analysis with analytical techniques. This makes it difficult to identify the material originally deposited (Wilson et al., 2009).
- The ease of removal (Wilson, 2005).

Within a fouling layer, the material is subject to a range of temperature histories so that ageing is non–uniform in space and highly time–dependent. Despite the importance of these effects, relatively little attention has been paid in the literature to these phenomena, particularly in the area of chemical reaction fouling (Figure 2.7). Timescales that enable to appreciate the effects of ageing are rather long and laboratory experiments rarely report deposit ageing (Wilson et al., 2009). Unlike the induction period, which happens at much shorter timescales, ageing plays a more important role in industrial equipment than in laboratory experiments.

2.4.4 Variables affecting fouling

Several experiments have been performed over the years to address the effects of all the variables affecting fouling. Tests have been performed in re–circulating closed loop apparatus in laboratory equipments (Wilson and Watkinson, 1997, 1996; Asomaning and Watkinson, 1999; Knudsen et al., 1999; Panchal et al., 1999; Wiehe et al., 2001; Crittenden et al., 1987a; Srinivasan and Watkinson, 2005; Crittenden et al., 2009; Bennett et al., 2009; Jamialahmadi et al., 2009) or in field units (Kuru et al., 1997).

Through these experiments, it has been found that mass transport in crude oil fouling increases weakly with both wall and bulk temperature and increases nearly linearly with velocity. Attachment, on the other hand, increases strongly with wall temperature but only weakly with bulk temperature and decreases with increased velocity (Watkinson, 2008). The fact that the fouling rate decreases with increasing velocity, suggests that crude fouling is controlled by adhesion or reaction.

In general, it has been shown that several interacting variables affect the extent of fouling:
2.4 Basic science in the fouling process

1. Crude oil composition and inorganic contaminants
2. Bulk and wall temperatures
3. Velocity (shear stress)
4. Surface conditions (e.g. roughness and roughness dynamics)

In turn, fouling has a direct effect on all these variables by affecting the overall heat transfer coefficient via three effects (Hewitt [2002]):

1. Reduction due to the thermal resistance of the fouling layer;
2. Increase due to the increased local velocity resulting from reduced flow area;
3. Change (usually an increase) in the roughness of the heat transfer surface.

Figure 2.10 summarises the interactions of the above variables involved in the tube–side fouling process and their combined effect on the two main measured quantities: pressure drops and outlet temperature. The overall effect can be significant: deposition of foulants increases the resistance to heat transfer, but it also affects the fluid–dynamics of the system by reducing the cross–sectional area which in turn increases the velocity, hence the convective heat transfer coefficient. The variables affecting fouling will be explored more in detail in the next sections.

2.4.4.1 Crude oil composition and inorganic contaminants

Although analytical techniques exist to characterise crude oil composition (a review of experimental methodologies is given by Merdrignac and Espinat [2007]), it is expensive and time consuming to perform such analysis on each crude slate that reaches the refinery. Moreover, composition of the crude processed in a refinery varies every day (Dickakian [1989]) as the crudes available are blended in different percentages. As a result, the detailed composition of crudes processed are usually unknown to the refinery which makes it difficult to relate fouling rates to crude compositions. Similar difficulties, already discussed, exist even in lab–controlled conditions where the crude used is usually constant and operating conditions fixed.

Nonetheless, it is possible to find some general guidelines by relating field and experimental observations to fouling behaviour. It is generally acknowledged that the heavier the crude, the higher is its fouling propensity. For this reason, light oils (e.g. European, West African, Middle Eastern), preferred by refiners to heavy ones (e.g. Canadian and Venezuelan oils) are in shortage in the market and the trend is increasingly towards the use of heavier crude feedstocks. US oil
refineries, for example, used to process crude oils with a weighted average of 32.46°API\textsuperscript{6} in 1985, processed in May 2007 heavier crudes — 30.59°API on average (EIA, 2007). This shift towards heavier feedstock is expected to continue, increasing fouling problems especially for refineries designed for a lighter quality of crudes.

Of course, determining the effects of composition on fouling behaviour is more complex than merely assessing the specific gravity of a given crude. The presence of sulphur, for example, has dramatic effects on fouling and its role has been analysed by Taylor and Wallace (1968) and summarised in ESDU (2000). Watkinson (2005) suggested that deposition by low–sulphur

\textsuperscript{6}The API gravity of a petroleum liquid is an inverse measure of its relative density compared to water and is related to the specific gravity (SG) by: API = 141.5/SG - 131.5. If the API gravity of a given fluid is greater than 10, then it is lighter and floats on water; if less than 10, it is heavier and sinks.
(sweet) light crude oils is largely due to particulates and gums whereas for medium–sulphur crude oils formation of iron sulphides plays a major role. [Taylor and Wallace (1967)] found that high paraffinic oils may lead to precipitation of gum–like material when heated. In unstable heavy oil systems, suspended asphaltenes are usually suspected to be the fouling species.

If oxygen is present in the crude, free–radical polymerisation reactions may occur [ESDU (2000)]. Thus, oxygen plays an important role in fouling and has been the subject of a number of investigations. [Watkinson et al. (1999)] ran experiments under inert and oxygenated conditions for a Canadian crude in a re–circulation heating loop to identify the role of oxygen in refinery preheater fouling. They found that, under oxygenated conditions the gum particle concentrations are increased due to autoxidation reactions, and the fouling rates are higher. [Watkinson (2005)] later noticed that trace quantities of impurities such as dissolved oxygen or suspended corrosion products add significantly to deposit formation.

[Srinivasan and Watkinson (2005)] summarized reported causes of fouling from crude oils:

- Impurities such as water, rust, and other particulates.
- Gum or polymeric species formed through oxidation of reactive species in the oils.
- Insoluble asphaltenes from self–incompatible oils or from blending.
- Iron sulfide formation.
- Coke formation due to reactions of polar fractions.

Several authors ([Wiehe, 2001a; Mason and Lin, 2003; Stark and Asomaning, 2003; Saleh et al., 2005a; Hong and Watkinson, 2009]) indicated asphaltene flocculation and deposition caused by asphaltene/oil incompatibility to be responsible for crude oil fouling, especially at high temperatures ([Eaton and Lux, 1984; Lambourn and Durrieu, 1986; Dickakian, 1989]). Asphaltenes, defined as the n–alkane insoluble/ toluene soluble fraction of the crude ([Watkinson, 2008]) have been described as the “cholesterol of the crude oil” and although they have been studied in a number of works ([Dickakian and Seay, 1988; Buenrostro-Gonzalez et al., 2004; Aguilera-Mercado et al., 2006]), there is ongoing debate among the scientific community on their exact structure ([Durand et al., 2010]). Compatibility was quantified by [Asomaning and Watkinson (1999)] via the colloidal instability index (CII):

\[
CII = \frac{\text{Saturates} + \text{Asphaltenes}}{\text{Aromatics} + \text{Resins}}
\]  

(2.3)
where the four different solubility classes can be determined experimentally by standard SARA analysis \cite{Hory2000}. At CII index $< 1$ no precipitation occurs. However, it has been argued that Equation 2.3 alone is not sufficient to predict asphaltene precipitation over a wide range of compositions thus Al-Atar and Watkinson (2001) included also the resin/asphaltene ratio as parameter influencing fouling.

It should be noted that, although asphaltene/oil compatibility issues plays an important role in deposition in PHTs, Wiehe (2001b) questioned that compatibility is the only issue related to asphaltenes depositions. He showed that asphaltenes do not require to be insoluble to produce fouling pointing out that:

- Crudes exist that are self–incompatible: they don’t need to be blended to produce fouling.
- Even compatible oils can undergo asphaltene fouling.

More recently, Venditti et al. (2009) characterised the deposits produced in lab–controlled conditions (through a micro–bomb reactor) finding evidence that contribution to fouling is not exclusive to asphaltenes but that heptane soluble fractions can also play an important role in the formation of fouling deposits. Discussion with refiners revealed that even crudes with just traces of asphaltenes do produce fouling in the hot end of the PHT. This is confirmed by industrial observations and experimental work by Saleh et al. (2005b) who studied fouling behaviour of an Australian crude oil with low sulfur, ash and asphaltene levels.

It should be noted that crude oil composition and its contaminants are not variables that can be manipulated whilst the process conditions, temperatures and, in particular, velocities can be adjusted by the designer in order to mitigate fouling.

From a modelling point of view, the number of components in the crude, the complexity of their interactions and uncertainties in the composition of the crude blend actually processed in the refinery makes it challenging describe from first principles crude deposition/removal. Research in this direction is currently under way but is, at the moment, in its infancy \cite{Sileri2009}.

2.4.4.2 Temperature

As a general rule, high temperatures are usually associated with the promotion of chemical reaction fouling and corrosion. Furthermore, temperature has a direct effect on the ageing speed of the foulant layer. The deposit may be hardened and become difficult to remove or, alternatively, become weaker and tend to spall under the influence of temperature and time.
There has been some debate (Polley et al. 2002a) in the literature over whether the rate of the fouling reaction is a function of surface (wall) temperature, \( T_w \), or rather the film temperature, \( T_f \), usually calculated as the average temperature between the bulk temperature, \( T_b \), and the wall one (Ebert and Panchal 1997):

\[
T_f = 0.5(T_b + T_w)
\]  

The temperature chosen to describe fouling rate dependence, is associated with the zone where the reaction is assumed to take place (i.e. Case 1, 2 or 3 in Section 2.4.2).

2.4.4.3 Pressure

Pressure is the least–studied parameter in heat exchanger fouling. Nevertheless, Asomaning et al. (2000) noted that pressure can have a significant effect on the fouling rate, especially in asphaltene precipitation during recovery of heavy crude oils. However, they noted it is not known whether the typical operating pressures in the laboratory and industrial fouling situations have an effect on the precipitation of asphaltenes or other heavy organics. Experimental data are lacking in literature.

2.4.4.4 Velocity and shear stress

Of all the variables, velocity is the one on which the designer has the greatest control (Bott 1995). An increase in velocity, on both sides of the exchanger, has a double–pronged effect on deposition by:

1. Increasing the wall shear stress.
2. Increasing the convective heat transfer coefficients.

The first is perhaps the more obvious effect on fouling: increased shear forces at the deposit/fluid interface impede fouling deposition and may even result in foulant removal. The role of shear stress in fouling behaviour is highlighted by a recent plot by Joshi et al. (2009) which relates fouling rates to shear stress for several heat exchangers in six different PHTs, covering a range of tube–side velocities from 0.9 m s\(^{-1}\) to 2.7 m s\(^{-1}\). The majority of the exchangers considered had a design shear stress range of 5–8 Pa. The graph shows that the higher the shear stress, the lower the fouling, as expected, but it is surprising that temperature appears to have no effect on fouling rates thus attributing a dominant role to shear stress.
The second is a less obvious but important effect that velocity has on fouling. An increase in velocity, assuming everything else remaining constant, produces an increase in the convective heat transfer coefficient thus a reduction in total thermal resistance. As a result, the wall temperature is reduced and fouling is thus reduced\(^7\). This is the principle exploited by fouling mitigation devices based on a fixed wire matrix inserted on the tube–side of industrial units (Ritchie et al., 2009). On the other hand, if the deposition involves mass transfer of insoluble species (e.g. Case 1a and 2a in Figure 2.8), higher velocities will increase the diffusion toward the surface in the presence of a concentration gradient thus enhancing deposition.

Controversial effects of velocity on initial fouling rate were reported by Crittenden et al. (1987a). At low surface temperatures the initial rate decreases with increasing flow rate. At high surface temperatures the opposite dependency was observed. They concluded that a combination of high surface temperatures and low flowrates can lead to mass transfer of deposit precursors to the surface becoming the rate determining step. This clashes with other observations, reported at the beginning of Section 2.4.4 that suggested adhesion or reaction are the rate determining steps. Industrial observations are that if the velocity is reduced, even for short periods, the result can be an increased deposition rate and, as a consequence, highly fouled surfaces. Once this is happened, even after the heat exchangers is brought back to normal operation, the deposits may have hardened their structure (aged) and not respond to increased velocities by detaching. This confirms the importance of maintaining the highest possible velocities allowed by other constraints given by an arbitrary earlier choice of allowable pressure drop (Butterworth, 2004) or by corrosion and vibration problems that may occur at large velocities (ESDU, 1989).

### 2.4.4.5 Surface conditions and roughness dynamics

The importance of surface conditions has been addressed in several articles (Crittenden and Kolaczkowski, 1979b; Zhao and Müller-Steinhagen, 2001; Forster and Bohnet, 2001; Santos et al., 2004; Kukulka et al., 2010). If the surface is corroded it not only provides resistance to heat transfer but it also creates sites that encourage deposition. Additionally, corrosion products released upstream become particulate fouling for downstream sections of the heat exchanger.

Another important aspect of the surface is its roughness as it affects the convective heat transfer coefficient (Walker and Bott, 1973). The disruption of the viscous sub-layer caused by a

\(^7\)See numerical example in Bott (1995) in which a two fold increase in velocity leads to 25°C lower wall temperature.
2.4 Basic science in the fouling process

rough surface generates an increase in the turbulence level compared to that of smooth surfaces (Yaglom and Kader [1974]) which in turn produces higher heat transfer coefficients. A constant value of equivalent sand roughness is typically used, calculated from shorthand correlations. However, not only the initial status of the clean surface matters, but also its changes over time. The accumulation of foulant material on heat transfer surfaces often results in a progressive increase in roughness, with associated effects on heat transfer coefficient and pressure drop.

Whilst in laminar flow the surface roughness has little effect on the friction factor and heat transfer coefficient (Shah and Dusan [2003]), it plays an important role in the turbulent regime typical of industrial applications.

Although the effect of roughness on the heat transfer coefficient is largely acknowledged in literature, the effect of fouling on surface roughness dynamics has received relatively little attention (Ceylan and Kelbaïyev [2003]). Enhancement of heat transfer due to an initial increase in surface roughness generated in fouling tests has been reported and analysed for particulate fouling by Crittenden and Alderman [1988], for crystallization fouling by Albert et al. [2009] and for corrosion fouling by Panchal [1988]. For chemical reaction fouling, most of the reported cases are qualitative. Bott [1990] noted that, due to the complex interaction of variables, no systematic study on the effects of roughness on fouling had been undertaken. However, some quantitative results have been presented. Cousineau et al. [1988] reported the increase in heat transfer coefficient for a Bayer process in which sodium aluminosilicate scales deposit with a kinetics of the second order. Yeap et al. [2004] noted that the apparent negative fouling resistance reported in the initial period (up to 40 h) of testing a crude oil by Knudsen et al. [1999] could be attributed to the progressive increase in surface roughness (Figure 2.11). Wilson and Watkinson [1996] reported both thermal and hydraulic roughness effects (from analysis of pressure drop measurements) in studies of autoxidation reaction fouling, while Asomaning et al. [2000] observed these in testing crude oils.

Quantitative modelling of roughness dynamics is in its infancy: for example, in their analysis of crude oil heat exchangers subject to fouling, Yeap et al. [2005] changed the surface roughness of clean tubes to that reported for bitumen by Kern [1988] to represent the foulant. An approach to modelling the increase in roughness due to fouling on tube surfaces was developed by Yiantsios and Karabelas [1994]. They proposed a population balance model based on a population of roughness elements to describe deposition and removal in crystallization fouling. However, their
focus was on the removal process and they did not discuss roughness in terms of hydrodynamics, pressure drop and more importantly, impact on heat transfer. To the author’s knowledge, no dynamic models exist for roughness effects in chemical reaction fouling, which is related to the paucity of experimental data. It should be pointed out that the dynamics of surface roughness are expected to apply mainly to laboratory testing, where more precise measurements of heat transfer are made, over short time–scales. Industrial applications feature larger timescales, so that short term variations in surface roughness are not noticed. Nonetheless, being able to capture this phenomenon is essential for the correct interpretation of accelerated fouling tests performed in pilot plants.

2.5 Fouling models

Fouling models are correlations that attempt to capture the dependency, discussed in the previous section, of fouling rate on process conditions and time. This section considers the development over the years of general fouling models and focuses in particular on chemical reaction models for crude oil fouling. Several reviews of fouling models for different mechanisms not covered here are available in literature ([De Deus, 1980] [Epstein, 1981a, 1988a] [Crittenden et al., 1987b] [Bott, 1995] [Wilson et al., 2005]).

2.5.1 General fouling models

Early attempts to model fouling in heat transfer equipment focused on developing rate models capable of explaining correlations between fouling rates and process conditions. One classical and simple way of dealing with fouling dynamics is based on the assumption that the fouling
2.5 Fouling models

resistance, $R_f$, grows asymptotically with time (Kern and Seaton [1959b]):

$$R_f = R^* (1 - e^{-a_1 t}) \quad (2.5)$$

where $R^*$ is the asymptotic value of the fouling thermal resistance and $a_1$ is a parameter. Equation 2.5 is an idealised fouling model and cannot capture fouling in a given unit when it departs from asymptotic behaviour. Moreover, it does not explain the variation of the fouling resistance as a function of process conditions.

Kern and Seaton (1959a,b) proposed to calculate the net mass of foulant deposited as a function of two competing mechanisms, namely deposition and removal. The difference between the rates of deposition, $\dot{m}_d$, and removal, $\dot{m}_r$, gives the net fouling rate:

$$\frac{dm_f}{dt} = \dot{m}_d - \dot{m}_r \quad (2.6)$$

which, in terms of fouling resistance, $R_f$, becomes:

$$\frac{dR_f}{dt} = \phi_d - \phi_r \quad (2.7)$$

where the deposition, $\phi_d$, and removal terms, $\phi_r$, are in $\text{m}^2 \text{K J}^{-1}$.

In particular, Kern and Seaton (1959b) proposed to calculate the thickness $\delta$ of the fouling layer as:

$$\frac{d\delta}{dt} = a_1 c_f \dot{m} - a_2 \tau \delta \quad (2.8)$$

where $\dot{m}$ denoted the mass flowrate whilst $a_1$ and $a_2$ are model constants. The deposition term is a function of the foulant concentration, $c_f$. The removal term assumes that deposits may be removed in chunks from the wall by effect of the shear action of the fluid, $\tau$, and is proportional to the layer thickness.

The Kern and Seaton model laid the foundations for capturing fouling as a function of process conditions and time. However, Equation 2.8 is a rather general fouling model which does not specifically take into account any particular fouling mechanisms. If the fouling mechanism is chemical reaction fouling, a model should take the kinetics of the reaction into account.
2.5 Fouling models

2.5.2 Chemical reaction fouling models

Watkinson and Epstein (1970) developed a transfer–adhesion–release model assuming that deposition was caused by mass transfer of suspended particles to the wall followed by adhesion:

$$\frac{dR_f}{dt} = a_1 \left(c_b - c_w\right) \exp\left(-\frac{E_f}{R_g T}\right) - a_2 u^2 C_f \delta$$

(2.9)

where $E_f$ denotes the activation energy of the fouling reaction, $u$ the bulk velocity, $C_f$ the friction factor and $a_1$ and $a_2$ denote coefficients in the equation. In Equation 2.9, the mass flux of foulant being deposited on the wall is assumed to be proportional to the difference between the particulate concentration in the bulk, $c_b$, and at wall $c_w$. Watkinson and Epstein showed that Equation 2.9 predicts the dependency of initial fouling rate on temperature as found in experiments. However, Crittenden et al. (1987b) suggested that Equation 2.9 does not predict the correct dependency of the asymptotic fouling factor on flow rate.

Taborek et al. (1972) used a simple Arrhenius kinetic in the deposition term which specifically accounts for its dependency on temperature:

$$\phi_d = \alpha \exp\left(-\frac{E_f}{R_g T_w}\right) (c_r)^k$$

(2.10)

where $\alpha$ denotes the Arrhenius pre–exponential term, $R_g$ the ideal gas constant and $c_r$ the concentration of the species reacting with reaction rate of $k^{th}$ order. In Equation 2.10, it is assumed that the chemical reaction producing fouling occurs at the wall ($T_w$ denotes the wall temperature). The removal term was assumed to be a function of a force balance between fluid shear and the strength of the deposit bonds:

$$\phi_r = a_2 \frac{\tau}{R_b}$$

(2.11)

where $R_b$ is defined as the “deposit bond resistance” and appears to be a difficult parameter to be estimated.

Fernandez-Baujin and Solomon (1976) developed a two–step model accounting for mass transfer and kinetics in the deposition of coke in steam cracking furnaces. They considered the
2.5 Fouling models

mass transfer flux of the precursor to the reaction site, \( N_{pr} \) as:

\[
N_{pr} = K_{pr}(c_{pr,b} - c_{pr,i})
\]  

where \( K_{pr} \) is the mass transfer coefficient and \( c_{pr,b}, c_{pr,i} \) the precursor concentrations in, respectively, the bulk and at the fluid/deposit interface. The fouling rate was then given by:

\[
\frac{dR_f}{dt} = \frac{1}{\rho_l \lambda_l} \left[ \frac{c_{pr,b}}{1/K_{pr} + 1/k} \right]
\]  

where \( \rho_l \) denotes the density of the foulant layer and \( \lambda_l \) its thermal conductivity. Crittenden and Kolaczkowski (1979b) extended this two–step model to include convection of the foulant back into the fluid bulk, \( N_f \):

\[
N_f = K_f(c_{f,i} - c_{f,b})
\]  

were \( K_f \) is the mass transfer coefficient. They calculated the thickness of the fouling layer, \( \delta \), as a function of the two mass fluxes:

\[
\frac{d\delta}{dt} = \frac{1}{\rho_l} (N_{pr} - N_f)
\]  

Assuming that \( c_{f,b} \) is very small they expressed the fouling resistance as:

\[
\frac{dR_f}{dr} = \frac{d(\delta/\lambda_l)}{dr} = \frac{1}{\rho_l \lambda_l} \left\{ \left[ \frac{c_{pr,b}}{K_{pr} + 1/k} \right] - \left[ K_f c_{f,i} \right] \right\}
\]  

Writing the mass transfer coefficients in terms of flowrate and physical properties using the Chilton and Colburn (1934) analogy Equation (2.16) becomes:

\[
\frac{dR_f}{dr} = \left[ \frac{c_{pr,b}}{\rho_l(d_i - 2\delta)^{1.8}Sc_{pr}^{0.67} + 1} \right] - \left[ \frac{0.607 \lambda_{pr,0.2} \mu^{0.8}}{\rho_l(d_i - 2\delta)^{1.8}Sc_{f,0.67} \mu f_{f,i}} \right]
\]  

where \( Sc \) is the Schmidt number. In this case deposition is a function of a first order reaction with an Arrhenius equation describing the rate–dependency on temperature and the effects of massflowrate on fouling are included. Crittenden and Kolaczkowski noted that for low temperatures, small tube diameters and large mass flowrates, the kinetics would be controlling in
2.5 Fouling models

Equation 2.17 whilst for high temperatures, large tube diameters and small mass flowrates, the precursor diffusion would be the controlling mechanism.

Crittenden and Kolaczkowski (1979a) further extended Equation 2.17 to consider the build-up of two layers (namely, tarry and coke) on the tube wall conceptualised by Atkins (1962). This is, noticeably, one of the first attempts to formalise in a mathematical way the ageing phenomenon (described in Section 2.4.3.5) by including its effect in Equation 2.7. They assumed that the increase in fouling resistance is governed by deposition of tarry layers but added two new terms to consider the interactions between the tarry and the coked layers:

\[
\frac{dR_f}{dr} = \phi_d - \phi_{tr} - \phi_{cr} - \phi_r
\]  
(2.18)

where \( \phi_{tr} \) and \( \phi_{cr} \) are, respectively, the fouling rate decrease by mass transfer of tars to the bulk of the fluid and by conversion of tarry layer to coke. By considering mass transfer and reaction kinetics in the system, they proposed the following form of the terms in Equation 2.18:

\[
\frac{dR_f}{dr} = \left[ \frac{1}{a_1(d_i - 2\delta)^{1.8} \exp\left(-E_{tr}/R_gT_{tr}\right)} \right] - \left[ \frac{a_3m^{0.8}}{(d_i - 2\delta)^{1.8}} \right] - \left[ \frac{a_4}{\exp\left(-E_c/R_gT_c\right)} \right] - \left[ \frac{a_5m^{0.8}R_f}{(d_i - 2\delta)^{3.8}} \right]
\]  
(2.19)

where \( T_{tr} \) and \( T_c \) denote, respectively, the temperature in the tarry and in the coke layer, \( d_i \) the tube inner diameter whilst \( a_i \) denote proportionality constants and other physical properties of the system. Crittenden et al. (1987b) used the equations above to model the experimental data for styrene deposition from kerosene by Crittenden et al. (1987a).

In his review of fouling models, Epstein (1981a) argued that there is a conceptual problem in defining the \( \phi_r \) term in Equation 2.7 as the \textit{removal} term due to re–entrainment. His argument was that as a foulant particle approaches the surface, it would not be deposited in first place because of the action of the fluid shear. He noticed how Kern himself, who first proposed the use of the term “removal”, in a later paper (Kern, 1966) re–defined it as a retardation process and called it \textit{suppression}. In this process, ageing is likely to play an important part as the structural change of the deposits to a harder material makes it difficult to remove. Wilson et al. (2005) noticed how in crude oil fouling there is no evidence that removal actually happens thus the word “suppression” is indeed more appropriate.
All the models reviewed so far have been validated (with limited success) against experimental data obtained under well defined, controlled laboratory conditions. Whilst this is important to improve understanding of the fouling process, the ultimate goal is to be able to predict fouling behaviour in industrial units. For this purpose, Crittenden et al. (1992) used plant data to fit the following relationship to refinery PHT data (i.e. fouling resistance calculated via the log mean temperature difference method summarised in Section 3.2):

$$\frac{dR_f}{dt} = \alpha \exp \left( - \frac{E_f}{R_g T_w} \right)$$

(2.20)

The authors found a value for the activation energy $E_f = 33 \text{ kJ mol}^{-1}$ and suggested that a value below $40 \text{ kJ mol}^{-1}$ indicates that both chemical and physical phenomena are important.

Epstein (1994) modified Equation 2.16 as follows:

$$\frac{dR_f}{dt} = \frac{1}{\rho l \lambda_l} \left[ \frac{K_f c_{p,b}}{1 + a_1 u^2 (C_f/2)(\mu/\rho)K_p \exp(E_f/R_g T_w)} \right]$$

(2.21)

where $\rho$ and $\mu$ denote the fluid density and dynamic viscosity respectively. Equation 2.21 was fitted to the experimental data by Crittenden et al. (1987a) with an average absolute deviation of 14.2%. Details on the regression accuracy were provided in the following paper by Vascaronáč and Epstein (1996).

### 2.5.3 Threshold fouling models

In a milestone conference article, Ebert and Panchal (1997) proposed the following form for the model in Equation 2.7:

$$\frac{dR_f}{dt} = \alpha \text{Re}^\beta \exp \left( - \frac{E_f}{R_g T_f} \right) - \gamma \tau$$

(2.22)

where the deposition term is as a function of the film temperature, $T_f$ (as opposed to $T_w$ in Equation 2.20) and the Reynolds number, Re whilst the suppression term depends on the wall shear stress, $\tau$. Parameters $\alpha = 8.3 \text{ K m}^2 \text{ W}^{-1} \text{ s}^{-1}$, $\beta = -0.88$, $E = 68,000 \text{ J mol}^{-1}$ and $\gamma = 4.03 \times 10^{-11} \text{ m}^3 \text{ N K}^{-1}$ were determined via regression to experimental data and are expected to vary between different crudes.

Equation 2.22 can be used to predict the film temperature, $T_f$, at which initiation of fouling would occur under the following assumptions:
Figure 2.12: Fouling threshold concept in heat exchanger design. If operating conditions are changed from A to B, the unit moves from a fouling to a no-fouling region.

1. The net deposition is given by formation minus suppression of foulant from the thermal boundary layer.
2. Foulant formed in boundary layer by a one-step reaction.
3. No concentration gradients of reactants in boundary layer.
4. Foulant transported by diffusion from the boundary layer to the bulk flow.
5. Linear temperature profile in the boundary layer.
6. Integrated reaction term expressed by film temperature in the boundary layer.
7. Rate of suppression independent of the film thickness.
8. Foulant removed from the thermal boundary layer by transport mechanisms and not from detachment process.

The model was developed after experimental evidence of the existence of a threshold for given operating conditions below which fouling would not occur. Since the threshold is given by the balance of the rate of deposition with the suppression one, its location can be determined by setting the rate to zero, equating the two terms and solving for \( T_f \), \( \tau \) and \( \text{Re} \). The importance of this is that it can be applied in a relatively simple way to the design of heat exchangers by determining a fouling threshold curve and changing design parameters so that operating conditions of the units are below it (Figure 2.12). This opened a new category of models defined as threshold fouling which have been used to take into account crude oil fouling when designing or retrofitting single units (Butterworth 2000; Polley et al. 2002b), whole PHTs (Yeap et al. 2001a; Bories and Patureaux 2003; Yeap et al. 2004; Polley et al. 2005) and to assist the scheduling of cleaning, thus improving network operability and mitigating costs related to
The threshold concept has also been implemented in the Poddar and Polley (1996) plot and exploited in commercial (ESDU 2000) and educational (Butterworth 2002) software to improve the design of heat exchangers (see Appendix C).

In a following work Panchal \cite{Panchal1999} determined a new set of constants using the experimental data for three different crudes and added the Prandtl number, $Pr$, to Equation \ref{eq:2.22} as this was seen to vary between 2.5 and 8.2. As for the previous model, in this new one the foulant is assumed to be removed from the boundary layer before it is deposited:

$$\frac{dR_f}{dt} = \alpha \text{Re}^\beta \text{Pr}^{-0.33} \exp\left(-\frac{E_f}{R_g T_f}\right) - \gamma \tau \quad (2.23)$$

In this new version of the model the regression with a larger data set returned lower values of parameters $\alpha = 0.0139$ K m$^2$ W$^{-1}$ s$^{-1}$, $\beta = -0.66$ and $E_f = 48,000$ J mol$^{-1}$ whilst $\gamma$ was not been changed from the original value of $4.03 \times 10^{-11}$ m$^4$ N K J$^{-1}$.

It should be noted that only 60% of experimental data points followed the fouling trend predicted by Equation \ref{eq:2.23} which was accepted as a “quite encouraging” agreement by the authors of the paper given the difficulty of obtaining high quality, reproducible data. However, Asomaning \textit{et al.} \cite{Asomaning2000} demonstrated that the model predicts field data with limited degree of success suggesting that this was due to the discrepancies existing between the laboratory data — obtained under controlled conditions — and the field data which tend to be situation–specific.

Polley \textit{et al.} \cite{Polley2002a} further modified Equation \ref{eq:2.23} assuming that the dependency of fouling on velocity is associated to transport phenomena and replaced the wall shear stress term, $\tau$, with the Reynolds number:

$$\frac{dR_f}{dt} = \alpha \text{Re}^{-0.8} \text{Pr}^{-0.33} \exp\left(-\frac{E_f}{R_g T_w}\right) - \gamma \text{Re}^{0.8} \quad (2.24)$$

The model with a new value for the exponent of the Reynolds number and the dependency on wall — rather than film — temperature, showed a better agreement with the experimental results by Knudsen and Hays \cite{Knudsen1997} compared to Equation \ref{eq:2.23}. The advantage of writing the suppression term as a function of Re number is that the need for the calculation of $\tau$ is removed. This enables to calculate fouling on the shell–side where shear stress can only be quantified with a CFD simulation (see section \ref{sec:2.24}).
Srinivasan and Watkinson (2005) fitted a simple correlation to experimental fouling data collected for three Canadian crudes in a re-circulation fouling loop:

\[
\frac{dR_f}{dt} = a_1 u_a^{-0.35} \exp\left(\frac{E_f}{R_e \hat{T}_f}\right)
\]  

(2.25)

where \(u_a\) denotes the annular velocity and \(\hat{T}_f\) is a modified film temperature weighted more heavily on the surface temperature:

\[
\hat{T}_f = 0.3T_b + 0.7T_w
\]  

(2.26)

the different definition of the film temperature allowed Srinivasan and Watkinson (2005) to better fit their rate data with Equation 2.25, achieving an accuracy of ±8%.

Saleh et al. (2005b) proposed a power–law equation to fit fouling data of a light Australian crude with a low asphaltene and sulfur contents obtained in a flow loop:

\[
\frac{dR_f}{dt} = a_1 P a_2 u^{a_3} \exp\left(-\frac{E_f}{R_e \hat{T}_f}\right)
\]  

(2.27)

where \(P\) denotes the pressure, \(a_1\) the power–law constant whilst \(a_2\) and \(a_3\) are the exponents of, respectively, pressure and velocity.

A further modification of Equation 2.24 was proposed by Nasr and Givi (2006):

\[
\frac{dR_f}{dt} = \alpha Re^\beta \exp\left(-\frac{E_f}{R_e \hat{T}_w}\right) - \gamma Re^{0.4}
\]  

(2.28)

in which the dependency on the Pr number is dropped. A better fit of fouling data by Saleh et al. (2005b) was shown by this form of the equation.

Yeap et al. (2004) compared the performance of three models in predicting fouling resistances calculated using 10 sets of data collected from experimental and plant measurements. The models considered were a modified version of the model by Epstein (1994) and other two models by Panchal et al. (1999); Polley et al. (2002a). Results of the comparison, reported in Figure 2.13, judged “only fair” by the authors, show that roughly only half of the (few) data point considered stay within ±50% error for the models by Panchal et al. (1999); Polley et al. (2002a) with an overall better agreement achieved by the modified Epstein (1994)’s model.

It should be noted that models reviewed so far and summarised in Table 2.3, aim at explaining
### Table 2.3: Summary of mathematical models relevant to chemical reaction fouling.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Fluid</th>
<th>System represented</th>
<th>Mass transfer</th>
<th>Ageing</th>
<th>Main Assumptions</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nelson (1939a)</td>
<td>Crude</td>
<td>Furnace tube</td>
<td>x</td>
<td>✓</td>
<td>Fouling rate dependent upon thickness of thermal boundary layer.</td>
<td>No removal term considered.</td>
</tr>
<tr>
<td>Kern and Seaton (1959b)</td>
<td>Water</td>
<td>HEX</td>
<td>x</td>
<td>x</td>
<td>Removal due to shearing action.</td>
<td>Conceptual model of fouling rate given by mass deposition - removal</td>
</tr>
<tr>
<td>Atkins (1962)</td>
<td>Crude</td>
<td>Furnace tube</td>
<td>✓</td>
<td></td>
<td>Deposit made up of two distinct layers.</td>
<td>Dependency of initial fouling rate on temperature predicted correctly but not of asymptotic fouling factor on flow rate.</td>
</tr>
<tr>
<td>Watkinson and Epstein (1970)</td>
<td>Hydrocarbons</td>
<td>HEX</td>
<td>✓</td>
<td>x</td>
<td>Fouling controlled by mass transfer and adhesion of suspended particles</td>
<td>No removal but considered ageing.</td>
</tr>
<tr>
<td>Crittenden and Kolaczkowski (1979a)</td>
<td>Hydrocarbons</td>
<td>Heated tube</td>
<td>✓</td>
<td>✓</td>
<td>$R_f$ governed by deposition of tarry layers and their interactions with coked layers.</td>
<td>One of the first attempts to formalise in a mathematical ageing.</td>
</tr>
<tr>
<td>Crittenden and Kolaczkowski (1979b)</td>
<td>Hydrocarbons</td>
<td>Heated tube</td>
<td>✓</td>
<td>x</td>
<td>1st order kinetics and mass transfer control.</td>
<td>Several parameters of difficult evaluation.</td>
</tr>
<tr>
<td>Crittenden et al. (1987a)</td>
<td>Hydrocarbons</td>
<td>Heated tube</td>
<td>x</td>
<td>x</td>
<td>Initial fouling rate is 1st order kinetics and mass transfer controlled.</td>
<td>Estimate model parameters from plant data.</td>
</tr>
<tr>
<td>Crittenden et al. (1992)</td>
<td>Crude</td>
<td>HEX</td>
<td>✓</td>
<td>x</td>
<td>$R_f$ controlled by reaction kinetics as a function of wall temperature.</td>
<td>Good agreement with experimental data by Crittenden et al. (1987a).</td>
</tr>
<tr>
<td>Epstein (1994)</td>
<td>Crude</td>
<td>Heated tube</td>
<td>✓</td>
<td>x</td>
<td>Mass transfer controlled.</td>
<td>Predicts the $T_f$ at which initiation of fouling would occur at a given velocity.</td>
</tr>
<tr>
<td>Ebert and Panchal (1997)</td>
<td>Crude</td>
<td>Heated tube</td>
<td>x</td>
<td>x</td>
<td>Fouulant formed in boundary layer by a one–step reaction. Rate of suppression independent on the film thickness.</td>
<td>Added the Pr number to Ebert and Panchal (1997). Only 60% of data followed the fouling trend predicted by the correlation.</td>
</tr>
<tr>
<td>Panchal et al. (1999)</td>
<td>Crude</td>
<td>HEX</td>
<td>x</td>
<td>x</td>
<td>Fouulant is removed from the boundary layer before it is deposited.</td>
<td>Can be used to predict shell–side fouling without the use of CFD.</td>
</tr>
<tr>
<td>Polley et al. (2002a)</td>
<td>Crude</td>
<td>HEX</td>
<td>x</td>
<td>x</td>
<td>Modification of the E–P model assuming deposition as a function of $T_w$, not $T_f$ and suppression term being diffusion–related thus a function of Re, not $\tau$.</td>
<td>Fitted on fouling data of three sour Canadian crude oils.</td>
</tr>
<tr>
<td>Srinivasan and Watkinson</td>
<td>Crude</td>
<td>Heated tube</td>
<td>x</td>
<td>x</td>
<td>$R_f$ is a function of film temperature weighted more heavily on $T_w$.</td>
<td>Fitted on data of a light Australian crude with low asphaltene and sulfur contents.</td>
</tr>
<tr>
<td>Saleh et al. (2005b)</td>
<td>Crude</td>
<td>Heated tube</td>
<td>x</td>
<td>x</td>
<td>$R_f$ follows a power–law.</td>
<td>Better fit than Polley et al. (2002a) on data by Saleh et al. (2005b).</td>
</tr>
</tbody>
</table>
2.6 Concluding remarks

From the review of the literature presented in this chapter it is clear that crude oil fouling is a major problem for oil companies as it results in enormous costs, environmental problems and

![Figure 2.13: Comparison between fouling models performed by Yeap et al. (2004) using models by (a) Epstein (1994), (b) Panchal et al. (1999) and (c) Polley et al. (2002a).](image)

with one simple equation all the complex phenomena described in Section 2.4.1 and their interactions summarised in Figure 2.10. Moreover, they rely on calculations of $R_f$ based on simple lumped models and are subject to several assumptions summarised in Table 2.4.

It is therefore not surprising that they cannot explain experimental data with great accuracy. Unless a rate model is integrated with a thermo–hydraulic description of the unit it would not be capable of capturing the complexity of the interactions existing in the system.

### Table 2.4: Summary of assumptions often used in fouling models.

<table>
<thead>
<tr>
<th>Assumption</th>
<th>Why used</th>
<th>Limitations</th>
</tr>
</thead>
<tbody>
<tr>
<td>No temperature variation across the HEX</td>
<td>Not integrated with a thermal model.</td>
<td>Errors in the calculations of heat transfer coefficients.</td>
</tr>
<tr>
<td>Constant physical properties</td>
<td>Variability of crudes compositions</td>
<td>Affects the calculations of the convective heat transfer coefficients and overall heat balance.</td>
</tr>
<tr>
<td>Constant heat transfer coefficient</td>
<td>Temperature distribution is not known.</td>
<td>Incorrect temperature driving forces being used.</td>
</tr>
<tr>
<td>No localized fouling</td>
<td>Temperature distribution is not known</td>
<td>Fouling process not fully described.</td>
</tr>
<tr>
<td>No shell–side fouling</td>
<td>Removes the need for shell–side calculations.</td>
<td>Only valid if tube–side fouling is dominating.</td>
</tr>
<tr>
<td>Heat of reaction is negligible</td>
<td>Detailed reaction kinetics not known.</td>
<td>Valid in most cases.</td>
</tr>
<tr>
<td>Ageing effects neglected</td>
<td>No validated ageing models exist, kinetics of ageing reaction not yet fully understood.</td>
<td>Spatial–temporal variation in thermal conductivity is not captured.</td>
</tr>
</tbody>
</table>
health and safety hazards.

Despite several experimental studies have been undertaken, little is known regarding the chemical reactions that produce precursor and fouling species in crude oil fouling. Complex chemical and physical phenomena that take place and interact with one another are extremely difficult to identify and isolate. However, there is evidence that several variables, such as crude composition, temperature, velocity and surface conditions, have an effect on fouling rates.

Key facts highlighted in the literature review are:

- Fouling is particularly severe at the hot end of the PHT where chemical reaction fouling is suspected to be the primary mechanism.
- Whilst it is important to consider the induction period and the role of roughness dynamics in interpretation of data obtained for short lab–scale experiments, ageing plays a more important role in capturing the fouling behaviour of industrial units operated for long periods.
- Heavy, sour crudes have a higher fouling propensity.
- The higher the operating temperature, the higher the fouling rate. The opposite it true for velocity.

Over the years, general fouling models have evolved and increased in complexity to account for specific fouling mechanisms. Models capable of capturing fouling dynamics as a function of operating conditions have been specifically developed for crude oil fouling. However, they rely upon heavy assumptions and often do not provide satisfactory accuracy in predicting the behaviour of industrial heat exchanger units. The following chapter will review the attempts made in literature to overcome these limitations in the design and modelling of heat exchangers and heat exchanger networks.
Chapter 3

Design, monitoring and modelling of heat exchangers and their networks: a review

Synopsis

This chapter examines traditional and emerging methodologies for heat exchanger design (Section 3.2) and fouling monitoring (Section 3.3). Heat exchanger network synthesis methodologies are discussed in Section 3.4. Detailed heat exchanger models, developed to improve existing design practices are reviewed in Section 3.5. Finally the conclusions in Section 3.6 summarise the outcomes of the literature review and set the basis for the development of the thesis.
3.1 Introduction

The previous chapter discussed the basic science of fouling and highlighted that the complex chemical and physical aspects of fouling deposition are highly dependent on local conditions (e.g. temperature, velocity etc.) which, in turn, are determined by the design of the heat exchangers and the arrangement of these heat exchangers in the pre–heat train. Here, the basic design and monitoring methodologies of heat exchangers (HEXs) and heat exchanger networks (HENs) are reviewed with particular focus on how fouling is accounted for. A promising way of overcoming these limitations is to capture the fouling behaviour as a function of process conditions and time. For this purpose two key ingredients are essential: a fouling rate model that captures the dynamics of the fouling process as a function of local conditions (previously discussed in Section 2.5) and a thermo–hydraulic model for heat exchangers capable of providing accurately such conditions (Section 3.5).

3.2 Heat exchanger design methodologies

The basic design of shell–and–tube heat exchangers was introduced in the early 1900s (Taborek, 2002a) but it was not until 1941 that the Tubular Exchangers Manufacturers Association (TEMA) produced a document to standardise the mechanical design thus improving safety, quality control, communication between parties and lowering costs. Although attention has been paid to improving some aspects of the design (e.g. baffle spacing: Li and Kottke (1998); Saffaravval and Damangir (1995); Eryener (2006)) and new methodologies, reviewed in Section 3.2.2, that approach the design to include fouling dynamics are emerging, the basic design practice has not changed much since then (Morton, 1960). The use of the latest version (9th edition, 2007) of the original TEMA document is considered a standard practice in industry all over the world.

Details of traditional design methodologies can be found in several publications (e.g. ESDU (1994); Hewitt (2002, 2007)). There exist mainly two design methodologies (Kakac and Agrawal, 1988), one based on the log mean temperature difference (LMTD), reviewed e.g. by Taborek (1978), the other on $\varepsilon$–NTU approach by Kays and London (1964), reviewed e.g. by Smith (1979). Although the latter approach has several benefits against the LMTD approach (e.g. it does not require initial guesses of inlet temperatures), the way in which fouling is considered in both is equivalent. For the purposes of illustrating the limitations given by traditional approaches,
3.2 Heat exchanger design methodologies

The LMTD methodology will be briefly described below.

A typical design problem is to find the required surface area for a given heat duty. Usually, the heat duty, $Q$ (in W), is calculated via an overall heat balance on the two sides of the exchanger:

$$Q = \dot{m}_h c_{p,h} (T_{in}^h - T_{out}^h) = \dot{m}_c c_{p,c} (T_{in}^c - T_{out}^c)$$ \hspace{1cm} (3.1)

where $\dot{m}_h$ and $\dot{m}_c$ denote the mass flowrate (in kg s$^{-1}$) of, respectively, the hot and the cold fluid of specific heat capacity $c_{p,h}$ and $c_{p,c}$ (in J kg$^{-1}$ K$^{-1}$). In Equation 3.1 $T_{in}^h$ and $T_{in}^c$ denote, respectively, the inlet hot fluid temperature whilst $T_{out}^h$ and $T_{out}^c$ denote the outlet temperatures for the two fluids.

The heat transferred between the two fluids is also given by:

$$Q = US f_t \Delta T_{lm}$$ \hspace{1cm} (3.2)

Where $U$ denotes the overall heat transfer coefficient in W m$^{-2}$ K$^{-1}$, $S$ the surface area in m$^2$, $f_t$ a dimensionless coefficient that takes into account configurations departing from pure counter–current flow and $\Delta T_{lm}$ the mean temperature driving force defined as:

$$\Delta T_{lm} = \frac{(T_{in}^h - T_{out}^c)}{\ln \left( \frac{T_{in}^h - T_{out}^c}{T_{out}^h - T_{in}^c} \right)}$$ \hspace{1cm} (3.3)

The overall heat transfer coefficient is given by the sum of the individual thermal resistances. For a clean heat exchanger it can be calculated based on the outer surface of the tube as:

$$\frac{1}{U_c} = \frac{S_o}{S_i h_t} + \frac{S_o \delta_w}{S_m \lambda_w} + \frac{1}{h_s}$$ \hspace{1cm} (3.4)

where $h_t$ and $h_s$ are, respectively, the tube–side (inner) and shell–side (outer) convective heat transfer coefficient, $S_i$ and $S_o$, the inner and outer heat transfer area. The thickness of the metal wall is $\delta_w$ and $\lambda_w$ its thermal conductivity. In Equation 3.4 $S_m$ is the logarithmic mean area:

$$S_m = \frac{S_o - S_i}{\ln(S_o/S_i)}$$ \hspace{1cm} (3.5)

Acknowledging that heat transfer is impaired by fouling, the traditional methodology prescribes to include in Equation 3.4 the two tube–side and shell–side thermal resistances, namely
3.2 Heat exchanger design methodologies

**Figure 3.1:** Temperature profiles on a heat transfer surface and nomenclature used.

\[ R_{f,t} \text{ and } R_{f,s}, \text{ added by the presence of fouling layers (of thickness } \delta_t, \text{ and } \delta_s \text{ respectively}): \]

\[
\frac{1}{U} = \frac{S_o}{S_i h_i} + \frac{S_o}{S_i} R_{f,t} + \frac{S_o}{S_m} \lambda_w + R_{f,s} + \frac{1}{h_s} \quad (3.6)
\]

The physical significance of the nomenclature is summarised in the Figure [3.1].

As a result of including fouling resistances in the calculation of the overall heat transfer coefficient (Equation [3.6]), the surface area required for the given duty is increased. Moreover, several uncertainties are often buried in the specification of the fouling resistances \( R_{f,t} \) and \( R_{f,s} \) (Chenoweth, 1988b). These may include the values of physical properties used in the calculations of the heat balances in Equation [3.1] the value of the correction factor for departure from pure counter–current flow, \( f_t \), etc.

Fouling is a central factor that influences the design of the heat exchangers (Gram, 1960; Hewitt, 2002). Once an exchanger has been designed, constructed and commissioned, the user has to live with the economic impact of its operation and maintenance during its useful life that typically spans 20-30 years (Sheikh et al., 2000). Guidelines have been suggested to deal with fouling (Taborek, 1979; Chenoweth, 1988a; Bott, 1997; 1995; Hewitt, 2002; Nesta and Bennett, 2004; Bennett et al., 2007) and case studies have been shown (Al-Bagawi and Said, 2001) that succeed in mitigating it, but these are based on heuristics and not on a sound systematic approach.

When using Equation [3.6] the problem arises of which value to attach to \( R_{f,t} \) and \( R_{f,s} \). As it was pointed out in previous sections, different fluids, at different process conditions foul in different ways. Traditional heat exchanger design methodology has relied for the past 70 years
on values provided by TEMA (1941). Values for the TEMA fouling resistances of typical PHT streams are reported in Table 3.1. These ‘fouling factors’ are perceived in industry as ‘safety’ factors that prevent the heat exchanger from losing performance over time. However, the use of the TEMA tables attracted criticism over the years by several authors (Epstein, 1983; Rabas and Panchal, 2000; Bott, 2001; Bennett et al., 2007) for a number of reasons discussed in the next section.

### 3.2.1 Criticism to the fouling factor design approach

Chenoweth (1997) listed 14 points limiting the fouling factors approach. He describes the developments over the years of the first edition of the TEMA tables questioning their very origin. He reported that no written records of the original source could be located by TEMA itself and he was able to track the origins back to a committee composed by eight experts.

Another criticism, often found in literature, regards the meaning of the values provided. The TEMA document states that the specified fouling resistances are a minimum value to be used in the design without reporting the operating conditions at which this value should be used. Epstein (1983) highlighted that there is inadequate indication of which value they are representing: on one hand these cannot be steady state values as fouling resistance develops with time, on the other hand, if they reflect the time of operation this time is not stated. These information, he pointed out, are needed to make an adequate economic evaluation.

Furthermore, Chenoweth (1997) highlighted that, when the tables were originated, a three–month run in a refinery was considered a great success. This time period is definitely not considered satisfactory anymore as refinery aim at operating over 4 to 5 year runs.

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2 It should be noted that the TEMA are not the only fouling factor values available. Other tables exist in literature (Nelson, 1958) and often companies use values based on in–house experience.

3 This version clashes with that by Kern, reported by Somerscales (1990), who proposed that they were originated by E.N. Seider in 1937.
Not only the TEMA fouling factors have a controversial history, but there is also debate on their future. Chenoweth (1990) reported fundamental disagreement within the members of a joint committee comprising experts from TEMA and HTRI on how fouling should be incorporated in the design of heat exchangers. Whilst the majority was supporting the use of the fouling resistances, some suggested that the use of 20–25% excess area is an easier and more appropriate way of dealing with fouling. This latter approach is also supported by Bennett et al. (2007).

Regardless of the historical and philosophical considerations on the TEMA tables, there is consensus on the following essential limitations:

- They barely recognize the variation of the fouling resistance with process variables (e.g. fluid velocity, bulk and surface temperature, crude composition).
- No dynamics is taken into account. An asymptotic fouling rate is considered even if most fouling–resistance curves are essentially linear in nature.
- Fouling is considered as if at start–up it was instantaneously reaching a steady–state with a fixed value of $R_f$.

The last two points (a direct consequence of the first one) imply that the designer is forced to select a bigger surface area for a given heat duty than that required for a clean heat exchanger. This not only increases the capital expenditure for the unit and for its foundations, but it also affects in a negative way the fouling process itself. The initial thermal over–performance (given by a larger surface area) produces higher initial temperatures and is usually adjusted by the use of a bypass which in turn reduces the velocity and shear stress within the unit. As a consequence of higher temperatures and lower velocities fouling is actually exacerbated.

Over–design is so rooted in industry that very often extra surface area is built into the design without any discussion or input from the refinery (Jones and Bott 2001a). As a demonstration of the ineffectiveness of this design philosophy, Yap (2003) reports a study of refinery fouling data by Jones and Bott (1999) which showed that the thermal resistances at the beginning of the fouling period for all the exchangers were on average 2.5 times greater than the fouling factors recommended by TEMA and by a factor of 3 over an eight month period. To keep increasing the ‘fouling allowance’ is definitely not the solution as this would generate design with larger surface areas which, in turn, will produce even higher temperatures or lower velocities, thus more fouling. New approaches to break this ‘self–fulfilling prophecy’ (as defined by Chenoweth (1988b) and Hays (1989)) are therefore required.
As noted by Fryer and Slater (1985), chemical reaction fouling does not occur evenly throughout the heat exchangers as it depends on local temperature conditions. Figure 3.2 visually substantiates this statement showing that the extent of fouling in different passes (a) and within the same pass (b) is substantially different. The use of lumped overall heat balances (Equation 3.1) prescribed by the traditional LMTD methodology, clearly fail in capturing this localised effects. However, the limitations of the used of lumped models are not confined to the way fouling is dealt with (Gardner and Taborek, 1977) but also reflect on the accuracy of the calculations of the heat transfer coefficient and the physical properties (often kept constant not only with respect to space, but also with respect to temperature).

### 3.2.2 New approaches

Whilst the calculations described above, together with those for the physical properties and the heat transfer coefficients, are simple enough to be performed by hand, automating the design via computer calculations is definitely desirable. Moreover, the implementation in computer programs opens the possibility of finding a mathematical optimum with respect to a certain design objective. Early programs (Tayyabkhan, 1962; Fontein and Wassink, 1978) allowed the rapid rating and design of heat exchangers via iterative procedures and included strategies to minimise costs. However, these were based on simple heat balances, used several assumptions on physical properties and featured crude optimisation methodologies to overcome the challenges
posed by the discrete nature of some design variables (e.g. number of tubes, baffles, etc.).

With recently developed optimisation techniques it has become possible to use a sound optimisation framework for the design of heat exchangers. These include the use of both non deterministic (e.g. genetic algorithm\textsuperscript{4}) as well as deterministic (e.g. mathematical programming) methods. In particular, optimisation methodologies based on mixed integer non linear programming (MINLP) allow the determination of non continuous variables such as the number of tubes, baffles etc. Table 3.2 reports a summary of optimisation approaches to the design of heat exchangers which includes the objective function, the design variables used in each case together with some remarks on how fouling is accounted for. With only one exception (discussed later), none of the optimisation approaches reviewed accounts for fouling dynamics.

A different (graphical) approach that reduces the computational effort needed by the conventional design methodologies and has the advantage of visualising several design options in one graph was proposed by Poddar in 1990 and later extended by Poddar and Polley\textsuperscript{[1996]} and Butterworth\textsuperscript{[1996]}. This methodology consists in plotting the tube count versus tube length in a two–dimensional graph, thus determining the region (the design space or envelope) of all exchanger designs that satisfies the constraints of maximum and minimum tube–side velocities, maximum allowable pressure drops, shell diameters, and tube lengths. Muralikrishna and Shenoy\textsuperscript{[2000]} used the same approach, based on Kern’s equations\textsuperscript{[Kern, 1988]} but also included targets for minimum area and cost designs. Serna-González et al.\textsuperscript{[2006]} improved accuracy of predictions implementing the Bell–Delaware method for the calculation of shell–side heat transfer coefficient and pressure drops as detailed in Taborek\textsuperscript{[2002a]}. The graphical representation provided by the design space methodology has the great advantage of supporting the designer with clear guidance regarding the influence of different design options and constraints (e.g. allowable pressure drop) on required geometry.

All the new methodologies presented thus far do not include fouling dynamics and still rely on fixed fouling factors to determine the area required for the given heat duty. Acknowledging the limitations in the use of fouling factors, different approaches have been proposed in literature. Pope et al.\textsuperscript{[1978a,b]} included fouling in the problem statement of the optimisation approach proposed to design heat exchangers in geothermal power plants. However, fouling was

\textsuperscript{4}Genetic algorithms were first proposed by John Holland in the early 1970s. These algorithms were inspired by the mechanism of natural selection in competitive environment where stronger individuals are selected for a particular task. Whilst this approach, detailed in Tayal et al.\textsuperscript{[1998]}, does not guarantee global optimality it offers significant savings in computational costs.
### Table 3.2: Summary of optimisation approaches to heat exchanger design. Symbols reported in Nomenclature.

<table>
<thead>
<tr>
<th>Author</th>
<th>Optimisation algorithm</th>
<th>Objective function</th>
<th>Design variables</th>
<th>Fouling dynamics</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fontein and Wassink (1978)</td>
<td>Steepest descend method</td>
<td>Depreciation and operating costs</td>
<td>$D_s, \text{NTU, } P_c, d_o$</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Pope et al. (1978a,b)</td>
<td>Proprietary</td>
<td>Total annual cost including W, maintenance, downtime</td>
<td>$\Delta T_{pp}, N_D, \Delta P_t, \Delta P_s$</td>
<td>Linear model</td>
<td>Developed for geothermal systems</td>
</tr>
<tr>
<td>Sun et al. (1993)</td>
<td>Flexible tolerance</td>
<td>Total entropy generation</td>
<td>$d_o, L, D_s, L_{bc}, B_c, N_b, N_t$</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Keppich and Kohoutek (1994); Keppich and Zagemann (1995)</td>
<td>2nd order derivatives</td>
<td>Capital, operating and maintenance annual costs for HEX and pumps</td>
<td>$N_t, L, D_s, N_b, L_{bc}$</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>Rao et al. (1991, 1996)</td>
<td>Search method</td>
<td>Cost, weight and volume</td>
<td>$D_s, d_o, L_{tp}, L_{bc}$</td>
<td>x</td>
<td>Coupled with HTRI design program.</td>
</tr>
<tr>
<td>Chaudhuri et al. (1997)</td>
<td>Simulated annealing</td>
<td>S or purchased cost index</td>
<td>$N_s, N_p, d_o, L_{tp}, L, \theta_{tp}$</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>Tayal et al. (1998)</td>
<td>GA</td>
<td>$S$ or purchase cost</td>
<td>$L, \theta_{tp}, d_o, L_{tp}, N_s$, baffle &amp; shell type, shell angle, vibration</td>
<td>x</td>
<td>First GA application to design of shell-and-tube.</td>
</tr>
<tr>
<td>Mizutani et al. (2003)</td>
<td>MINLP</td>
<td>Total annualized investment and operating costs</td>
<td>$N_s, N_p, d_s, d_p, N_b, \theta_p$, head type, fluid allocation.</td>
<td>x</td>
<td>Introduced Bell–Delaware method.</td>
</tr>
<tr>
<td>Ponce-Ortega et al. (2006)</td>
<td>MINLP</td>
<td>Investment cost</td>
<td>$N_s, S, f_l, \text{LMTD, } \epsilon, \text{param}$</td>
<td>x</td>
<td>Multiple shell units</td>
</tr>
<tr>
<td>Selbaş et al. (2006)</td>
<td>GA</td>
<td>Capital, operating and maintenance costs</td>
<td>$d_s, \theta_{tp}, N_p, D_s, B_c, L_{bc}$</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>Ravagnani and Caballero (2007)</td>
<td>MINLP</td>
<td>Costs including $S$, W</td>
<td>$d_s, d_p, L_{tp}, L, N_p, N_s, D_s, D_{col}$, $N_t, N_b, B_c, L_{bc}$</td>
<td>x</td>
<td>Implemented TEMA standards.</td>
</tr>
<tr>
<td>Costa and Queiroz (2008)</td>
<td>Search method</td>
<td>Minimum area</td>
<td>$D_s, d_s, N_p, L, B_c, L_{bc}$</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>Fesanghary et al. (2009)</td>
<td>Harmony search algorithm</td>
<td>Capital and operating costs</td>
<td>$D_s, d_s, N_p, \theta_p, P_s, L/D_s, B_c$, $L_{bc}/D_s, N_{bc}$, materials of construction</td>
<td>x</td>
<td>Sensitivity analysis on geometric parameters.</td>
</tr>
<tr>
<td>Ravagnani et al. (2009)</td>
<td>Particle Swarm</td>
<td>Cost for $S$ and $W$ or $S$</td>
<td>$L, D_s, D_{col}, d_s, L_{tp}, \theta_p, N_p, N_s$, fluid allocation</td>
<td>x</td>
<td>Implemented TEMA standards.</td>
</tr>
</tbody>
</table>
simplistically assumed to be linear.

The design space method was also extended to account for crude oil fouling dependence on temperature and velocity by Butterworth (2002) and ESDU (2000). They implemented the Ebert–Panchal fouling model (Equation 2.22) in their respective software, DEVIZE and Express Plus (see Appendix C). The estimation on fouling parameters is performed by fitting values of the fouling resistance calculated (via the LMTD method) from plant measurements. Polley et al. (2009a) used this approach to propose a design methodology that allowed the identification of geometries providing acceptable fouling levels throughout a pre–determined operating period.

Shilling et al. (2009) proposed a risk–based design margin methodology aimed at quantitatively identify uncertainties related with the design process. According to this new approach, area margins are still added but the way these are determined take into account errors in the heat transfer correlations, probability and severity of fouling and operating uncertainties related to the specific process. Whilst this is an attempt of improving the fouling factor approach, this approach still requires a good level of engineering judgment and experience, for example, in determining the fouling propensity of a particular service.

### 3.3 Fouling monitoring techniques

Monitoring heat exchanger fouling consists in the use of available plant measurements (typically, the four temperature measurements and the two flowrates) needed to calculate the LMTD (Equation 3.3) and heat duties (Equation 3.1 on each side of the unit) to quantify the extent of the extra resistance to heat transfer produced by the presence of the low–conductive deposits.

Monitoring of fouling has long been recognised as a pivotal activity in plant operations. Gunness and Baker (1938) described a simple monitoring procedure based on the LMTD concept which is still in use by refineries worldwide. Over the years, fouling monitoring methodologies (Jones and Bott 2001b; Glen et al. 2001) became more sophisticated but remain substantially based on the same simple overall heat balances and require several assumptions which, inevitably, affect the accuracy of calculations. For example, the very presence of the fouling layer reduces the cross–sectional area thus calculations made by using the clean tube diameter are bound to underestimate the values of velocity, pressure drops and wall shear stress. Other authors acknowledged that errors are introduced in the estimation of fouling resistance when using
Figure 3.3: Fouling monitoring over 200 days based on LMTD methodology for a 2 shells unit (2 tube pass per shell) from a UK refinery. Inlet and outlet temperatures are shown in (a). When process conditions are such that temperature crossing happens, the fouling resistance cannot be calculated (b) and is automatically set to 0.

Traditional calculations (Glen et al., 1999). Merry and Polley (1981) discussed the difficulties in obtaining accurate estimation of the fouling resistances in four heat exchangers associated to a nitrogen compressor. They reported an error in the difference between heat duty on the tube–side and shell–side of around ±7% and suggested that calculations of fouling resistances have larger errors. Crittenden et al. (1992) clearly showed how errors in plant measurements and heat duty calculations can readily propagate to give large errors in the values of the fouling resistances. They assumed an error of ±1% in the measured flowrates, ±1°C in the temperatures and provided a way of assessing the error in the calculations of the fouling resistance, estimated in ±20%.

Another major limitation in using the LMTD approach, which seems not to have received much attention in literature, is that it fails to provide a value for the fouling resistance if temperature crossing happens in the unit being monitored. Figure 3.3 reports one such example
for a typical heat exchanger in a UK refinery. When the tube–side inlet and the shell–side outlet temperature cross (Figure 3.3(a)), the argument of the logarithm at the denominator in Equation 3.3 becomes negative. As a result, no value can be calculated for $R_f$ (reported as 0 in Figure 3.3). For this particular unit, process conditions are such that temperature crossing is a frequent event, occurring in 851 days over a monitoring period of 1819 days available (ca. 47% of data).

Despite all the discussed limitations, most refineries still rely on the log mean temperature difference approach as monitoring methodology for its simplicity to use. Howarth et al. (1999) discussed the importance of having appropriate tools for fouling monitoring and the barriers to the technology transfer of these tools to industry. It should be pointed out, though, that oil companies are now putting effort in improving the way they monitor fouling especially in CDUs (Liporace and de Oliveira, 2007).

### 3.4 Heat exchanger network synthesis methodologies

The aim of heat exchanger network (HEN) synthesis is to determine the optimal interconnection of heat exchanger units, together with the optimal design of these units, with the objective of maximising energy integration between streams in a given process that need to be heated with those that need to be cooled. The HEN synthesis problem was introduced by Ten Broeck (1944) although it was more rigorously defined by Masso and Rudd only in 1969. Since then, research in this area lead to many substantial developments aimed at maximising energy efficiency.

Extensive reviews of different approaches in HEN synthesis are available in literature (Fryer, 1988a; Furman and Sahinidis, 2002). Given the large number of publications dealing with this subject (Furman and Sahinidis, 2002 identified over 460 relevant papers), here the discussion will be limited to the industry standard, the so called “Pinch Technology” (Linnhoff and Hindmarsh, 1983), and to a brief overview of the new approaches based on advanced mathematical programming methodologies (Papoulias and Grossmann, 1983) with particular focus on treatment of fouling.

#### 3.4.1 Pinch Technology

The origin of Pinch Technology (PT) is controversial. According to Ebrahim and Kawari (2000), it was developed in the late 1970s by Ph.D. student Bodo Linnhoff from Imperial Chemical
3.4 Heat exchanger network synthesis methodologies

Industries (ICI) under the supervision of John Flower at the University of Leeds (Linnhoff, 1978) in response to the energy crisis of the 1970s and the need to reduce steam and fuel consumption in oil refineries and chemical plants by optimising the design of heat exchanger networks (Linnhoff, 1993). Linnhoff further developed the methodology at the University of Manchester Institute of Technology (UMIST) and setup a consultancy firm known as Linnhoff March International Ltd. (later acquired by KBC Energy Services plc.).

In PT the overall thermal energy demand and availability profiles for a whole process are represented by composite curves for heating and cooling streams on a temperature–enthalpy graph. By the means of this graph it is possible to determine the location of the process pinch point (of closest, pre–selected, temperature approach), and the minimum thermodynamic heating and cooling requirements or energy targets. This approach allows to then systematically design heat exchanger networks which aim to achieve those energy targets with a minimum number of units. Hohmann (1971) in this PhD thesis showed that the minimum number of units required in a network was one less than the total number of streams and laid some of the groundwork for the pinch method.

The benefits of using PT are clear and many successful plant implementations around the world exist. Worrell and Galitsky (2005) report total–site pinch analysis (integrating heating and cooling demands of various processes in the refinery) been applied to refineries operated by major oil companies. Typical energy savings identified in these site–wide analyses were around 20–30%, although the economic potential was found to be limited to 10–15% (Linnhoff–March, 2000). The PT approach has proven particularly useful also in retrofitting existing PHTs to improve their energy efficiency (Markowski, 2000, Bulasar et al., 2009). However, the pinch point is highly affected by fouling (Szklo and Schaeffer, 2007) and pinch–based methodologies suffer of several limitations:

- They consider steady–state performance of exchangers (i.e. no fouling dynamics).
- They seek to match the hottest process streams with the crude at its highest temperature. This leads to wall temperatures being maximised. In turn fouling, which is a function of temperature and velocity, is exacerbated.
- They rely on simple, lumped models that are limited by a number of assumptions on physical properties and temperature profiles inside the units.

The importance of including fouling at heat exchanger level and accounting for the way in which
several units interact in a network has been highlighted by Fryer (1988b). He considered the robustness of network design with regards to both the response to fouling and the controllability of the HEN when fouling occurs.

Brodowicz and Markowski (2003) proposed a modification of the classic PT to account for fouling based on the minimum sensitivity to the fouling effects by a single heat exchanger and the HEN. However, several aspects, such as the thermo–hydraulic interactions between fouling and pressure drops, remain to be addressed. Optimisation approaches, reviewed in the next section, seem to be better suited to accommodate dynamic fouling models and generate optimal layouts of heat exchanger networks.

### 3.4.2 New approaches

Optimisation techniques offer a powerful way to automatically generate heat exchanger network configurations that satisfy specified targets and constraints, while minimising total costs (i.e. including capital expenses and utility costs).

Optimisation approaches in the synthesis of networks include the use of genetic algorithm (Ponce-Ortega et al., 2007), mathematical programming techniques based on the sequential solution of continuous and integer linear programs (Papoulias and Grossmann, 1983) and nonlinear optimization problems (Floudas et al., 1986).

The basic mathematical programming approach was expanded to account for pressure drops (Frausto-Hernández et al., 2003; Serna-Gonzalez et al., 2004), flexibility (Floudas and Grossmann, 1987; Papalexandri and Pistikopoulos, 1994a,b) and used for the retrofit of existing networks (Papalexandri and Pistikopoulos, 1993; Bjork and Nordman, 2005). However, a number of assumptions are used to simplify the definition of the mathematical problem and fouling dynamics is not taken into account. As noted by Yeap et al. (2005), if this is not taken into account, it may lead to the design of network layouts which are optimal for energy recovery at clean conditions but not from a practical operating and, ultimately, economic point of view. This is also confirmed by practical refinery experience that highly optimised networks may not work due to fouling dynamics (personal communication).

Table 3.3 summarises the key contributions to the heat exchanger network synthesis problem identified by Furman and Sahinidis (2002).

Limitations highlighted above of traditional HEX and HEN design methodologies can be
Table 3.3: Summary of main contributions to the heat exchanger network synthesis problem adapted from Furman and Sahinidis (2002).

<table>
<thead>
<tr>
<th>Reference</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ten Broeck (1944)</td>
<td>First HEN synthesis related paper.</td>
</tr>
<tr>
<td>Westbrook (1961)</td>
<td>First use of mathematical programming in HEN synthesis.</td>
</tr>
<tr>
<td>Hwa (1965)</td>
<td>First grassroots design and superstructure.</td>
</tr>
<tr>
<td>Masso and Rudd (1969)</td>
<td>First formal definition of the HEN synthesis problem.</td>
</tr>
<tr>
<td>Umeda et al. (1978)</td>
<td>Identification of the pinch point.</td>
</tr>
<tr>
<td>Linnhoff and Flower (1978a)</td>
<td>Dual temperature approach.</td>
</tr>
<tr>
<td>Linnhoff and Flower (1978b)</td>
<td>Pinch design method.</td>
</tr>
<tr>
<td>Colbert (1982)</td>
<td>Transportation model.</td>
</tr>
<tr>
<td>Li and Motard (1986)</td>
<td></td>
</tr>
<tr>
<td>Yuan et al. (1989)</td>
<td></td>
</tr>
<tr>
<td>Yee and Grossmann (1990)</td>
<td></td>
</tr>
</tbody>
</table>

overcome by integrating a fouling rate model with a detailed and dynamic description of the heat exchange in an industrial unit as detailed in the next section.

### 3.5 Mathematical models of heat exchangers undergoing chemical reaction fouling

In his book dedicated to fouling Bott (1995) stated that:

“...The purpose of any fouling model is to assist the designer or indeed the operator of heat exchangers, to make an assessment of the impact of fouling on heat exchanger performance given certain operating conditions.”

To be able to accomplish this goal, Schreier and Fryer (1995) noted that fouling models should take into account:

- The rates of the processes that lead to deposition.
- The temperature distribution and deposit thickness profile.
- The effect of flow on deposition and if relevant re–entrainment (removal).

To successfully model fouling in a tubular heat exchanger, two main aspects need to be considered: the thermal–hydraulic model used to describe the heat exchanger in clean conditions and the
fouling model used to describe the rates of deposition. It should be noted that these are not separate, but they closely interact.

The fouling rate models, reviewed in Section 2.5, are relatively simple correlations that provide a means to capture the fouling dependence on process conditions and time. Whilst these models are very easy to use, their accuracy in fitting the data is often not satisfactory and their applicability appears to be very limited. One reason for this is that fouling rate models do not include a thermal model (e.g. they do not allow calculation of outlet temperatures in the system considered) thus they cannot be fitted to primary measurements (i.e. temperatures). Fouling resistance data, which are derived quantities (from experimental measurements) that suffer from propagation of errors, must be used instead. On the other hand, heat exchanger models that do not incorporate fouling will clearly provide completely erroneous predictions.

### 3.5.1 Advanced heat exchanger models

The importance of considering the transient behaviour of heat exchange equipment was highlighted in a recent editorial by Master and Chunangad (2008). Literature shows that some effort has been put in developing dynamic models of shell–and–tube heat exchangers in order to study the transient response of these units (Meyers et al., 1970; Hold, 1974; Tan and Spinner, 1978; Shah, 1980; Roppo and Ganić, 1981; Roetzel and Xuan, 1992; Xuan and Roetzel, 1993; Lakshmanan and Potter, 1994; Romie, 1999; Yin and Jensen, 2003; Ansari and Mortazavi, 2006). An extensive list of existing models of heat exchangers is reported by Skoglund et al. (2006).

When developing a model for shell–and–tube heat exchangers, the description of the shell–side flow and the related calculation of the heat transfer coefficient and pressure drop present several challenges. Very often in plant calculations, the heat transfer coefficient is considered as a linear function of the inlet flowrates. This provides an easy to compute albeit crude way to deal with the problem and it appears to be too simplistic for the purposes of this thesis. Tinker (1958) proposed a method that takes into account the effect of leakage streams (baffle–shell and baffle–tube) on heat transfer coefficient and pressure drop. These are not of secondary importance with respect to the predominant cross–flow stream as it was proven by the experiments performed at the University of Delaware by Bergelin and co–workers. Based on the Delaware data, Sullivan and Bergelin (1956) proposed the first differential model for the shell–side calculations.

Baptista and Castro (1993) noted that changes in flow direction imposed by the baffles are
3.5 Mathematical models of heat exchangers undergoing chemical reaction fouling

hard to describe by means of a differential model and require complex equations and elaborate computing strategies. A discrete approach was proposed by [Brambilla and Nardini (1972)] which divided the shell into a number of cells conveniently located in different zones where the prevalent direction of the fluid is either parallel to the tube bundle or in cross-flow with it. This approach accounts for the changes in flow direction typical of a baffled shell and has been further developed by other groups (e.g. [Correa and Marchetti (1987); Baptista et al. (1992)].

[Taborek (2002b)] reviewed the correlations available in literature for the description of shell-side heat transfer coefficient and pressure drop suggesting that the Bell–Delaware method (which will be used in this thesis) is the most suitable for the design of heat exchangers. In an attempt to improve the predictions of the heat transfer coefficient given by traditional methodologies described above, at the expenses of computational complexity, some papers focused on improving calculation of shell–side flow by using different approaches: [Gaddis and Schluder (1979); Kukral and Stephan (1992) considered axial dispersed plug flow, (Patankar and Spalding, 1972; Pataknar and Spalding 1974; Butterworth 1978b,a; Prithiviraj and Andrews 1998, 1999) developed multi-dimensional models whilst Tierney (1992); Karlsson and Vamling (2005) used full–blown CFD simulation. Moreover, [Kapale and Chand (2006)] focused on the accurate calculation of shell–side pressure drops.

The accurate calculation of the shell–side heat transfer coefficient has drawn also the attention of researchers investigating multitubular reactors where the accurate calculation of temperature profiles is paramount (Stankiewicz and Eigenberger, 1991; Baptista et al. 1992; Baptista and Castro, 1993; Shin et al., 2007). It is interesting to note that a shell–and–tube heat exchanger undergoing chemical reaction fouling acts essentially as a tubular reactor where no catalyst is needed to activate the reaction.

Regardless of the complexity involved in the description of the shell–side, only few papers focused on developing a dynamic and distributed model for heat exchangers which incorporates fouling. [Roetzel and Xuan (1999)] proposed dynamic and distributed models for several types of heat exchangers including plate, shell–and–tube and cross flow heat exchangers. They suggested the simultaneous solution of simple asymptotic models to represent fouling combined to a detailed, distributed heat exchanger model. However, their work focused primarily on studying the dynamic response of the different types of heat exchangers to step and ramp disturbances and no results are reported on the fouling behaviour.
3.5 Mathematical models of heat exchangers undergoing chemical reaction fouling

3.5.2 Integrated heat exchange and fouling models

Thermal models of heat exchangers that integrate fouling equations have the key feature of providing calculations of the fouling resistance as a function of process conditions within the system (tube or heat exchanger). This approach allows, for example, to capture not only the thermal interactions between tube–side and shell–side but also the thermo–hydraulic effects generated by the presence of the fouling deposits, leading to more accurate calculations of the velocity, wall shear stress, and convective heat transfer coefficient. Some models also include a detailed mass balance of precursors and fouling species together with a complex reaction scheme. This is particularly useful, for example, for milk fouling models where — unlike crude oil fouling — the reaction kinetics is better known.

Although more complex, integrated heat transfer and fouling models have the advantage of being able to be fitted to temperature and (if available) pressure drop measurements. They also provide a more flexible approach to the simulations of single tubes (representative of laboratory equipment) as well as different HEX and HEN configuration (as they allow the interconnection of units in a network).

An example of the integration of rate models with detailed heat transfer calculations was proposed by Takatsuka et al. (1989) who developed a distributed model for residual thermal cracking in a single furnace tube where the cracked products were assumed to come from the n–heptane soluble component of the feedstock.

As mentioned in Section 2.4.2, Panchal and Watkinson (1993, 1994) proposed one of the most detailed models so far that includes kinetics of the fouling reaction, mass transport to the wall along with thermal effects. However, the model was developed on the basis that the reaction mechanisms are known and includes several parameters of difficult estimation. Whilst they provided some values for their particular system, it seems difficult to apply them to a different system. A distributed model for a single tube was also developed by Watkinson and Zhang (2005) to simulate the material deposition from heavy hydrocarbon vapors. The model incorporates a physical condensation rate–mass transfer model for the condensation of the vapours.

Fryer and Slater (1985) developed a dynamic and distributed model for a single pass heat exchanger undergoing milk fouling. Although the fluid treated was different from crude oil, fouling mechanisms are very similar (i.e. chemical reaction fouling) and the fundamental thermal equations are relevant to the discussion. They calculated fouling rates as a function of local
temperature in terms of the Biot number for fouling, $\text{Bi}_f$:

$$\text{Bi}_f = h_0^t \frac{\delta}{\lambda_f}$$  \hspace{1cm} (3.7)$$

where $h_0^t$ is the tube–side convective heat transfer coefficient in clean conditions. The Biot number is a dimensionless fouling coefficient. Fryer and Slater (1985) captured the dependence of the Biot number as a function of both $T_w$ and $T_f$:

$$\frac{d\text{Bi}_f}{dt} = k_d(\tau) \exp\left(-\frac{E_f}{R_g T_s + (\sigma + \text{Bi}_f) T_f}\right) - k_r(\tau) \text{Bi}_f$$  \hspace{1cm} (3.8)$$

where $k_d$ and $k_r$ denote, respectively, the rate constants for deposition and removal as a function of $\tau$. In Equation (3.8), $\sigma$ is:

$$\sigma = h_0^t \left(1 + \frac{\delta}{\lambda_f}\right)$$  \hspace{1cm} (3.9)$$

The assumption underlying the model is that the convective heat transfer coefficient, $h_t$, does not change over time and is not a function of fouling layer thickness (i.e. $h_t = h_0^t = \text{const}$). For the specific system they examined, Fryer and Slater were able to determine a correlation between the rate constants and shear stress from Arrhenius plots of initial fouling rates. The model has also been used to explore alternative control strategies (Fryer and Slater, 1986).

Georgiadis (1998) and Georgiadis et al. (1998a) developed a dynamic and distributed model for milk fouling in shell–and–tube heat exchangers which included radial velocity, temperature and foulant concentration profiles capable of distinguishing between bulk, boundary layer and surface reaction rates. The fouling resistance was expressed in terms of the $\text{Bi}_f$ number:

$$\frac{d\text{Bi}_f}{dt} = a_1 k_m c_f$$  \hspace{1cm} (3.10)$$

In this case a detailed first principle, distributed mass balance was used, which includes the reaction of the foulant species to calculate $c_f$. The model was then used to find optimal design and operation of single units (Georgiadis et al., 1998b) and networks (Georgiadis et al., 2000).

Yeap et al. (2001b) presented a model for simulating crude oil fouling in shell–and–tube heat exchangers. They used the Panchal et al. (1999) fouling model coupled with a quasi–steady state distributed thermal model. They divided the exchanger into segments of equal length along the unit where the effectiveness and the number of transfer units were calculated. In this simple way
they were able to determine a temperature profile within the unit and associated local fouling rates. Whilst there exist more sophisticated thermal models (e.g. dynamic, with the heat transfer coefficient calculated as a function of process conditions), this is the first attempt in literature to develop a distributed model of a full unit undergoing crude oil fouling.

Yeap et al. (2004) coupled the Epstein (1994) rate model with a thermo–hydraulic model for a shell–and–tube heat exchanger. The thermal model used was a simple lumped \( \varepsilon \)–NTU model but they coupled it with an hydraulic model that allowed to capture also the interactions of fouling with pressure drops. However, the model is limited by the thin slab approximation to cases in which the thickness of the fouling layer is less than 10% the tube diameter. An important contribution of this work is that the authors used the thermo–hydraulic simulations to visualise through the so called ‘temperature field plot’ the fouling effects for the case study PHT presented by Panchal and Huangfu (2000) and proposed retrofit structures that mitigated fouling.

Table 3.4, which summarises the mathematical models for chemical reaction fouling in heat exchangers reviewed, shows that a single work coupling thermal and hydraulic models capable of describing local variations of the fouling layer (and with it local velocities and temperature profiles) in a shell–and–tube heat exchanger is not yet available.

Integrated models have been used in network simulations to retrofit pre–heat trains (Yeap et al., 2001a, Wilson et al., 2002, Yeap et al., 2004, 2005, Polley et al., 2005, de Oliveira Filho et al., 2007, Polley et al., 2009b, Tavares et al., 2009) and assist the scheduling of cleaning (Wilson and Vassiliadis, 1999, Smaïli et al., 2001, Ishiyama et al., 2009a, Sikos and Klemes, 2010). In a three part article, Lavaja and Bagajewicz (2004, 2005a,b) introduced the use of a mixed integer linear programming (MILP) model that includes fouling dynamics in the planning of cleaning scheduling. Although the fouling model used is linear to eliminate the complications of nonlinearities in the definition of the problem and the underlying heat exchanger model is based on simple, lumped heat balances, they set–up a sound framework for approaching maintenance planning in a CDU. A similar approach was also proposed by Wilson and Polley (2001). Numerical difficulties involved in integrating MINLP approach with non linear fouling models (e.g. threshold models described in Section 2.5) have been addressed by Wilson et al. (2001) and have limited the application of more realistic models to cleaning scheduling MINLP optimisations.
Table 3.4: Summary mathematical models for chemical reaction fouling in heat exchangers.

<table>
<thead>
<tr>
<th>Reference</th>
<th>Fluid</th>
<th>System</th>
<th>Side model</th>
<th>Dynamic</th>
<th>Distribution and functionality</th>
<th>Ageing</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fryer and Slater (1985)</td>
<td>Milk</td>
<td>HEX</td>
<td>✓/x</td>
<td>✓/✓/✓</td>
<td>✓/x/x</td>
<td>x</td>
<td>Single pass units only. HTC not function of fouling layer thickness. Numerical solution procedure depends upon the flow configuration.</td>
</tr>
<tr>
<td>Takatsuka et al. (1989)</td>
<td>Vacuum resid. Furnace tube</td>
<td>✓/x</td>
<td>✓/✓/✓</td>
<td>✓</td>
<td>x/x/x</td>
<td>✓</td>
<td>Fouling is related to sedimentation of precursors. Several parameters of difficult evaluation required.</td>
</tr>
<tr>
<td>Panchal and Watkinson (1994)</td>
<td>Hydrocarbons</td>
<td>Tube</td>
<td>✓/x</td>
<td>✓/✓/✓</td>
<td>✓/x/x</td>
<td>✓/x/x</td>
<td>Compared model simulations with experimental data to determine which one of the three fouling mechanisms proposed may be occurring.</td>
</tr>
<tr>
<td>Georgiadis et al. (1998a)</td>
<td>Milk</td>
<td>HEX</td>
<td>✓/x</td>
<td>✓/✓/✓</td>
<td>✓/x/x</td>
<td>x</td>
<td>Considered the radial dependency of velocity, temperature, and concentrations.</td>
</tr>
<tr>
<td>Yeap et al. (2001)</td>
<td>Oil</td>
<td>HEX</td>
<td>✓/x</td>
<td>✓/✓/✓</td>
<td>✓/x/x</td>
<td>✓/x/x</td>
<td>Thin slab approximation. Pumping power cost low compared to thermal penalty.</td>
</tr>
<tr>
<td>Yeap et al. (2004)</td>
<td>Oil</td>
<td>HEN</td>
<td>✓/x</td>
<td>✓/✓/✓</td>
<td>✓/x/x</td>
<td>x</td>
<td>Thin slab approximation. Pumping power cost low compared to thermal penalty.</td>
</tr>
<tr>
<td>Watkinson and Zhang (2005)</td>
<td>HC vapours</td>
<td>Furnace tube</td>
<td>✓/x</td>
<td>✓/✓/✓</td>
<td>✓/x/x</td>
<td>x</td>
<td>Thin slab approximation. Pumping power cost low compared to thermal penalty.</td>
</tr>
</tbody>
</table>

†T=thermal, H=hydraulic, M=mass transport model. ‡Models that do not rely on quasi-steady state approximation. * T(z): temperature dependence on the axial coordinate, ω(T)/ω(z): generic physical property (i.e. ρ, µ, A, c_p) dependence on temperature and/or axial coordinate, h(T)/h(z)/h(ω): dependence of heat transfer coefficient on temperature, axial coordinate and/or physical properties.
3.5 Mathematical models of heat exchangers undergoing chemical reaction fouling

3.5.3 Other approaches

To overcome the difficulties involved in modelling the complex fouling phenomena, several authors have attempted non deterministic approaches to describe the fouling process.

Sheikh et al. (1996) presented an economic analysis based on a probabilistic generalization of the deterministic modelling strategy proposed by Casado (1990) that developed a cost-based optimisation model to calculate the optimum operation of a shell–and–tube heat exchanger in a PHT. Sheikh et al. (1996) further generalized the Casado’s analysis by incorporating the stochastic nature of the linear fouling growth law as discussed by Zubair et al. (1997b,a, 1999). They incorporated a power–law, falling rate and asymptotic random falling growth laws developed by Zubair and Sheikh (2000); Sheikh et al. (2000); Zubair et al. (2001). However, these models consider fouling as being essentially random in nature and thus fail to explain in a satisfactory way the interactions between different phenomena involved in the deposition/removal process.

Sheikh et al. (1999) developed a probabilistic approach with which they described fouling as a time random process where the fouling resistance is determined by:

\[ R_f(t) = f(a_1, a_2, t) \]  

(3.11)

where \( a_1 \) and \( a_2 \) are parameters of the model that contain all the cumulative effect of the uncertainties related to the process.

Artificial neural network techniques have been successfully utilized to correlate the data during the entire fouling process in several types of fouling mechanisms (Malayeri and Müller-Steinhagen, 2001; Sheikh et al., 2001; Malayeri and Müller-Steinhagen, 2007; Radhakrishnan et al., 2007) and also in crude oil Aminian and Shahhosseini (2008, 2009).

Li (2005) based his analysis on the fact that fouling data typically present fluctuations which are difficult to model. He proposed to separate the fouling rate into two parts: a mean component that exhibits a smooth and asymptotic behaviour and a fluctuating component that exhibits an oscillatory behaviour. However, this approach fails to explain the reason of the fluctuations and cannot be considered a reliable way of predicting fouling behaviour.

In general, all the statistical methodologies reviewed above are essentially black box approaches that do not offer any physical understanding of the process. Another drawback is that
this kind of models require extensive data for “training” and appear to have limited extrapolation capabilities compared to either first principle or empirical models. Other approaches to assess fouling behaviour of industrial heat exchangers, include the use of principal component analysis (Zabiri et al., 2006), expert systems (Afgan and Carvalho, 1996) and computational fluid dynamics (Appendix B).

3.6 Concluding remarks

In this chapter the several limitations of the traditional TEMA fouling factor approach to the design of heat exchangers and heat exchanger networks have been highlighted. Many authors criticised the use of fixed values of the fouling resistance as this approach fails to capture fouling dynamics and its dependence on process conditions. As a result, fouling in heat exchangers remains a major problem for refinery operators. Two main factors have favoured over the years the use of these design methodologies. The difficulties in capturing knowledge and translating it into a reliable model capable of accurately predicting fouling on one hand and the lack of an effective implementation of available models into user–friendly tools on the other.

Existing models for fouling in heat exchangers seem to be either lumped thermal models (of low accuracy in the description of dynamics and distributed phenomena), or dynamic and distributed heat exchanger models which do not incorporate (or use only simple) fouling models. Moreover, the trend in literature is to fit fouling models parameters not to primary data such as temperatures but to fouling resistances calculated with the classic LMTD or $\epsilon$–NTU methods. Such derived fouling resistance embeds all the uncertainties not only in the measurements but also in the assumptions, such as constant density and specific heat capacity, used for its calculation. The combination of these assumptions used together with a simplistic way of determining the values of model parameters often lead to inaccurate fit of model simulations to fouling data. Predictions of future trends (i.e. not fitting) is even more challenging and predictive ability is often not attempted or reported.

To be able to improve design, retrofit and monitoring of both heat exchangers and networks of heat exchangers, several key aspects must be addressed:

- Fouling, ageing, surface roughness dynamics phenomena and their effect on the thermo–hydraulic behaviour of the system considered must be captured simultaneously as a
function of process conditions.

- A suitable modern integration tool should be used to allow the solutions of a large number of equations in a user–friendly way. The implementation should be flexible enough to allow the analysis of important phenomena at several levels of investigation and serve a variety of purposes:

  - Analysis of laboratory data (typically obtained in tube sections). At this time and length scale of investigation, it is important to include phenomena such as surface roughness dynamics.
  - Performance monitoring of individual industrial units and networks. This may include on–line and/or control applications and assessment of running costs. The correct estimation of model parameters is pivotal. A model–based parameter estimation approach using primary measurements (i.e. flowrates and temperatures) rather than derived quantities should be preferred.
  - Single unit design and retrofit. Here ageing plays an important role and should be accounted for. Model validation with available plant data, although challenging, is important to give confidence in the accuracy of the predictions.
  - Heat exchanger networks design and retrofit that take into account fouling dynamics. Assessment of the impact of selected network structures should be based not only on energy recovery at clean conditions, but on key performance indicators that inform not only design but also operational decisions.
  - It should be possible to easily replicate the single heat exchanger model in a flow-sheeting environment to readily generate specific network topology. This would allow eventually to optimise the impact of each single heat exchanger design together with the network structure to minimise fouling and maximise economic performance over time.

The following chapters will focus on the development of a mathematical models capable of predicting fouling behavior at the tube (Chapter 4), unit (Chapter 5) and network (Chapter 6) levels that incorporate all the features above.
Chapter 4

A dynamic, distributed model of a single tube undergoing crude oil fouling

Synopsis

The focus of this chapter is the development of a dynamic and distributed model for a single tube undergoing crude oil fouling. Models for the description of important phenomena such as surface roughness dynamics and the structural changes of the deposits over time (ageing) are proposed. Simulations are carried out for two operating conditions, namely uniform heat flux (representative of experimental configurations) and uniform wall temperatures. Results are presented to demonstrate the impact of ageing and surface roughness dynamics on the thermal and hydraulic behaviour of the system.
4.1 Introduction

The multi–scale approach to the modelling of shell–and–tube heat exchangers undergoing crude oil fouling proposed in this thesis starts off in this chapter with the development of the equations for crude oil fouling in a single tube.

The system considered is schematically defined in Figure 4.1. The dimensions and operating conditions used are representative of those employed in refinery applications. However, the

\[ \begin{align*}
\Omega_t & \quad \Omega_i & \quad \Omega_w \\
r = 0 & \quad r = R_{f,ow} & \quad r = R_i & \quad r = R_o \\
(z) & \quad \delta(z)
\end{align*} \]

\[ \begin{align*}
\Omega_t & \quad \tilde{\Omega}_i & \quad \Omega_w \\
\tilde{r} = 1 & \quad \tilde{r} = 0
\end{align*} \]

Figure 4.1: Single tube model domains definition and reference system in (a) dimensional and (b) dimensionless coordinate.
model is readily adapted to other geometries representative of laboratory or pilot plant scale experiments, such as the annular flow configuration used in the HTRI heated rod testing system (Bennett et al., 2009) or the HIPOR (high pressure oil rig) built at Imperial College London (Macchietto et al., 2009). The physical system is divided into the 3 following domains (illustrated in Figure 4.1):

\( \Omega_w \): The tube wall domain, defined as the region between the inner radius of the tube, \( R_i \) and its outer radius, \( R_o \).

\( \Omega_l \): The deposit layer domain, defined as that between the crude oil/deposit layer interface (at the flow radius, \( r = R_{flow} \)) and the inner radius of the tube, \( R_i \).

\( \Omega_t \): The tube–side flow domain, defined between the tube centre (\( r = 0 \)) and \( R_{flow} \).

The model is defined in each domain along the length of the tube (from \( z = 0 \) to \( z = L \)). In the deposit layer and tube wall domains (\( \Omega_l \) and \( \Omega_w \)) model equations are also distributed along the radial coordinate. This allows to model phenomena which vary in the radial direction, such as the ageing of deposit.

The tube–side flow is treated as being locally well mixed in the radial direction (i.e. in plug flow) as it is turbulent thus the components in the model are not related to radial variations in the flow domain. The location of the fluid/deposit interface, \( R_{flow} \), is determined by the deposit thickness and changes along \( z \) with time, depending on local fouling conditions. The physical properties of the crude oil flowing in the tube such as density, \( \rho \), dynamic and kinematic viscosities, \( \mu \) and \( \nu \), thermal conductivity, \( \lambda \) and heat capacity, \( c_p \), are calculated using API relationships (Riazi, 2005) as a function of temperature and space.

Entrance and exit effects in the tube are neglected (i.e. the flow is considered thermally and hydraulically fully developed at \( z = 0 \)). Gravity effects are also assumed to be negligible and symmetry is assumed in the angular coordinate, \( \vartheta \).

The general framework used also allows incorporating sub–models that capture important and complex phenomena such as roughness dynamics and ageing of deposits developed, discussed respectively in Section 4.2.3.3 and Section 4.2.2.1.

Results are presented for two operating cases, namely uniform wall temperature, UWT, and uniform heat flux, UHF.
4.2 Model equations

In the following sections, the main model equations are derived for each domain together with suitable boundary and initial conditions.

The temperature profiles in each domain calculated with a thermal balance on a differential control volume $\Delta z$ (Figure 4.2) based on first principles (Bejan, 1984):

\[
\begin{align*}
\text{Rate of energy accumulation in control vol.} = & \text{Net energy transfer by fluid flow} - \text{Net energy transfer by conduction} + \text{Rate of internal heat generation} - \text{Net work transfer to environm.} \\
\end{align*}
\]  

(4.1)

4.2.1 Tube wall

Heat transfer occurs via conduction in domain $\Omega_w$. The second term in Equation 4.1 is thus neglected as well as the net work transfer to the environment (5th term in Equation 4.1):

\[
\rho_w c_{p,w} \frac{\partial T_w}{\partial t} = \nabla (\lambda_w \nabla T_w) + q''''_w
\]  

(4.2)

where $T_w$ is the local temperature at time $t$ and location $(z, r)$ whilst $\lambda_w$ is the thermal conductivity, $\rho_w$ the density and $c_{p,w}$ the heat capacity of the metal wall assumed constant. Assuming no heat sources, $q''''_w$, neglecting phenomena in the axial direction and symmetry w.r.t. angular coordinate $\theta$, yields:

\[
\rho_w c_{p,w} \frac{\partial T_w}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} (r \partial T_w/\partial r) + \frac{\partial^2 T_w}{\partial r^2}
\]  

(4.3)

**Figure 4.2:** Differential control volume.
4.2 Model equations

The heat flux across the tube wall, $q'_w(z, r, t)$, is calculated as:

$$
q'_w = -\lambda_w \frac{\partial T_w}{\partial r}
$$

(4.4)

4.2.2 Deposit layer

The deposit layer, domain $\Omega_l$ (defined for $z = [0, L]$ and $r = [R_i, R_{flow}]$), is also modelled as a conductive domain. Neglecting variations in the axial direction and assuming symmetry w.r.t. angular coordinate $\theta$, no heat sources and no net work to the environment:

$$
\rho_l c_{p,l} \frac{\partial T_l}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \lambda_l \frac{\partial T_l}{\partial r} \right)
$$

(4.5)

Here, $T_l$ is the local temperature and $\lambda_l$ the thermal conductivity, both of which are a function of spatial coordinates $r, z$ and time (i.e. $T_l(z, r, t)$ and $\lambda_l(z, r, t)$). Conversely, the density of the deposit layer, $\rho_l$, and its specific heat capacity, $c_{p,l}$, are here assumed uniform and constant. It should be noted that Equation [4.5] also accounts for the variation of the thermal conductivity in the radial direction. Moreover, the model formulation in cylindrical coordinates allows accounting for curvature effects in the heat flux thus overcoming the thin slab approximation used in other models.

The radial heat flux at any point in the deposit layer, $q''_l(z, r, t)$, is calculated as:

$$
q''_l = -\lambda_l \frac{\partial T_l}{\partial r}
$$

(4.6)

Equations [4.5] and [4.6] are defined in the domain between $R_i$ and the moving boundary coordinate $R_{flow}(z, t)$:

$$
R_{flow} = R_i - \delta
$$

(4.7)

where the deposit thickness, $\delta$, is a function of the axial coordinate and time (i.e. $\delta = \delta(z, t)$) and is calculated as shown later by Equation [4.38].

To solve the set of partial differential and algebraic equations (PDAE) with a moving boundary, Equations [4.5] and [4.6] are re-formulated in dimensionless form with respect to the radial coordinate, utilising a coordinate transformation. The following dimensionless radial
coordinate is introduced:

\[ \tilde{r} = \frac{r - R_i}{R_{flow} - R_i} \]  

(4.8)

so that, \( \forall \tilde{r} \):

\begin{align*}
\text{at} & \quad r = R_i \quad \text{(wall)} \quad \rightarrow \quad \tilde{r} = 0 \\
\text{at} & \quad r = R_{flow} \quad \text{(deposit/ fluid boundary)} \quad \rightarrow \quad \tilde{r} = 1
\end{align*}

(4.9)

From the definition of the flow radius in Equation 4.7, the new radial coordinate can be written as:

\[ \tilde{r} = \frac{R_i - r}{\delta} \]  

(4.10)

Figure 4.1(b) shows a schematic of the deposit domain coordinate transformation. In terms of the new radial coordinate \( \tilde{r} = [1, 0] \), Equation 4.5 becomes:

\[ \delta^2 \rho_l c_{pl} \frac{\partial T_l}{\partial t} = \frac{\partial \lambda_l \frac{\partial T_l}{\partial \tilde{r}}}{\partial \tilde{r}} - \frac{\lambda_l \delta}{R_i - \tilde{r}} \frac{\partial T_l}{\partial \tilde{r}} + \lambda_l \frac{\partial^2 T_l}{\partial \tilde{r}^2} \]  

(4.11)

Similarly, Equation 4.6 becomes:

\[ q''_l = \frac{\lambda_l}{\delta} \frac{\partial T_l}{\partial \tilde{r}} \]  

(4.12)

### 4.2.2.1 Ageing model

As noted in Section 2.4.3.5, exposure of the deposit layer to distinct temperature histories over time causes its structure to change (ageing). Ageing is expressed via a change in the deposit thermal conductivity, between that of the freshly deposited material (the lower limit), \( \lambda_l^0 \), and a maximum value, \( \lambda_l^\infty \) viz.

\[ \lambda_l = \lambda_l^\infty + (\lambda_l^0 - \lambda_l^\infty) \cdot y \]  

(4.13)

Typical thermal conductivity values (Watkinson, 1988) are \( \lambda_l^0 = 0.2 \text{ Wm}^{-1}\text{K}^{-1} \) (initial gel–like deposit, \( \lambda \) similar to oil) and \( \lambda_l^\infty = 1 \text{ Wm}^{-1}\text{K}^{-1} \) (coked deposit). These values were employed in the simulations presented here.

The ‘youth’ variable, \( y(z, \tilde{r}, t) \), in Equation 4.13 is introduced assuming first order exponential decay dynamics:

\[ \frac{dy}{dt_{age}} = -A_a \exp \left( -\frac{E_a}{R_g T_l} \right) \cdot y \]  

(4.14)

where \( E_a \) and \( A_a \) are, respectively, the activation energy (i.e. the temperature dependency) and pre–exponential constant characteristic of the ageing process. It should be noted that ageing is
4.2 Model equations

Figure 4.3: Schematic showing ageing time–deposit thickness construction for (a) constant deposition rate; (b) deposition rate with autoretardation.

very sensitive to the local deposit temperature, $T_l$.

The ageing time, $t_{age}(z, r, t)$, in Equation 4.14 refers to the lifetime of the deposit and therefore depends on when it was formed. For an element formed at instant $t_A$,

$$t_{age} = t - t_A; \forall t \geq t_A$$  \hspace{1cm} (4.15)

Each element of deposit in a deposit layer will feature a particular lifespan, between 0 and $t$, which needs to be tracked through time in order to evaluate the change in $y$. Ishiyama et al. (2009b) captured these dynamics by discretising the layer into elements formed at regular time intervals and integrating Equation 4.14 for each element, via a series of ordinary differential equations (ODEs). Here, a continuous formulation that captures the age of individual elements in the fouling layer is proposed. This approach is exact for the particular case of constant deposition rate, i.e. the deposit thickness increases linearly with time which corresponds to the condition expected for fouling experiments performed under conditions of constant heat flux (and no change in surface roughness). It is shown later that it represents a conservative estimate for the other commonly used experimental mode of uniform wall temperature.

Consider the case of deposit growing at constant rate, as shown in Figure 4.3(a). At time $t_I$ the deposit has grown to a thickness $\delta_I$ and the age of the fresh deposit is zero. The radial location of the element of fresh deposit is $R_{flow}$, and thus $\tilde{r} = 1$. At time $t_{II}$ the deposit layer has grown to an overall thickness $\delta_{II}$. The age of the deposit formed at time $t_I$ is now $t_{II} - t_I$, which
by similar triangles is given by:

\[ t_{\text{age}} = t_{II} \left( \frac{\delta_{II} - \delta_{I}}{\delta_{II}} \right) = t_{II} \cdot (1 - \tilde{r}) \] (4.16)

A general relationship between temporal and spatial variables, which applies from the time of formation of the element of deposit, can be written:

\[ t_{\text{age}} = t (1 - \tilde{r}) \] (4.17)

Using Equation [4.17], the L.H.S. of Equation [4.14] may then be rewritten as:

\[ \frac{dy}{dt_{\text{age}}} = \frac{dy}{dt} \frac{dt}{dt_{\text{age}}} = \frac{dy}{dt} \frac{d}{dt_{\text{age}}} \left( \frac{t_{\text{age}}}{1 - \tilde{r}_I} \right) \] (4.18)

hence:

\[ \frac{dy}{dt_{\text{age}}} = \frac{1}{1 - \tilde{r}} \frac{dy}{dt} \] (4.19)

Therefore Equation [4.14] becomes:

\[ \frac{dy}{dt} = (1 - \tilde{r}) \left[ -A_d \exp \left( -\frac{E_a}{R_l T_l} \right) \cdot y \right] \] (4.20)

Differential Equation [4.20] is expressed in the same time coordinate as the other differential equations and can therefore be integrated simultaneously with them.

When the deposition rate (here, referring to the change in deposit thickness) is not constant, the ageing transformation (Equation [4.17]) is not exact. Consider the autoretardation (falling rate) scenario in Figure 3(b). The age of the deposit element formed at instant \( t_{III} \) at time \( t_{IV} \) is \( (t_{IV} - t_{III}) \). The deposit layer has grown to thickness \( \delta_{IV} \), which is smaller than that given by linear growth, \( \delta_{IV}^* \). The dimensionless co-ordinate of the material formed at \( t_{III} \) is \( \tilde{r} = \delta_{III}/\delta_{IV} \), which is greater than that given by the linear deposition case \( \delta_{III}/\delta_{IV}^* \). The age of this element given by Equation [4.17] will be smaller than the true value and Equation [4.20] will therefore under predict the rate of ageing. The transformation is therefore an approximation for this scenario and provides a conservative estimate of the effect of ageing. This is considered to be acceptable, particularly as the underlying physics and associated parameters are not well known.

Equations [4.13] and [4.20] together give the thermal conductivity, \( \lambda_l \) at each point in the deposit
layer undergoing ageing (i.e. \( \lambda_l = \lambda_l(z, r, t) \)), and its use in Equation 4.11 gives the temperature evolution in the layer at any time.

### 4.2.3 Tube–side flow

Deposition inside the tube, which depends on the local conditions, reduces the cross-sectional area for flow, \( A_{\text{flow}} \), over time and space affecting both heat transfer and pressure drop along the tube. The changing cross-sectional area, \( A_{\text{flow}}(z, t) \) is:

\[
A_{\text{flow}} = \pi R_{\text{flow}}^2
\]  

(4.21)

where \( R_{\text{flow}} \) is the flow radius, defined earlier in Equation 4.7.

The first term in Equation 4.1, the rate of energy accumulation in the control volume (in Joules), is:

\[
\{1\} = \left. \left( \rho c_p T A_{\text{flow}} \Delta z \right) \right|_{z, t} \Delta t - \left. \left( \rho c_p T A_{\text{flow}} \Delta z \right) \right|_{z + \Delta z, t} \Delta t
\]  

(4.22)

where \( T_n \) is the tube–side fluid temperature whereas \( \rho \) and \( c_p \) are, respectively, its density and specific heat capacity.

The energy flowrate (second term in Equation 4.1) at the inlet and outlet of the differential element is:

\[
\{2\} = \left( \rho c_p T u A_{\text{flow}} \right)_{z, t} \Delta t - \left( \rho c_p T u A_{\text{flow}} \right)_{z + \Delta z, t} \Delta t
\]  

(4.23)

The heat conduction (third term in Equation 4.1) in the axial direction is:

\[
\{3\} = q'' A_{\text{flow}} \Delta z \Delta t - q'' A_{\text{flow}} \Delta z \Delta t
\]  

(4.24)

Where \( q''(z, t) \) is the tube–side heat flux in the axial direction:

\[
q'' = -\lambda \frac{\partial T}{\partial z}
\]  

(4.25)

The heat source term (from the wall, fourth term in Equation 4.1) is:

\[
\{4\} = q''' A_{\text{flow}} \Delta z \Delta t
\]  

(4.26)
4.2 Model equations

where \( q''', \) the heat source per unit volume in W m\(^{-3}\), is given by:

\[
q''' = \frac{S}{\Delta z A_{flow}} h \left( T_{|r=R_{flow}} - T \right) \quad (4.27)
\]

where \( h \) is the convective heat transfer coefficient (as calculated with Equation 4.35) and \( S \) is the heat transfer area as a function of \( P_t \), the tube–side inner perimeter:

\[
S = P_t \cdot \Delta z = 2\pi R_{flow} \cdot \Delta z \quad (4.28)
\]

The source term in Equation 4.26 therefore becomes:

\[
\{4\}_4 = q''' = \frac{P \Delta z}{A_{flow} \Delta z} h \left( T_{|r=R_{flow}} - T \right) A_{flow} \Delta z \Delta t = P_t h \left( T_{|r=R_{flow}} - T \right) \Delta z \Delta t \quad (4.29)
\]

The net work from the control volume to its environment is neglected:

\[
\{5\}_5 = 0 \quad (4.30)
\]

Dividing the total heat balance by \( \Delta t \) and \( \Delta z \) (but not by \( A_{flow} \) as it changes both with time and \( z \)), substituting Equation 4.25 in Equation 4.24 and taking the limit for \( \Delta t \to 0 \) and \( \Delta z \to 0 \), yields:

\[
\frac{\partial}{\partial t} \left( \rho c_p T A_{flow} \right) = \frac{\partial}{\partial z} \left( \rho c_p T u A_{flow} \right) + \frac{\partial}{\partial z} \left[ A_{flow} \frac{\partial T}{\partial z} \right] + P_t h \left( T_{|r=R_{flow}} - T \right) \quad (4.31)
\]

It should be noted here that no assumptions on the physical properties (e.g. constant density, thermal conductivity or heat capacity) have been made. Equation 4.31 takes into account the variation of the cross–sectional area given by the fouling layer.

4.2.3.1 Hydraulics

The hydraulic effect of fouling (reduction of flow section in pipes on velocities and pressure drop) and its interaction with the fouling process itself is paramount. This is captured through the definition of the flow radius, \( R_{flow} \), in Equation 4.7 and the flow area, in Equation 4.21. The velocity, \( u \), is function of this flow radius:

\[
u = \frac{m}{\rho A_{flow}} \quad (4.32)\]
The pressure drop inside the tube also reflects the fouling growth and is calculated by:

$$ \frac{dP}{dz} = C_f \frac{\rho u^2}{R_{flow}} $$ (4.33)

The Fanning friction factor, $C_f$, for tubes of roughness $e$, is calculated in the turbulent regime via (Wilkes, 2005):

$$ C_f = \left\{ -1.737 \ln \left[ 0.269 \frac{e}{2R_{flow}} - \frac{2.185}{\text{Re}} \ln \left( 0.269 \frac{e}{2R_{flow}} + \frac{14.5}{\text{Re}} \right) \right] \right\}^2 $$ (4.34)

The role and importance of the surface roughness are discussed in Section 4.2.3.3.

Both $R_{flow}$ and the surface roughness (via $C_f$) affect the local tube–side heat transfer coefficient, $h(z, t)$. This is accounted for in the correlation (Gnielinski, 1976):

$$ h = \left( \frac{\lambda}{2R_{flow}} \right) \left( \frac{C_f}{2} \right) \frac{(\text{Re} - 1000) \text{Pr}}{1 + 12.7 \sqrt{\frac{C_f}{2} \left( \text{Pr}^{0.67} - 1 \right)}} $$ (4.35)

where Re and Pr are the local Reynolds and Prandtl numbers, respectively, evaluated at the bulk temperature. For a given mass flowrate, Equation 4.35 shows that $h$ is enhanced by a progressive reduction in cross–sectional area, showing that fouling can have a positive effect on heat transfer albeit at the expense of increased pressure drop.

A tube–long average convective heat transfer coefficient, $\bar{h}(t)$, is defined as:

$$ \bar{h} = \frac{1}{L} \int_0^L h dz $$ (4.36)

which will be used in the next section to calculate an overall heat transfer coefficient.

### 4.2.3.2 Fouling model

It has been noted in Chapter 2 that chemical reaction fouling, particularly in the area of crude oil fouling as considered here, is a complex phenomenon. There are presently no theoretical models that can reliably describe the inception, growth (and where applicable, removal) of chemical reaction fouling layers from first principles. Amongst the several semi–empirical
models that correlate the fouling resistance to process conditions and time reviewed in Chapter 2, the threshold model proposed by Panchal et al. (1999) is chosen here to calculate the fouling rate:

\[
\frac{dR_f}{dt} = \alpha \text{Re}^{-0.66} \text{Pr}^{-0.33} \exp\left(\frac{-E_f}{R_g T_f}\right) - \gamma \tau
\] (4.37)

where \(R_f(z, t)\) denotes the local fouling resistance, \(T_f(z, t)\) the local film temperature and \(\tau(z, t)\) the shear stress on the fluid/deposit interface whilst \(\alpha, \gamma,\) and the fouling activation energy, \(E_f\), are adjustable parameters that vary between different crudes. A sensitivity analysis for the parameters and variables involved in Equation 4.37 is reported in Appendix A.

This model is typically used to give an aggregate fouling resistance over a whole heat exchanger, with parameters adjusted to fit overall thermal balances based on measured temperatures and flows. In this work the above fouling model is used to calculate the rate of deposition, at each point along the axial direction, based on local conditions. The increase in fouling layer thickness, at any axial point \(\delta(z, t)\), can be calculated knowing the thermal conductivity of a newly deposited layer, which is taken to be \(\lambda^0_l\), being that of an oily gel as discussed in section 4.2.3:

\[
\frac{d\delta}{dt} = \lambda^0_l \frac{dR_f}{dt}
\] (4.38)

Integration of Equation 4.38 together with the other model equations, allows calculation of the deposit thickness and flow radius, \(R_{flow}\), at each point along the axis.

The standard method to represent the thermal effect of fouling is by means of an overall ‘fouling resistance’. The detailed, distributed information on thermal conductivity at each point in the fouling layer is used to compute the average fouling resistance, \(\bar{R}_f(t)\):

\[
\bar{R}_f = \frac{1}{L} \int_0^L \left( \int_0^1 \frac{\delta(z)}{\lambda_l(z, \tilde{r})} d\tilde{r} \right) dz
\] (4.39)

Although the distributed information is useful for identifying and analysing performance at different allocations in the tube, the average fouling resistance defined in Equation 4.39 can be used to assess the overall thermal performance of a tube undergoing fouling in a way that is more commonly understood. The overall heat transfer coefficient, \(U\), is defined as:

\[
\frac{1}{US_o} = \frac{1}{S_i \bar{h}} + \frac{\bar{R}_f}{S_i} + \frac{1}{S_m \lambda_w} \delta_w
\] (4.40)
where $\delta_w$ is the wall thickness, $S_o$ is the outer surface area of the tube, $S_i$ the inner one and $S_m$ is the logarithmic mean area defined in Equation 3.5. The average fouling resistance defined in Equation 4.39 can be compared against other aggregate ways of calculating it.

4.2.3.3 Surface roughness dynamics

Surface roughness is often expressed in terms of an equivalent sand roughness, $e$, (Brown, 1950): typical values for clean, tubes range (Perry and Green, 1997) from 1.5 $\mu$m (for drawn steel tubes) to 46 $\mu$m whereas that of bitumen layers has been reported as 120 $\mu$m (Kern, 1988). Although chemical reaction fouling is often accompanied by observable changes in surface roughness (e.g. Yang et al. 2009b), there are currently no established models to calculate surface roughness of chemical reaction fouling deposits from first principles and indeed there are few data available. Here, surface roughness dynamics is modelled as increasing from a minimum value (that of a clean tube), $e^0$, as deposition increases until a maximum value, $e^\infty$ is reached.

In the absence of experimental data, two functional forms for the roughness $e$ in Equation 4.34 are proposed in order to illustrate the effect of the increase in roughness given by fouling deposition on heat transfer.

The first model is a simple linear ramp related to the thickness of the fouling layer:

$$e = e^0 + \min(k_p\delta, e^\infty)$$

(4.41)

where $k_p$ is a rate constant. When the maximum value, $e^\infty$, is reached, the roughness does not change anymore. This introduces a mathematical discontinuity which is unlikely to occur in reality (see results section, Figure 4.7(a)). It is acknowledged that this is a simple model, which suggests that deposition occurs via the build up a uniform layer, the surface of which increases in roughness. The change in deposit thickness, $\delta$, is calculated from the thermal fouling model (Equation 4.35), which does not, however, include roughness effects. There is therefore considerable scope for development of these dynamic models.

A second model treats the surface roughness as evolving asymptotically over time to its final value (with $k_t$ the time it takes to achieve 1/2 of the final roughness):

$$e = e^0 + (e^\infty - e^0) \frac{t}{t + k_t}$$

(4.42)
However, if deposition does not occur, the roughness should not change. For this reason, a different model, although exhibiting the same asymptotic behaviour of Equation 4.42, is proposed to relate the roughness to the thickness of the fouling layer:

\[
e = e^0 + \left( e^\infty - e^0 \right) \frac{\delta}{\delta + k_a e^\infty}
\]

(4.43)

Equation 4.43 states that the roughness of the interface between oil and deposit layer evolves asymptotically from the clean tube value, \( e^0 \), to a final value, \( e^\infty \), characteristic of the deposit type, with the rate of change depending on the foulant thickness and a dimensionless (adjustable) constant \( k_a \). A suitable choice of \( k_a \) allows defining faster or slower evolution of the roughness to its final value.

These conceptual models are used here in the absence of reliable, dynamic data and a mechanistic model. The results do, nevertheless, highlight the importance of including a suitable roughness model.

### 4.2.4 Boundary conditions

Two typical operating conditions are considered here: uniform heat flux (UHF) and uniform wall temperature (UWT) which require two different sets of boundary conditions.

The UHF case corresponds to the tube being heated through the wall (for example, by an electric cartridge heater) with a fixed value of the heat flux at the outer tube surface, \( q''_o \). The boundary condition is therefore:

\[
q''_w \bigg|_{r=R_o} = q''_o
\]

(4.44)

In the UWT case the temperature of the tube outer surface is fixed at \( T_o \) for all times and axial values:

\[
T_w \bigg|_{r=R_o} = T_o
\]

(4.45)

In both the above cases the following boundary conditions apply at the interface with the other domains. At the interface between \( \Omega_w \) and the fouling layer, \( \Omega_l \), there is continuity in the heat
4.2 Model equations

flux and the temperature at all times:

\[ q''|_{r=R_i} = q''|_{r=R_i} \]  \hspace{1cm} (4.46)
\[ T_w|_{r=R_i} = T_j|_{r=R_i} \]  \hspace{1cm} (4.47)

Or, for the dimensionless domain, ˜Ω:

\[ q''|_{\tilde{r}=0} = q''|_{\tilde{r}=0} \]  \hspace{1cm} (4.48)
\[ T_w|_{\tilde{r}=0} = T_j|_{\tilde{r}=0} \]  \hspace{1cm} (4.49)

At the moving boundary between the fouling layer, Ω, and the tube–side domain Ω, there is continuity in the heat flux:

\[ q''|_{r=R_{flow}} = -h(T|_{r=R_{flow}} - T) \]  \hspace{1cm} (4.50)

Or, for the dimensionless domain, ˜Ω:

\[ q'|_{\tilde{r}=1} = -h(T|_{\tilde{r}=1} - T) \]  \hspace{1cm} (4.51)

At the tube inlet (all \( t, r \)) the oil temperature, \( T_{in}(t) \) and pressure, \( P_{in}(t) \) are supplied functions of time:

\[ T|_{z=0} = T_{in} \]  \hspace{1cm} (4.52)
\[ P|_{z=0} = P_{in} \]  \hspace{1cm} (4.53)

4.2.5 Initial conditions

At all points \( z \) along the axis, at time \( t = 0 \), the tube is clean (i.e. no fouling layer):

\[ R_j|_{z=0} = 0 \]  \hspace{1cm} (4.54)

The thickness of fouling layer, \( \delta \), is initialised to a small positive value (10\(^{-7}\) m), for numerical reasons:

\[ \delta|_{z=0} = 10^{-7} \]  \hspace{1cm} (4.55)
The temperature profiles at time 0 are assumed to be in steady in all domains

\[ \frac{dT_w}{dt} \bigg|_{t=0} = \frac{dT_l}{dt} \bigg|_{t=0} = \frac{dT_t}{dt} \bigg|_{t=0} = 0 \quad (4.56) \]

The ageing model given by Equation 4.20 introduces a differential equation which needs an initial value of the youth variable, \( y \):

\[ y \bigg|_{t=0} = 1 \quad (4.57) \]

### 4.3 Solution method

The model outlined in the previous section consists in a set of PDAE. The simultaneous solution of Equations 4.3 and 4.4 in the wall domain, \( \Omega_w \), Equations 4.11, 4.11 and 4.12 in the fouling layer domain, \( \Omega_l \), Equations 4.21, 4.31, 4.32, 4.33, 4.34, 4.35, 4.37, 4.38, 4.39 and 4.42 in the tube domain, \( \Omega_t \), allows to obtain, amongst other useful information such as the overall heat transfer behaviour, the distributed temperature profiles across the heat exchanger (and the fouling layer) which allow the calculation of the fouling resistance, \( R_f \), according to the Ebert–Panchal model (Equation 4.37) at any axial coordinate. This provides a point value of the fouling resistance necessary to calculate the thickness of the fouling layer, \( \delta \) (Equation 4.38). However, the \( R_f \) value calculated via Equation 4.37 does not take into account the effects of ageing on the thermal behaviour of the system. For this reason, and ageing model (Equation 4.20) is introduced and an effective fouling resistance (Equation 4.39) that accounts for the variation in thermal conductivity of the fouling layer is calculated.

The boundary conditions between domain \( \Omega_w \) and \( \Omega_l \) in Equation 4.48, between domain \( \Omega_l \) and \( \Omega_t \) in Equation 4.51 and at the tube inlet in Equation 4.52 together with the initial conditions (Equations 4.54, 4.55, 4.56, 4.57) complete the set of equations that describe the model. A summary of the equations used for each simulation is reported in Table 4.1.

All equations, summarised in Table 4.1 were modelled and solved using the gPROMS™ modelling environment (Process Systems Enterprise, 2009). The partial differential equations are solved using a 2nd order centered finite difference method with all domains uniformly discretised in 10 points in the axial direction.

Whilst solution for no ageing and slow ageing conditions does not present substantial challenges for the numerical solver, calculations for the constant heat flux cases at fast ageing
4.3 Solution method

Table 4.1: Summary of main model equations.

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<thead>
<tr>
<th>Equation No.</th>
<th>Domain</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.3</td>
<td>$\Omega_w$</td>
<td>Thermal balance.</td>
</tr>
<tr>
<td>4.4</td>
<td>$\Omega_w$</td>
<td>Heat flux.</td>
</tr>
<tr>
<td>4.11</td>
<td>$\Omega_l$</td>
<td>Thermal balance.</td>
</tr>
<tr>
<td>4.12</td>
<td>$\Omega_l$</td>
<td>Heat flux.</td>
</tr>
<tr>
<td>4.20</td>
<td>$\Omega_l$</td>
<td>Ageing model.</td>
</tr>
<tr>
<td>4.21</td>
<td>$\Omega_l$</td>
<td>Calculation flow area.</td>
</tr>
<tr>
<td>4.31</td>
<td>$\Omega_t$</td>
<td>Thermal balance.</td>
</tr>
<tr>
<td>4.32</td>
<td>$\Omega_t$</td>
<td>Heat flux.</td>
</tr>
<tr>
<td>4.33</td>
<td>$\Omega_t$</td>
<td>Flow velocity calculation.</td>
</tr>
<tr>
<td>4.34</td>
<td>$\Omega_t$</td>
<td>Friction factor calculation.</td>
</tr>
<tr>
<td>4.35</td>
<td>$\Omega_t$</td>
<td>Heat transfer coefficient calculation.</td>
</tr>
<tr>
<td>4.37</td>
<td>$\Omega_t$</td>
<td>Fouling model.</td>
</tr>
<tr>
<td>4.38</td>
<td>$\Omega_t$</td>
<td>Fouling thickness calculation.</td>
</tr>
<tr>
<td>4.39</td>
<td>$\Omega_t$</td>
<td>Effective fouling resistance calculation.</td>
</tr>
<tr>
<td>4.32, 4.43</td>
<td>$\Omega_w/\Omega_l$</td>
<td>Surface roughness models.</td>
</tr>
<tr>
<td>4.48</td>
<td>$\Omega_w/\Omega_l$</td>
<td>Boundary conditions.</td>
</tr>
<tr>
<td>4.51</td>
<td>$\Omega_t/\Omega_l$</td>
<td>Boundary conditions.</td>
</tr>
<tr>
<td>4.32</td>
<td>$\Omega_l$</td>
<td>Boundary conditions at tube inlet.</td>
</tr>
<tr>
<td>4.34</td>
<td>$\Omega_t$</td>
<td>Initial condition for fouling resistance.</td>
</tr>
<tr>
<td>4.35</td>
<td>$\Omega_t$</td>
<td>Initial condition for fouling layer thickness.</td>
</tr>
<tr>
<td>4.36</td>
<td>$\Omega_w,\Omega_l,\Omega_t$</td>
<td>Initial conditions for temperature.</td>
</tr>
<tr>
<td>4.37</td>
<td>$\Omega_t$</td>
<td>Initial condition for youth variable in the ageing model.</td>
</tr>
</tbody>
</table>

conditions proved to be more critical. The reason is that fast ageing produces steep profiles of the thermal conductivity in the radial direction (as reported in the results section) in regions close to the interface between domains $\Omega_l$ and $\Omega_t$. To ensure accuracy of the solution a mesh independency test was performed for the most challenging conditions (combination of fast ageing and fast fouling rates). Figure 4.4(a) reports the results of this test, showing that satisfactory accuracy is achieved using 3001 or more equally-spaced discretisation points. Figure 4.4(b)

![Figure 4.4](image)

**Figure 4.4:** Mesh independency test. Radial heat flux after a year in case of (a) fast and (b) intermediate ageing. Legend indicates the number of discretisation points used.
shows the absence of numerical problems when integrating under slow ageing conditions. For the simulations performed in this chapter, 3001 equally-spaced points were therefore used in the radial direction for the $\Omega_l$ domain, whereas 10 points were considered sufficient for $\Omega_w$.

### 4.4 Application

The geometric and physical property parameters for a base case representing a tube in a refinery exchanger are reported in Table 4.2 which also reports the fouling parameters, selected as being representative of typical refinery heat exchangers [Yeap et al., 2004], together with ageing and roughness model parameters. The inlet oil temperature and pressure were kept constant at 250°C and 30 bar. The model is initially used to assess the dynamic evolution of fouling resistance inside this typical refinery tube. The tube is operated in UHF conditions with no ageing (i.e. $A_a = 0$ s$^{-1}$ $E_a = 0$ kJ mol$^{-1}$ in Equation 4.20), which is investigated in Section 4.6, and no roughness dynamics (i.e. $e = e^0 = 10$ $\mu$m in Equation 4.41 and 4.43), explored in Section 4.5.

Figure 4.5(a) shows the variation of $R_f$ and $\delta$ over time at the inlet and outlet of the tube. Over time, the fouling layer builds up reaching a thickness of over 3.4 mm after one year of operation, equivalent to 15% of the clean tube diameter. Distributed effects can be appreciated in

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Units</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tube length</td>
<td>$L$</td>
<td>m</td>
<td>6.1</td>
<td>Typical plant value</td>
</tr>
<tr>
<td>Outer tube diameter</td>
<td>$d_o$</td>
<td>mm</td>
<td>25.4</td>
<td>Typical plant value</td>
</tr>
<tr>
<td>Inner tube diameter</td>
<td>$d_i$</td>
<td>mm</td>
<td>22.9</td>
<td>Typical plant value</td>
</tr>
<tr>
<td>Minimum roughness</td>
<td>$e^0$</td>
<td>$\mu$m</td>
<td>10</td>
<td>Reference</td>
</tr>
<tr>
<td>Maximum roughness</td>
<td>$e^\infty$</td>
<td>$\mu$m</td>
<td>150</td>
<td>[Kern, 1988]</td>
</tr>
<tr>
<td>Inlet temperature</td>
<td>$T_{in}$</td>
<td>˚C</td>
<td>250</td>
<td>Typical plant value</td>
</tr>
<tr>
<td>Mass flowrate</td>
<td>$m$</td>
<td>kg s$^{-1}$</td>
<td>0.3</td>
<td>Typical plant value</td>
</tr>
<tr>
<td>Inlet pressure</td>
<td>$P_{in}$</td>
<td>bar</td>
<td>30</td>
<td>Typical plant value</td>
</tr>
<tr>
<td>Uniform wall temperature</td>
<td>$T_0$</td>
<td>˚C</td>
<td>270</td>
<td>Typical plant value</td>
</tr>
<tr>
<td>Crude gravity</td>
<td>$^\circ$API</td>
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<tr>
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<td>$\rho$</td>
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<td>Crude specific heat at 250°C</td>
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<td>J kg$^{-1}$ °C$^{-1}$</td>
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<tr>
<td>Universal gas constant</td>
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<td>J K$^{-1}$ mol$^{-1}$</td>
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<td>[Perry and Green, 1997]</td>
</tr>
<tr>
<td>Fouling activation energy</td>
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<td>J mol$^{-1}$</td>
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<td>Yeap et al., 2004</td>
</tr>
<tr>
<td>Fouling deposition constant</td>
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<td>Yeap et al., 2004</td>
</tr>
<tr>
<td>Fouling suppression constant</td>
<td>$\gamma$</td>
<td>m$^2$ K N$^{-1}$ J$^{-1}$</td>
<td>7.3 x 10$^{-12}$</td>
<td>Yeap et al., 2004</td>
</tr>
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<td>Intermediate ageing pre–exponential factor</td>
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<td>–</td>
</tr>
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<td>Fast ageing pre–exponential factor</td>
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</tr>
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Figure 4.5: Fouling resistance and deposit layer thickness over time at tube inlet and outlet (a) and over space after 10 and 365 days (b) in UHF conditions.

Figure 4.5(b). After 10 days, the fouling layer is 9.4 µm thicker at the tube outlet than at the tube inlet whilst after a year of operations the difference becomes 230 µm. The associated reduction of cross-sectional area (over 50% of the clean cross-sectional area is occupied by deposits), has a dramatic effect on the pressure drop which increases by over 600% after one year reaching a value of over 0.2 bar (Figure 4.6).

In the following sections, the model above is used first to study the effect of roughness dynamics (Section 4.5) and then the impact of deposit ageing (Section 4.6) on heat transfer. Different timescales of investigation are considered in the two cases to reflect experimental evidence. Increase in roughness due to fouling affects the overall heat transfer coefficient within hours (Knudsen et al. 1999), whereas ageing is expected to manifest its effects over days or months of operation (Ishiyama et al. 2009b).

Figure 4.6: Pressure drop increase over time produced by the occlusion of the cross-sectional area caused by fouling in a single tube with UHF operation.
4.5 Impact of surface roughness dynamics

The effect of surface roughness on the initial stages of fouling was explored in the absence of deposit ageing (by setting $A_a$ to 0 s$^{-1}$) in order to de-couple the two effects. The time frame used is 80 h of operation, starting from an initially clean tube surface. Roughness is expected to give rise to measurements of apparent negative fouling resistance, as reported experimentally by [Knudsen et al., 1999] in the first 50 h of operation. Over this relatively short time scale the operating mode does not have a great influence on deposition, thus only the UWT case was investigated, with Equation 4.45 as the boundary condition at the tube outer wall. The linear and asymptotic models proposed to capture the roughness dynamics are investigated with particular reference to the impact of deposit roughness on overall heat transfer coefficient and thereby fouling resistance.

The parameter $k_p$ in the linear model (Equation 4.39) was arbitrarily fixed to 4, so that the timescale in which a negative fouling resistance is predicted by the model is within that experimentally observed by [Knudsen et al., 1999]. Simulations for other values of this parameter can be easily performed, as required. Figure 4.7(a) shows the variation of roughness over time in a section in the middle of the tube (i.e. $z = L/2 = 3$ m) for the linear model (Equation 4.41). At the deposition rate achieved in this case (to which the roughness is related) the final roughness value of 150 $\mu$m is reached after ca. 70 h of operation. Figure 4.7(b) shows the evolution of roughness at the same location given by the asymptotic model, Equation 4.43, for different

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**Figure 4.7:** Evolution of surface roughness at the tube mid–point ($z = L/2$) as a function of time for (a) linear (Equation (27)) and (b) asymptotic (Equation 4.41) models with different values of the constant $k_a$ compared to the no fouling case. When no fouling occurs, the roughness value remains at that of the clean tube, $e^0$, i.e. 10 $\mu$m.
values of the constant $k_a$, compared to the no fouling case. Depending on the value set for the $k_a$ parameter, the time at which the asymptotic value of roughness is reached changes. For $k_a = 1000$, 15 h are sufficient to reach the 150 $\mu$m considered as maximum roughness whereas for smaller values of the same parameter ($k_a = 50$ and $k_a = 100$), more than 80 h are needed. Due to the short time horizon, there is no significant difference in thickness along the length of the tube (only 1 $\mu$m after a year of operation). However, it becomes much larger inside the tubes for longer periods (see later Figure 4.14).

Figure 4.8(a) shows how the increase of surface roughness affects the tube–side convective heat transfer coefficient, $h$. For comparison the plot also shows the results for cases with constant roughness (at $e^0$ and $e^\infty$) and with no fouling. In the no fouling case, there are no variations in cross–sectional area or roughness to affect the heat transfer coefficient which therefore remains constant at the clean tube value, over the whole time horizon. With deposition and constant roughness, the reduction in cross–sectional area in both cases considered increases the oil velocity, giving a small rise to $h$ (barely noticeable in Figure 4.8(a) by comparison with the no fouling case). A linear variation in roughness, on the other hand, produces a large increase in the film convective heat transfer coefficient, from a clean tube value of 1800 W m$^{-2}$ K$^{-1}$ to about 2400 W m$^{-2}$ K$^{-1}$ after 70 hours, when the final deposit roughness of 150 $\mu$m is reached. When the asymptotic roughness model is used (Figure 4.8(b)), the increase in convective heat transfer is more rapid, depending upon the value for the parameter $k_a$ used. With both models, the value

![Figure 4.8](image_url)

**Figure 4.8:** Effect of surface roughness dynamics on the tube film heat transfer coefficient over time: (a) linear and (b) asymptotic models with different values of the parameter $k_a$. Figure (a) also shows the effect of deposit layer growth without any change in roughness (solid line, $e = 10$ $\mu$m).
4.5 Impact of surface roughness dynamics

Figure 4.9: Effects of surface roughness dynamics on overall heat transfer resistance over time: (a) linear and (b) asymptotic roughness models with different values of the constant $k_a$ compared to the no fouling case. Plot (a) also shows the result obtained for deposit growth with no change in roughness.

The increase in convective heat transfer coefficient is evident in the plot of the overall thermal resistance (Figure 4.9), calculated as the inverse of the overall heat transfer coefficient in Equation 4.40. In case of constant surface roughness (Figure 4.9(a)), set at a minimum value of $e = 10\,\mu m$, a linear increase in the overall thermal resistance, from the no fouling value (horizontal dashed-dotted line) is seen. The same linear behaviour is exhibited by the system for a constant $e = 150\,\mu m$; however the clean surface heat transfer resistance (at time zero) is smaller ($0.0010\, m^2K/W$) owing to the larger contribution to the convective heat transfer from a rougher surface. The linear roughness model (continuous line in Figure 4.9(a)) produces an initial decline in the overall thermal resistance below that of no fouling conditions over the first 17 h of operation. At this time the heat transfer enhancement given by the increase in roughness balances the decrease in heat transfer given by fouling deposition, i.e. the sum of the following two contributions is zero:

$$\frac{d}{dt}\left(\frac{1}{h}\right) + \frac{d\bar{R}_f}{dt} = 0$$  \hspace{1cm} (4.58)

At this time, the thickness of the fouling layer is 8.9 $\mu m$. Thereafter, the increase in the deposit layer resistance becomes larger but the overall resistance is still smaller than the no fouling value, which is reached after 40 h, when the thickness of the fouling layer is 20.6 $\mu m$. Figure 4.9(b) shows the results obtained with the asymptotic roughness model. A strong decline in heat
transfer resistance is observed over the first 10 h of operation for small values of parameter $k_a$, whereas it is limited to the first 5 h for larger values ($k_a = 500$). In the case of $k_a = 1000$, the two contributions in Equation 4.58 counterbalance after 2.5 h, when the thickness of the fouling layer is only 1.4 µm. In all cases, the overall heat transfer resistance is below the no fouling value for up to 52–55 h.

### 4.6 Impact of ageing

In this section, the impact of ageing on fouling and hence thermal and hydraulic performance of the exchanger tubes is investigated. Unlike deposit roughness, these effects typically impact medium and long term operation (timescales of weeks to months). The benefits of a distributed model are also highlighted.

Presently, due to a lack of detailed experimental data, the values of the parameters for the ageing kinetic model cannot be estimated. A parametric study showing the relative importance of the pre–exponential factor, $A_a$, and the activation energy, $E_a$, in Equation 4.20 was proposed by Ishiyama et al. (2009b), based on realistic estimates of the ageing parameters. In this thesis, the activation energy of the ageing reaction, $E_a$, was set at 50 kJ mol$^{-1}$. The ageing speed is governed by the values of the pre–exponential factor, $A_a$, and three cases were considered corresponding to fast ageing ($A_f = 10^{-2}$ s$^{-1}$), intermediate ageing ($A_i = 10^{-3}$ s$^{-1}$) and slow ageing ($A_s = 10^{-4}$ s$^{-1}$). Values for this parameter were set based on previous simulations (Ishiyama et al., 2009b).

The results in the following sections are reported for the two operating modes discussed earlier:

- Uniform heat flux (UHF). For comparison, the value of the heat flux in this case was selected to give the same initial wall outer temperature as in the following UWT mode.
- Uniform wall temperature (UWT), with an outer wall temperature of 270°C.

In both cases, the mass flowrate was fixed at 0.3 kg s$^{-1}$. The reduction in cross-sectional area caused by fouling is accompanied by an increase in pressure drop which must be compensated for by increasing pumping power. An alternative scenario, of constant pressure drop (i.e. mass flowrate decreasing over time), was explored by Ishiyama et al. (2009b), and is not repeated here. The inlet oil temperature was constant, at 250°C, in both cases.
4.6 Impact of ageing

4.6.1 Uniform heat flux (UHF) operation

In this case the deposition rate is almost constant, and the time transform in Equation 4.17 holds good.

The effects of ageing can be appraised by considering the temperature and thermal conductivity profiles within the deposit at different times. Figure 4.10 depicts, graphically, the thickness of the fouling layer in the case of fast ageing at three different times, namely after 30, 150 and 360 days of operation. The flow radius $R_{flow}$ defined in Equation 4.7 at each instant is termed as $R_{30d}$, $R_{150d}$, $R_{360d}$, respectively. The sizable reduction in duct flow diameter of 30%, (ca. 50% in cross-sectional area) after one year is evident.

Radial temperature profiles across the tube wall and the fouling layer located at the middle of the tube (i.e. $z = L/2 = 3$ m), at the above times, are reported in Figure 4.11 for the four cases of (a) no ageing, (b) slow, (c) intermediate, and (d) fast ageing. For consistency in the comparison with the next operating mode, the value for the heat flux fixed at the boundary is the same as the initial value at mid-point section of the tube in the UWT case. It is clear that in order to sustain the required rate of heat transfer the temperature at the wall has to increase. With no ageing (Figure 4.11(a)) and slow ageing (Figure 4.11(b)) the high thermal resistance given by a low-conductivity layer results in a large increase in this wall temperature (above 500°C after 6 months). Unrealistic values would clearly be reached over this and longer timescales. With intermediate and fast ageing (Figure 4.11(c) and (d)), for these operating parameters, the wall temperature remains below 450°C owing to the higher thermal conductivity of the aged deposit.

Figure 4.10: Graphical representation of fouling layer thickness after 10, 150 and 360 days for the case of UHF and fast ageing. After a year of operation, the cross-sectional area available for the fluid flow is reduced by ca. 50%.
which in turn reduces the impact of fouling on the overall heat transfer coefficient. Similar profiles were observed at other locations along the tube.

The consequence of UHF operation is that the surface temperature increases as fouling progresses, whereas with UWT operation the temperatures decrease. As a result, UHF operation causes a large change in thermal conductivity, even at the low ageing speed (Figure 4.12(b)). The asymptotic value of $\lambda_\infty$ is not reached after one year, but over half of the layer has doubled its thermal conductivity by this time. The limiting value, $\lambda_\infty^l$, is reached both with intermediate and fast ageing speeds ((Figure 4.12(b) and (c)). In particular, the combination of high temperature and fast ageing results in zones of steep change in thermal conductivity in the foulant layer close to the interface with the crude flow. In the limiting case, ageing would occur instantaneously.

In order to relate these results to current practice, it is useful to aggregate the distributed
values into the customary measure of fouling, the overall fouling resistance. The effect of ageing on the average fouling resistance, $\overline{R_f}$ (calculated via Equation 4.39) is presented in Figure 4.13. The higher the ageing rate, the lower the fouling resistance, as expected. The important result, that this thermal measure of fouling does not give an accurate representation of the deposit layer thickness (and associated pressure drop etc.), is evident.

The small deviation from linearity of the fouling profile for the no-ageing case shown in Figure 4.13 is due to the significant change in cross-sectional area available for flow caused by the high deposition rate (i.e. the parameters used in the fouling model). Curvature of the deposit layer affects the estimation of thermal resistance, but the main factor is the change in the suppression contribution to the deposition rate (Equation 4.37) causing the deposition rate to change from its initial value.
4.6 Impact of ageing

![Graph showing fouling resistance over time for different ageing speeds.](image)

**Figure 4.13:** UHF case: aggregate fouling resistance over time for different ageing speed.

### 4.6.2 Uniform wall temperature (UWT) operation

The distributed model is able to incorporate the effects of changing temperature conditions across the tube. In this case the deposition rate is expected to change owing to the change in deposit/liquid interface temperature. However, as noted in previous sections, when the deposition rate is not constant, Equation 4.17 represents a conservative estimate of the age of each element. The error introduced can be estimated by comparing, through simulations, the actual thickness with that obtained if the deposition rate throughout the operation was constant, at the initial values. As the fouling rate is temperature dependent, the assumption of linearity is least accurate for the case of constant wall temperature with slow ageing, where the surface temperature will change noticeably with time. In this particular case, the difference in thickness between the linear and the non–linear deposit–time profiles was not considered to be significant (less that 1% difference) over the first 80 days of operation, whereas the deviation reaches ca. 19% after a year of operation.

Figure [4.14](a) shows how the ageing speed affects the fouling layer thickness along the length of the tube after one year of operation. The faster the ageing, the larger is the portion of the fouling layer which, at a given time, has changed to a higher thermal conductivity value. This results in higher temperatures within and across the deposit, which in turn promotes deposition...
4.6 Impact of ageing

Figure 4.14: Fouling layer thickness along the tube with UWT: (a) after one year of operation, for different ageing speeds. Plot (b) shows the fouling layer thickness at the tube entry and exit over the last 60 days of operation for the fast ageing case.

and yields larger layer thicknesses. At the exit of the tube, there is a 40 µm difference between the no–ageing and fast ageing cases. Figure 4.14(b) shows the deposit thickness at the entry and exit sections of the tube over the last 60 days of one year of simulated operation for the fast ageing case (i.e. the worst case). The deposit thickness is greater at the exit, owing to the higher fluid–deposit interface temperature at this location. The difference is not large, mainly because the change in temperatures across the tube considered here is quite modest: much larger temperature changes can occur in operating units and the model can handle these readily. Figure 4.15 shows radial temperature profiles in the tube wall and the fouling layer at the mid–point of the tube (i.e. $z = L/2 = 3$ m), after 30, 150 and 360 days of operation in UWT mode for the four cases of (a) no ageing, (b) slow, (c) intermediate, and (d) fast ageing. After a year of operation, in all cases considered, there is a significant drop in temperature at the interface between the fouling layer and the flowing liquid. In the case of no–ageing (Figure 4.15(a)) and slow ageing (Figure 4.15(b)) the temperature profile shows a similar, linear trend. However, with intermediate and fast ageing (Figure 4.15(c) and (d)), the temperature profiles are no longer linear as a result of the changing thermal conductivity in the radial direction (see Figure 4.16). Most of the heat transfer resistance is developed across the younger, lower conductivity deposit layers located near the deposit/liquid interface. The layer–liquid interface temperatures at any one time in the four cases (a) to (d) are increasingly different, although this may not be so apparent from Figure 4.15 even after 360 days, due to the scales used in the graph. This is more clearly reflected in the tube exit temperature profiles, shown later in Figure 4.18. In the no–ageing case the thermal
Figure 4.15: Radial temperature profiles for a section at the tube mid–point with UWT in the case of (a) no–ageing, (b) slow, (c) intermediate, and (d) fast ageing. The vertical dotted line indicates the location of the tube wall, $R_i$.

conductivity is, by definition, constant at the initial value, $\lambda_0$, throughout the time horizon (Figure 4.16(a)). Ageing causes an increase in thermal conductivity at coordinates close to the tube metal wall as a consequence of the combined effect of exposure time and high temperature. In the case of slow ageing (Figure 4.16(b)), this increase is modest (ca. 20%) compared to that in case of intermediate ageing in Figure 4.16(c) (ca. 150%). Both cases show a linear variation of $\lambda_i$ along the radial coordinate and the final value of thermal conductivity typical of coke deposits, $\lambda_\infty$, is not reached over this timescale. With fast ageing (Figure 4.16(d)), the profile is no longer linear and after six months of operation a 5 fold increase in $\lambda_i$ (from $\lambda_0$ to $\lambda_\infty$) is reached in regions close to the tube wall. With time, other sections along the radial coordinate increase their thermal conductivity, approaching the asymptotic value, $\lambda_\infty$. After a year of operation, ca. 8% of the deposit layer has a thermal conductivity above 0.99 W m$^{-1}$K$^{-1}$, indicating an almost complete
4.6 Impact of ageing

Figure 4.16: Deposit thermal conductivity distribution for a section at the tube mid–point with UWT in the case of (a) no–ageing, (b) slow ageing, (c) intermediate, and (d) fast ageing.

change to ‘coke’ in that section.

For comparison with the previous UHF case, Figure 4.17 reports the average fouling resistance, \( \bar{R}_f \) (calculated via Equation 4.39). The trend shown with the changing speed of ageing is the same as the UHF case (Figure 4.13), however, a larger deviation with respect to the no–ageing case is seen in the latter case which further highlights the importance of considering ageing in accelerated fouling tests.

At a macroscopic level, a beneficial effect of ageing can be observed on the oil temperature at the tube outlet (Figure 4.18). The increase in thermal conductivity given by fast ageing (as reflected by the fouling resistance in Figure 4.17) produces a slower decline in outlet temperature compared to the case with slower or no ageing. This difference in outlet temperature results in
a significant difference between the fouling Biot number, $\text{Bi}_f = \bar{R}_f \bar{h}$, in the different cases considered. After a year of operation, in fact, $\text{Bi}_f$ for the no ageing case is ca. 86 whereas it is ca. 40% less in the case of fast ageing ($\text{Bi}_f = 52$).

**Figure 4.17**: Aggregate fouling resistance over time for different ageing speed in case of UWT as calculated via Equation 4.39.

**Figure 4.18**: Effect of ageing speed on crude oil outlet temperature in case of UWT.
4.7 Concluding remarks

A distributed model for a single tube undergoing crude oil fouling has been developed in this chapter. This uses a novel way of modelling the continuous growth of deposit distributed over time and space, via a moving boundary approach which provides a sound and general formulation as a set of partial differential and algebraic equations in cylindrical coordinates. A suitable transformation in the time domain allowed incorporating an ageing model. It has been shown that this approach is rigorously valid for the special case of linear deposition, whereas it represents a reasonable approximation in other cases. However, several assumptions introduced by previous authors were overcome:

- The underlying fouling model includes a suppression term (the Ebert–Panchal model was used here, but in principle other deposition–suppression models could be used).
- The use of cylindrical coordinates overcomes the need for a ‘thin slab’ assumption and allows modelling large deposits relative to tube diameter.
- A local ageing history can be calculated for each point along the length of the deposit, rather than an overall, ‘lumped’ value for averaged conditions.
- The assumption of constant deposit roughness was relaxed with the use of two novel models proposed to capture the effects of deposition on roughness and heat transfer. Whilst the underlying physics of the evolution of roughness is unknown, the models represent plausible approximations.

Geometry, flowrate (fixed to a constant value) and fouling behaviour used in the studies presented are typical of oil refineries.

Results show that the roughness model can explain some puzzling phenomena such as (apparent) initial negative fouling resistance that cannot be captured otherwise. Accounting for roughness dynamics is therefore important to aid interpretation of short time–scale pilot–scale tests.

To appreciate the effects of ageing, simulations were performed for two typical operating modes (UWT and UHF). The results highlight the importance of considering deposit formation and ageing in industrial applications where the timescale is of weeks to several months. They show that even for the case considered as slow ageing the impact on the fouling resistance is significant. Moreover, it has been highlighted how ageing thermal measure of fouling alone does
not give an accurate representation of the deposit layer thickness (and associated pressure drop etc.).

Finally it should be noted that the fouling and ageing models are independent from each other and the latter can be applied to different fouling mechanisms as long as the evolution in thermal conductivity can be satisfactorily described by first order kinetics.

Overall, the model enables capturing and improving our understanding of the complex interaction between thermal, hydraulic and ageing effects in a fouling heat exchanger tube. The results presented are clearly applicable to other geometries (annular tubes) and full scale equipment (multi–pass heat exchangers). Validation of various model components (e.g. surface roughness, ageing) and estimation of key parameters for others (e.g. fouling model) will require quality experimental data currently not available.

The capabilities of the detailed model developed in this chapter will be exploited in the following one to build a model for an entire shell–and–tube heat exchanger undergoing crude oil fouling.
Chapter 5

A dynamic, distributed model of shell–and–tube heat exchangers undergoing crude oil fouling

Synopsis

The mathematical model for a single tube undergoing crude oil fouling developed in the previous chapter is used here as building block to model one tube–side pass of a shell–and–tube heat exchanger. Single–pass models are then linked together to describe a multi–pass unit. Coupling the multi–pass tube–side model to a shell–side model, also presented here, allows capturing the dynamic behaviour of an industrial heat exchanger as a function of local conditions and time. Furthermore, a procedure to analyze refinery data and support the estimation of a set of model parameters is established. The model is validated using data from existing refineries operated by major oil companies and shows excellent agreement (less than 2% error) with primary plant temperature measurements even when it is tested for its predictive capabilities over long periods (i.e. up to 550 days).
5.1 Introduction

The heat exchanger model derived in this chapter inherits the key properties of the single tube model derived in Chapter 4. It is dynamic and distributed and takes into account local fouling rates as a function of process conditions and time. The ageing model, also developed in Chapter 4, is included to account for the change in thermal conductivity of the deposits over the radial direction and time. However, given the large time–scale considered in industrial units, the roughness model is not included and a different expression for the tube–side heat transfer coefficient and friction factor are considered in the full heat exchanger model. In particular, this chapter aims at:

1. Extending the tube model presented in Chapter 4 to a multi–pass shell–and–tube heat exchanger.
2. Devising a procedure to systematically analyse plant data and to estimate necessary model parameters using raw plant measurements (i.e. temperatures and flowrates) rather than derived fouling resistances.
3. Validating the model with plant measurements and testing it for its predictive capabilities, against primary quantities directly measured (temperatures).

5.2 System definition

The mathematical model proposed here is for a multi–pass tubular heat exchanger undergoing crude oil fouling on the tube–side. It is acknowledged that fouling can also occur on the shell–side (for example, when heavy crude fractions are used as heating fluid or if the crude is switched to the shell–side for design reasons). Unless independent pressure drops measurements (typically not available) are used, it is not easy to determine with certainty whether fouling is occurring on the tube–side only. However, visual inspection when the exchangers are dismantled for cleaning indicate that very often tube–side fouling is the dominant resistance to heat transfer. This is due to a number of reasons. First, the most foulant liquid is often allocated on the tube side for ease of cleaning purposes. Second, the more complex flow path prevents deposition to occur on the shell–side. Counter–intuitively, initial fouling on the shell–side can also have a beneficial effect as deposits accumulate on the leakage areas (i.e. clearance tube–to–baffle hole, shell–to–baffle and shell–to–tube bundle) which typically depress the convective heat transfer coefficient.
### Table 5.1: Input geometric parameters required for the shell–and–tube model.

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<thead>
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<th>Parameter</th>
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<th>Parameter</th>
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<td>(B_c)</td>
<td>%</td>
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<td>mm</td>
<td>Tube outer diameter</td>
<td>(N_b)</td>
<td>–</td>
<td>Number of baffles</td>
</tr>
<tr>
<td>(d_i)</td>
<td>mm</td>
<td>Tube inner diameter</td>
<td>(N_t)</td>
<td>–</td>
<td>Total number of tubes</td>
</tr>
<tr>
<td>(L)</td>
<td>m</td>
<td>Tube length</td>
<td>(N_p)</td>
<td>–</td>
<td>Number of tube pass</td>
</tr>
<tr>
<td>(L_{tp})</td>
<td>mm</td>
<td>Tube pitch</td>
<td>(N_{ss})</td>
<td>–</td>
<td>Number of sealing strips (pairs)</td>
</tr>
<tr>
<td>(\theta_{tp})</td>
<td>deg</td>
<td>Tube pitch angle</td>
<td>(L_{bb})</td>
<td>mm</td>
<td>Diametral clearance (d_o)–to–baffle</td>
</tr>
<tr>
<td>(L_{bi})</td>
<td>mm</td>
<td>Inlet baffle spacing</td>
<td>(L_{bb})</td>
<td>mm</td>
<td>Diametral bypass clearance shell–to–tube bundle</td>
</tr>
<tr>
<td>(L_{bc})</td>
<td>mm</td>
<td>Central baffle spacing</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>(L_{bo})</td>
<td>mm</td>
<td>Outlet baffle spacing</td>
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</table>

The exchanger considered is of TEMA type AET (i.e. single pass shell, front end stationary head with removable cover and floating head at the rear end) of length \(L\). However, the model can be used for shell type E with different front and rear head types (e.g. bonnet, floating head, U tube bundle etc.) but will require some adaptation to consider different shell types (e.g. two pass with longitudinal baffle, F shell, or divided flow, J shell). The geometry of each exchanger is defined by typical geometric parameters summarised in Table 5.1 and can be readily extracted by technical drawings typically available at the refineries.

Figure 5.1 depicts the physical system, which is divided in 4 distinct control volumes (domains):

\(\Omega_s\) : The shell–side domain. It is the volume of the exchanger shell outside the tubes.

\(\Omega_{w,n}\) : The tube wall domain, defined as the region between the inner radius of the tube, \(R_i\), and its outer radius, \(R_o\).

\(\Omega_{l,n}\) : The deposit layer domain, defined as that between the crude oil/deposit layer interface (at the flow radius, \(r = R_{flow}\)) and the inner radius of the tube, \(R_i\).

\(\Omega_{t,n}\) : The tube–side domain, defined between the centre of a tube \((r = 0)\) and the interface with the fouling layer, \(R_{flow}\).

The subscript \(n\) is used to indicate the pass number and varies between 1 and the total number of passes on the tube–side, \(N_p\). The model is one dimensionally distributed along the \(z\) axis for the tube–side and shell–side domains (\(\Omega_t\) and \(\Omega_s\)). In the fouling layer and wall domains (\(\Omega_l\) and \(\Omega_w\)) the model is distributed along both the axial and the radial coordinate to capture phenomena occurring in the radial direction. An example of such phenomena is the ageing of the deposits outlined in Section 2.4.3.5 and modelled in Section 4.2.2.1.

Being distributed only axially, the shell–side is assumed to have the same temperature radially,
at a given $z$ coordinate in the heat exchanger. Each tube in the same pass is assumed to experience the same temperature difference relative to the shell. The driving force for heat exchange is therefore the same for each tube in the same pass $n$. As all tubes in each pass behave similarly, the system can be conceptualized as shown in Figure 5.2 where a single tube per pass is actually modeled and considered representative of all other tubes in the same pass (however, in practice the shell–side flow is not parallel to the tubes, as discussed later). Headers are considered perfectly mixed and all entrance effects at the tube entrances and exits (i.e. $z = 0$ and $z = L$) and heat losses are neglected.

![Figure 5.2: Schematic representation of a 1 shell, 2 tube pass heat exchanger in case of first tube pass flow in co-current (a) and counter-current (b) with the shell–side flow. The heat transfer coefficient for the shell–side takes into account deviation from co/counter-current flow due to cross-flow.](image)

**Figure 5.1:** Shell–and–tube heat exchanger model domains definition and reference system.
The physical properties of the crude oil flowing in the tube such as density, \( \rho \), viscosities, \( \mu \) and \( \nu \), thermal conductivity, \( \lambda \) and heat capacity, \( c_p \), are calculated using API relationships (Riazi, 2005) as functions of temperature and space.

5.3 Model equations

In the following sections the governing equations of the model are given, together with suitable boundary and initial conditions. Equations for domain \( \Omega_{w,n} \), \( \Omega_{l,n} \) and \( \Omega_{t,n} \) are similar to those derived in Section 4.2. The model equations for the heat balance in the \( \Omega_s \) domain are derived from first principles below.

5.3.1 Shell–side

The heat balance on the shell as the control volume (domain \( \Omega_s \) defined for \( z = [0, L] \)) is as follows.

The rate of energy accumulation (term in first bracket in Equation 4.1) in the control volume (in Joules) is given by:

\[
\{1\} = \left( \rho_s c_{p,S} T_s A_s \Delta z \right)_{z+\Delta z, t} - \left( \rho_s c_{p,S} T_s A_s \Delta z \right)_{z, t} \tag{5.1}
\]

where \( T_s \) is the shell–side fluid temperature function of the axial coordinate (i.e. \( T_s(z) \)) whereas \( \rho_s \) and \( c_{p,S} \) are, respectively, its density and specific heat capacity also function of the axial coordinate. The cross–sectional area of the shell, \( A_s \), is given by:

\[
A_s = \frac{\pi}{4} \left( D_s^2 - d_o^2 N_t \right) \tag{5.2}
\]

In Equation 5.2, \( N_t \) is the number of tubes of external diameter \( d_o = 2R_o \), and \( D_s \) is the inner shell diameter.

The energy flowrate (term in the second bracket in Equation 4.1) at the inlet and the outlet of differential control volume \( \Delta z \) is:

\[
\{2\} = \left( \rho_s c_{p,S} T_s u_s A_s \right)_{z, t} \Delta t - \left( \rho_s c_{p,S} T_s u_s A_s \right)_{z+\Delta z, t} \Delta t \tag{5.3}
\]
The heat conduction (term in the third bracket in Equation 4.1) in the shell is:

\[
\{3 \} = q_s'' A_s \frac{\Delta t}{z_f} - q_s'' A_s \frac{\Delta t}{z_f + \Delta z_f} \Delta t
\]

(5.4)

where \(q_s''\) is the shell–side heat flux in the axial direction:

\[
q_s'' = -\lambda_s \frac{\partial T_s}{\partial z}
\]

(5.5)

Substituting \(q_s''\) in Equation 5.4 yields:

\[
\{3 \} = \left[ -A_s \lambda_s \frac{\partial T_s}{\partial z} \right]_{z_f}^{z_f + \Delta z} \Delta t - \left[ -A_s \lambda_s \frac{\partial T_s}{\partial z} \right]_{z_f + \Delta z_f}^{z_f + \Delta z} \Delta t
\]

(5.6)

Assuming an adiabatic unit (i.e. no heat loss to the environment through the shell), The heat source term (fourth bracket in Equation 4.1) is given by total heat exchanged between the shell–side fluid and the tube walls over all passes:

\[
\{4 \} = q_s''' = \sum_{n=1}^{N_p} Q_{\Delta z,n} \cdot \Delta t
\]

(5.7)

In Equation 5.7, \(Q_{\Delta z,n}\) is the heat exchanged between shell–side fluid and the tube wall in each pass (0 \(\leq n \leq N_p\)):

\[
Q_{\Delta z,n} = P_{S,n} \Delta z h_f \left( T_s - T_{w,n} \right)_{r=R_o}
\]

(5.8)

where \(N_p\) is the number of tube passes and \(P_{S,n}\) is the wetted perimeter from which heat is exchanged:

\[
P_{S,n} = 2\pi R_o \frac{N_t}{N_p}
\]

(5.9)

As noted, all tubes in the same pass, \(n\), of the unit are considered to exchange the same amount of heat with the shell as the driving force, \(Q_{\Delta z,n}\) in Equation 5.8 is the same.

The net work from the control volume to its environment is neglected:

\[
\{5 \} = 0
\]

(5.10)

Putting the above terms together into Equation 4.1 dividing by the constant quantities \(A_s, \Delta t, \Delta z\)
5.3 Model equations

Figure 5.3: Flow stream though the sell–side according to [Tinker (1958)]. Stream A is the leakage stream baffle tube hole to tube wall, Stream B is the main effective cross–flow stream, Stream C is the bundle bypass stream between the bundle and the shell wall, Stream E is the leakage stream between baffle edge and shell wall, Stream F is the bypass stream in flow channels due to omission of tubes in the tube pass partition.

and taking the limit for $\Delta t \to 0$ and $\Delta z \to 0$ yields:

$$\frac{\partial}{\partial t} \left( \rho_s c_{p,s} T_s \right) = -\frac{\partial}{\partial z} \left( \rho_s c_{p,s} T_s u_s \right) + \frac{\partial}{\partial z} \left( \lambda_s \frac{\partial T_s}{\partial z} \right) + \frac{1}{A_s} \sum_{n=1}^{N_p} P_{S,n} h_s \left( T_s - T_{w,n} \right)_{r=R_o}$$  \hspace{1cm} (5.11)

A variable direction term, $\text{dir}_s=\pm 1$ is introduced to take into account the internal arrangement, with respect to the direction of the flow in the first tube pass:

$$\frac{\partial}{\partial t} \left( \rho_s c_{p,s} T_s \right) = -\text{dir}_s \frac{\partial}{\partial z} \left( \rho_s c_{p,s} T_s u_s \right) + \frac{\partial}{\partial z} \left( \lambda_s \frac{\partial T_s}{\partial z} \right) + \frac{1}{A_s} \sum_{n=1}^{N_p} P_{S,n} h_s \left( T_s - T_{w,n} \right)_{r=R_o}$$  \hspace{1cm} (5.12)

where $\text{dir}_s=1$ if the first tube pass is in co–current flow (Figure 5.2a), $\text{dir}_s=-1$ otherwise (Figure 5.2b). The shell–side heat transfer coefficient, $h_s(z,t)$ are calculated through the Bell–Delaware method as modified by [Taborek (2002a)]:

$$h_s = h_{id} J_c J_l J_b J_s J_r$$  \hspace{1cm} (5.13)

where $h_{id}(z,t)$ is the heat transfer coefficient for ideal cross–flow. The deviation from ideality of the heat transfer coefficient caused by leakage streams (Figure 5.3) is taken into account by introducing the correction factors $J_c, J_l, J_b, J_s$, and $J_r$ for, respectively, the baffle cut, the baffle leakage (A and E streams), the bypass tube bundle to shell (C and F streams), the laminar heat transfer and the non equal inlet/outlet baffle spacing. Details of the calculations are given by
5.3 Model equations

Taborek (2002a) and not reported here. The only difference with the standard calculation is the dependence on the spatial position of the ideal heat transfer coefficient:

\[ h_{id} = h_{id}(z, t) \]  

(5.14)

It should be noted that, whilst in Equation 5.12 the fluid velocity is assumed to be parallel to the tubes, the heat transfer coefficient in Equation 5.13 does take into account the variation in heat transfer produced by a more complex flow path. This is clearly an approximation in the calculation of the convective term in Equation 5.12 used to reduce computational effort. More complex ways of describing shell–side flow and the heat transfer coefficient, reported in Section 3.5, would require extra computational power at the parameter estimation stage or when a network simulations is performed (see Chapter 6). An a posteriori model validation against plant data (reported in Section 5.7 and Section 5.8) shows that the overall error introduced with this approximation is acceptable.

The shell–side pressure drop, \( \Delta P_s \), are calculated, following the Bell–Delaware method, as the sum of the cross–flow pressure drop between baffle tips, \( \Delta P_c \), the pressure drop in the baffle window, \( \Delta P_w \), and the pressure drops in the inlet and outlet baffles, \( \Delta P_e \):

\[ \Delta P_s = \Delta P_c + \Delta P_w + \Delta P_e \]  

(5.15)

The reader is again referred to Taborek (2002a) for details on the calculations.

5.3.2 Tube wall

For the tube wall (domain \( \Omega_w \), defined for \( z=[0, L] \), and \( r=[R_i, R_o] \)), the heat conduction equation 4.3 is used for each pass, \( n \), under the same assumptions given in Section 4.2.1:

\[ \frac{\rho_w c_{p,w}}{\lambda_w} \frac{\partial T_{w,n}}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T_{w,n}}{\partial r} \right) + \frac{\partial^2 T_{w,n}}{\partial r^2} \]  

(5.16)

where \( T_{w,n} \) denotes the temperature in each pass as a function of \( (z,r,t) \) whilst \( \rho_w \), \( c_{p,w} \) and \( \lambda_w \), are, respectively, the density, the specific heat capacity and the thermal conductivity of the tube.
metal wall, considered constant. The heat flux, for each pass, is calculated as:

\[ q''_{w,n} = -\lambda_w \frac{\partial T_{w,n}}{\partial r} \]  

\[ (5.17) \]

### 5.3.3 Deposit layer

Similarly to what reported in Section 4.2.2, the deposit layer (dimensionless domain \( \tilde{\Omega}_l \), defined for \( z=[0, L] \), and \( r=[0, 1] \)) is modelled as a conductive domain, neglecting variations in the axial direction:

\[ \frac{\delta^2}{\delta \tilde{r}^2} \rho_l c_{p,l} \frac{\partial T_{l,n}}{\partial t} = \frac{\partial \lambda_{l,n} \frac{\partial T_{l,n}}{\partial \tilde{r}}}{\partial \tilde{r}} - \frac{\lambda_{l,n} \delta_n}{R_l - \tilde{r} \delta_n} \frac{\partial T_{l,n}}{\partial \tilde{r}} + \lambda_{l,n} \frac{\partial^2 T_{l,n}}{\partial \tilde{r}^2} \]  

\[ (5.18) \]

Here, \( T_{l,n} \) is the local temperature and \( \lambda_{l,n} \) the thermal conductivity, both of which are functions of the spatial coordinates \( z, \tilde{r} \) and time (i.e. \( T_{l,n} = T_{l,n}(z, \tilde{r}, t) \) and \( \lambda_{l,n} = \lambda_{l,n}(z, \tilde{r}, t) \)). The density of the deposit layer, \( \rho_l \) and its heat capacity, \( c_{p,l} \), are assumed uniform and constant. As already noted in Chapter 4, formulating the model in cylindrical coordinates allows accounting for curvature effects in the radial heat flux thus overcoming the thin slab approximation used in other models. The radial heat flux at any point in the deposit layer is in fact calculated from Equation 4.12 as:

\[ q'_{l,n} = \frac{\lambda_{l,n}}{\delta_n} \frac{\partial T_{l,n}}{\partial \tilde{r}} \]  

\[ (5.19) \]

Equation 5.18 and 5.19 account for the variation of the thermal conductivity in the radial direction which is calculated using the ageing model in Equation 4.13.

### 5.3.4 Tube–side

The energy balance equation used for a given pass, \( n \), is the same as the one derived in Equation 4.31:

\[ \frac{\partial}{\partial t} \left( \rho_n c_{p,n} T_n A_{flow,n} \right) = -\frac{\partial}{\partial z} \left( \rho_n u_n c_{p,n} T_n A_{flow,n} \right) + \frac{\partial}{\partial z} \left( \lambda_n A_{flow,n} \frac{\partial T_n}{\partial z} \right) + P_n h_n \left( T_n \bigg|_{r=R_{flow}} - T_n \right) \]  

\[ (5.20) \]

As previously noted for Equation 4.31, Equation 5.20 takes into account the variation of the cross–sectional area given by the fouling layer and no assumptions on the physical properties (e.g. constant density, thermal conductivity or heat capacity) have been made. A variable \( dir = \pm 1 \) is
introduced to take into account the direction of the velocity depending on the pass:

\[
\frac{\partial}{\partial t} \left( \rho_n c_{p,n} T_n A_{\text{flow},n} \right) = -\text{dir}_n \frac{\partial}{\partial z} \left( \rho_n c_{p,n} T_n u_n A_{\text{flow},n} \right) + \frac{\partial}{\partial z} \left( \lambda_n A_{\text{flow},n} \frac{\partial T_n}{\partial z} \right) + P_n h_n \left( T_{l,n}\big|_{r=R_{\text{flow}}} - T_n \right)
\]  

(5.21)

where \( \text{dir} = 1 \) in case of an odd pass, \( \text{dir} = -1 \) in case of even pass.

### 5.3.4.1 Hydraulics

The hydraulic effect of fouling (reduction of flow section in pipes on velocities and pressure drop) is captured through the definition of the flow radius, \( R_{\text{flow}} \), in Equation 4.7, and the flow area, \( A_{\text{flow}} \), in Equation 4.21 as detailed in Section 4.2.3.1. The velocity, \( u_n \), the same in each tube of a given pass, is function of this flow radius:

\[
u_n = \frac{\dot{m}}{\rho_n A_{\text{flow},n} N_t/N_p}
\]  

(5.22)

where \( N_t \) is the total number of tubes. The pressure drop inside each tube also reflects the interaction with the growth of the fouling inside the tubes and is calculated in each pass by:

\[
\frac{dP_n}{dz} = C_{f,n} \frac{\rho_n u_n^2}{4 R_{\text{flow},n}}
\]  

(5.23)

In this case, given that roughness dynamics effects is neglected, the Fanning friction factor, \( C_{f,n} \), is solely dependent on the Reynolds number, \( Re \). For rough tubes it is possible to write (Yeap et al., 2004):

\[
C_{f,n} = 0.0035 + 0.264 \text{Re}_n^{-0.42}
\]  

(5.24)

The overall tube–side pressure drop, \( \Delta P \) across the heat exchanger is calculated as the difference between inlet and outlet value of the pressure calculated with Equation 5.23:

\[
\Delta P = P_{out} - P_{in}
\]  

(5.25)

The total pumping power required, \( W \), is related to the mass flowrate, \( \dot{m} \) and the total pressure drop across the tubes, \( \Delta P \) as follows:

\[
W = \frac{\dot{m}}{\rho} \Delta P
\]  

(5.26)
Another effect of the interaction of the fouling layer with the fluid flow is through the heat transfer coefficient on the tube–side. It is well acknowledged in literature that one of the main limitations in the design of heat exchangers is the use of constant values of the heat transfer coefficient (Gardner and Taborek, 1977). Takemoto et al. (1999) showed that by neglecting the effect of heat transfer coefficient variation through an exchanger, it is possible to become misled into believing that a heat exchanger may be fouled when actually it is clean.

Here, the heat transfer coefficient in each pass, \(h_n\), is considered distributed across the axial direction and affected by the growth of the fouling layer within the tube:

\[
h_n = \frac{\lambda_n \text{Nu}_n}{2R_{\text{flow},n}} \quad (5.27)
\]

where \(\text{Nu}_n(z, t)\), the Nusselt number in each tube pass, function of the Reynolds and Prandtl ones, can be calculated through the Dittus–Boelter relationship (Hewitt et al., 1994):

\[
\text{Nu}_n = 0.023 \text{Re}_n^{0.87} \text{Pr}_n^{0.4} \quad (5.28)
\]

Equation \(5.27\) is valid (with a standard deviation of 13%) for \(0.7 < \text{Pr} < 160, \text{Re} > 10^4\) and a ratio between the length of the pipe and its diameter \(> 10\) (Hewitt et al., 1994). It can also be noted from Equation \(5.28\) that \(h_n\) is enhanced by the progressive reduction in cross–sectional area.

The wall shear stress in each tube pass, \(\tau_n(z, t)\), is calculated as a function of the Reynolds number through the following (Wilkes, 2005):

\[
\tau_n = C_{f,n} \left( \frac{\rho_n u_n^2}{2} \right) \quad (5.29)
\]

where \(C_{f,n}\) is the Fanning friction factor, given by Equation \(5.24\).

### 5.3.4.2 Fouling model

Fouling is captured by the modified Ebert–Panchal model (Panchal et al., 1999) and extended to distributed systems:

\[
\frac{dR_{f,n}}{dt} = \alpha \text{Re}_n^{-0.66} \text{Pr}_n^{-0.33} \exp \left( \frac{-E_f}{R_n T_{f,n}} \right) - \gamma \tau_n \quad (5.30)
\]
where $T_{f,n}$ is the film temperature calculated as (see Equation 2.4):

$$T_{f,n} = T_n + 0.55(T_{ln,R_{film}} - T_n) \quad (5.31)$$

Once the fouling rate is known through Equation 5.30, the fouling layer thickness in each pass, $n$, can be calculated by:

$$\frac{d\delta_n}{dt} = \lambda_0 \frac{dR_{f,n}}{dt} \quad (5.32)$$

The average fouling resistance per pass, is calculated as follows:

$$\bar{R}_{f,n} = \frac{1}{L} \int_0^L \left( \int_0^1 \frac{\delta_n}{\lambda_{l,n}} d\tilde{r} \right) dz \quad (5.33)$$

An overall average fouling resistance, $\bar{R}_f$, useful for comparison reasons with aggregate models can be defined:

$$\bar{R}_f = \frac{1}{N_s} \sum_{i=1}^{N_p} \frac{\bar{R}_{f,n}}{N_p L} \quad (5.34)$$

where, $N_p$ is the number of tube–side passes per shell whilst, for a multi–shell unit, $N_s$ is the number of shells per unit.

### 5.3.5 Boundary conditions

At the shell–side inlet:

$$T_{s|z=0} = T_{s,\text{in}} \quad (5.35)$$

At the interface between the shell–side domain, $\Omega_s$, and the tube wall, $\Omega_w$:

$$q''_{w,n|r=R_w} = -h_s \left( T_s - T_{w,n|r=R_w} \right) \quad (5.36)$$

At the interface between $\Omega_w$ and $\Omega_i$ there is continuity in heat flux and temperature:

$$q''_{w,n|r=R_i} = q''_{l,n|r=R_i} \quad (5.37)$$

$$T_{w,n|r=R_i} = T_{l,n|r=R_i} \quad (5.38)$$
At the moving boundary between the fouling layer, $\Omega_l$, and the tube–side domain $\Omega_t$ there is continuity in the heat flux:

$$q''_{ln}|_{r=R_{flow}} = -h(T_{ln}|_{r=R_{flow}} - T_n)$$  \hspace{1cm} (5.39)

At the tube inlet, for a counter–current pass ($dir_n = 1$):

$$T_{n|z=0} = T_{in}$$  \hspace{1cm} (5.40)

$$P_{n|z=0} = P_{in}$$  \hspace{1cm} (5.41)

whereas for a for co–current pass ($dir_n = -1$):

$$T_{n|z=L} = T_{in}$$  \hspace{1cm} (5.42)

$$P_{n|z=L} = P_{in}$$  \hspace{1cm} (5.43)

### 5.3.6 Initial conditions

At time 0 the heat exchanger is assumed to be clean (i.e. no fouling resistance):

$$R_{f,n}|_{t=0} = 0$$  \hspace{1cm} (5.44)

The thickness of fouling layer, $\delta_n$, in each pass, $n$, is initialised to $10^{-7}$ m for numerical reasons:

$$\delta_{n|t=0} = 10^{-7}$$  \hspace{1cm} (5.45)

The temperature profiles at time 0 are assumed to be in steady state in all domains:

$$\left.\frac{dT_s}{dt}\right|_{r=0} = \left.\frac{dT_w,n}{dt}\right|_{r=0} = \left.\frac{dT_{ln}}{dt}\right|_{r=0} = \left.\frac{dT_n}{dr}\right|_{r=0} = 0$$  \hspace{1cm} (5.46)

The ageing model given by Equation introduces a differential equation which needs an initial value of the youth variable:

$$y_{t=0} = 1$$  \hspace{1cm} (5.47)
5.4 Estimation of model parameters

Fluid physical properties, namely density, $\rho$, viscosities, $\mu$ and $\nu$, thermal conductivity, $\lambda$ and heat capacity, $c_p$; can vary substantially depending on the blend processed in the refinery — typically changed every 2–3 days — and are also temperature dependent. The same crude therefore changes its physical properties within a unit. Ideally, if the composition is known at all times, it can be used as input to thermodynamic packages that can be interfaced with the heat exchanger model to capture variations in physical properties. However, this is usually not the case and the properties of the fluids passed on both sides of the exchanger are unknown. The same established relationships used in Chapter 4 are used here (Riazi, 2005) to capture the temperature dependence of the physical properties. These are based on few inputs, namely °API, mean average boiling point, MeABP, and kinematic viscosity at 100°F, $\nu_{100^\circ F}$. If, as it usually happens in practice, these inputs are not known a priori, they are treated as a set of parameters that is to be estimated from plant data according to the procedure detailed in this section. This set of parameters will be referred to as Set A and includes the physical properties (i.e. °API, MeABP and $\nu_{100^\circ F}$) of the fluids on both shell–and–tube–side.

Another set of parameters, Set B, including the activation energy, $E_f$; pre–exponential deposition constant, $\alpha$ and suppression constant, $\gamma$ in the fouling model (Equation 5.30) is also to be estimated from plant data for each shell comprised in the unit under investigation. They are expected to vary from crude to crude but are also specific of the unit under consideration. Table 5.2 reports a summary of the 9 model parameters in the two different sets.

In order to decouple the estimations accordingly to the related phenomena, parameters included in Set A, which do not depend on fouling, should be estimated over a period of time in which fouling is not yet initiated and the exchanger can be considered clean. On the contrary, parameter set B should be estimated over a longer period where fouling is affecting

<table>
<thead>
<tr>
<th>Parameter set A</th>
<th>Units</th>
<th>Parameter set B</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shell–side fluid API</td>
<td>°API</td>
<td>$\alpha$</td>
<td>K m$^2$ W$^{-1}$ s$^{-1}$</td>
</tr>
<tr>
<td>Shell–side fluid $\nu_{100^\circ F}$</td>
<td>cSt</td>
<td>$E_f$</td>
<td>J mol$^{-1}$</td>
</tr>
<tr>
<td>Shell–side fluid MeABP</td>
<td>°C</td>
<td>$\gamma$</td>
<td>m$^3$ N K W$^{-1}$ s$^{-1}$</td>
</tr>
<tr>
<td>Tube–side fluid API</td>
<td>°API</td>
<td></td>
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</tr>
<tr>
<td>Tube–side fluid $\nu_{100^\circ F}$</td>
<td>cSt</td>
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</tr>
<tr>
<td>Tube–side fluid MeABP</td>
<td>°C</td>
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</tbody>
</table>
the performance of the unit. To achieve predictive capabilities it is not sufficient to simply fit the model by adjusting the values of the parameters to one set of plant data but it is required to test model accuracy in predicting outlet temperatures from the unit against a set of plant data different from the one used for the estimations. The following periods are therefore defined (Figure 5.4):

**Figure 5.4:** Periods definition.

Period I - estimation period. This is divided in two sub-periods:

a. Clean period. During this time the unit is considered clean. Data are used to estimate values of parameters in set A.

b. Operation period. Parameter set B is estimated.

Period II - prediction period. Data are only used for comparison with simulation results.

Given the large variability in the quality of the feedstock, changed every few days, Period Ia must therefore be sufficiently long, so that fluid properties are not fitted to a single oil slate (which may be not representative) but averaged out over of the typical crudes processed by the refinery. Conversely, if the period is too long, the assumption that no fouling is present may become invalid.

### 5.4.0.1 Plant data analysis

Plant data (i.e. measurements of inlet and outlet temperatures and flowrates for each side of the exchanger) are notoriously difficult to obtain in a reliable way [Wilson and Vassiliadis, 1999; Takemoto *et al.*, 1999; Crittenden *et al.*, 1992] highlighted how fouling resistance calculated with refinery data after cleaning are non zero, showing an off-set which was attributed not only to the poor quality of plant data but also to the propagation of errors in the calculation of fouling resistances. As a result, the ratio of the heat duties calculated on the shell–side, $Q_s$ and tube–side,
5.4 Estimation of model parameters

\( Q_t \), typically does not satisfy the overall heat balance:

\[
\frac{Q_t}{Q_s} = \frac{\dot{m}c_p\Delta T_t}{\dot{m}c_p\Delta T_s} = 1
\]  

(5.48)

Relying on inaccurate data can cause numerical errors when estimating parameters and even cause estimation failure infeasible regions are encountered. This is often an input data problem rather than purely a numerical one. To make meaningful use of plant data, it is necessary to check their quality and remove gross errors in the measurements. To this end, it is useful to consider the percentage difference between the shell-side heat duty and the tube-side heat duty, \( \varphi \):

\[
\varphi = \frac{Q_s - Q_t}{Q_s} \times 100\%
\]

(5.49)

In ideal conditions \( \varphi \) is 0%, small positive or negative deviations point out that the heat balance is not closed but can be accepted. Large deviations indicate errors in the measurements (larger than the inaccuracies due to the simplified mode in Equation 5.48).

A filtering procedure to consistently analyse plant measurements and eliminate gross errors is devised based on calculating \( \varphi \) from Equation 5.49 on raw temperature and flowrate data (step 1), its average over time, \( \bar{\varphi} \) and standard deviation \( \sigma \) (step 2). A first filtering is done by excluding outliers, data that are statistically not significant (Step 3). Mean \( \bar{\varphi}' \) and standard deviation \( \sigma' \) are calculated again on the remaining data. Remaining data usually show an offset which does not depend on statistical errors but a systematic error in the calculations of Equation 5.49. A further filtration is performed by discarding data which do not satisfy the following criterion:

\[
|\varphi - \bar{\varphi}'| < \zeta
\]

(5.50)

where \( \zeta \), in %, is an arbitrary number which gives the maximum distance from average allowed satisfying the criterion (Step 4). Data satisfying this criterion are defined as filtered.

The next step is to estimate parameter set A and B. Input data used are the inlet temperatures \( (T_{in}^s, T_{in}^t) \) and the volumetric flowrates \( (\dot{V}_{in}^s, \dot{V}_{in}^t) \) which are assumed to have no errors, whilst the measured outlet temperatures, \( T_{out}^s \) and \( T_{out}^t \), have an assumed constant variance of \( \pm 1^\circ C \) (see Section 5.5). The model is fit to filtered data in Period Ia, estimating parameter set A through gPROMS (numerical details are reported in the following section). Estimated values are called
5.5 Solution method

The model outlined in Section 5.2 comprises a set of PDAE and was implemented and solved using the gPROMS modelling environment (Process Systems Enterprise, 2009) exploiting its hierarchical structure. This allowed defining a single tube model once and re–using it as many times as needed within a multi–pass exchanger configuration, for the description of the full unit. A graphic user interface in the gPROMS flowsheeting environment and an Excel interface via CAPE–OPEN (2010) were developed to input the heat exchanger geometries. These made extremely simple to set–up the geometries of the unit under investigation.

The PDAE were discretised in 10 point in the axial direction in each domain using the same 2nd order centered finite difference scheme used to solve the single tube model presented in Chapter 4. As previously noted in Section 4.3, the ageing phenomenon produces steep profiles of the thermal conductivity in the radial direction in regions close to the interface between domains Ω_l and Ω_t. To ensure accuracy of the solution a mesh independency test was performed for typical model parameters. Figure 5.6 shows that satisfactory accuracy is achieved with 1000 or more uniform radial discretization points. The computational load required to solve the set of PDAE is substantial when solving a full heat exchanger unit with multiple pass. A better

---

**Figure 5.5**: Data filtering for gross error elimination and parameter estimation procedure.

set A’. In the following step, the model is fit to filtered data in Period Ib using parameter set and estimating parameter set B. Estimated values are called set B’. Parameter sets A’ and B’ are then fixed to simulate Period II. Finally, simulation results are compared against plant data using overlay plots, residuals and normal distribution curves of residuals. The data filtering for gross error elimination and parameter estimation procedure are graphically summarised in Figure 5.5.

---

5.5 Solution method

set A’. In the following step, the model is fit to filtered data in Period Ib using parameter set and estimating parameter set B. Estimated values are called set B’. Parameter sets A’ and B’ are then fixed to simulate Period II. Finally, simulation results are compared against plant data using overlay plots, residuals and normal distribution curves of residuals. The data filtering for gross error elimination and parameter estimation procedure are graphically summarised in Figure 5.5.

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Figure 5.5: Data filtering for gross error elimination and parameter estimation procedure.

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5.5 Solution method

The number of grid points required to achieve the same accuracy given by the uniform grid with 1000 elements is reduced to 150 thus increasing the efficiency of the solution. Figure 5.6 also shows a comparison between the uniform and non-uniform discretization one for different number of nodes. The wall domain $\Omega_w$ does not present particular numerical challenges, therefore a uniform discretization in the radial domain with 10 points was satisfactory.

Optimal estimates of model parameter sets A and B, as prescribed in point 7 and 8 above, are found with the gPROMS in-built parameter estimation facility based on a Maximum Likelihood formulation (Process Systems Enterprise, 2004). For the estimation, parameters were scaled according to their respective initial guesses in order to avoid numerical problems.

The sensor used for the measurement is a thermocouple for which a constant variance model is used with its value assumed to be 1°C (Crittenden et al., 1992). Real plant data of inlet
temperatures and volumetric flowrates are fed to the model for both the parameter estimations and the simulations.

5.6 Model validation: case studies

To validate the model over a wide range of operating conditions, data were collected for 4 industrial units in two refineries operated by different major oil companies:

- RA–E01, RA–E02. Two double shell units in Refinery A.
- RB–E01, RB–E02. Two single shell units in Refinery B.

For refinery A, the measured inlet temperatures and flowrates on both shell–side and tube–side were used as input for the model. The measured outlet temperatures were used to estimate the parameters in Period I and to assess the quality of model predictions over Period II. For Refinery B, the same procedure was used. However, there was no physical sensor installed and thus no direct readings were available for the shell–side inlet temperature. For this variable, the ’measurements’ supplied had been estimated by the refiner through data reconciliation techniques.

The use of data from different refineries is particularly important to guarantee that the model is not refinery–specific. It is well known that whilst refineries change crude blends every 2–3 days, the crude types processed by one refinery are usually from a limited number of geographic origins. As a result, testing the model on data from different refineries has the significance of generalizing its validity to several crude blends. Moreover, considering units from different refineries also means dealing with different design and operating philosophies.

The heat exchanger geometries considered here vary in respect of shell size, number of tube passes, tube diameter, pitch angle (45 and 90°), baffle number and spacing, etc. The range of operating temperatures considered is 150–350°C on the shell–side and 130–245°C on the tube–side (see Section 5.8). One of the units, RB–E02, operates at a relatively low temperature (crude is between ca. 130 and 150°C) just below the range in which chemical reaction fouling is believed to be the dominant fouling mechanism. The hydraulic conditions on the tube–side considered also vary sensibly. The design velocity of the heat exchanger considered ranges between 1 and 2.5 m s⁻¹.
For all the units considered, Period Ia was set to include the first 15 accurate measurements. Depending on the quality of the data (assessed with the procedure described above) it ends at different dates for each unit. Period I was 60 days for all units. The length of the prediction period, Period II, is related to the length of the run specific for each exchanger, which is between 162 and 550 days (last column of Table 5.6). The prediction periods considered here therefore range from 5.5 months for unit RA–E02 up to 16 months for unit RB–E01.

5.7 Analysis of unit RA–E01

First, to illustrate the methodology used as well as the model capabilities, results are shown for one unit, namely RA–E01AB in an ExxonMobil PHT. The unit comprises two identical shells with 4 tube pass per shell (geometric parameters are summarised in Table 5.3). The crude is passed on the tube–side of the unit, whereas hot residuum from the distillation column flows on the shell–side (Figure 5.7). Plant personnel indicated that typical oils processed, although not light, produced severe fouling in this unit. Refinery observation when dismantling the unit for cleaning indicated that, whilst some shell-side fouling was detected, the dominant fouling resistance was on the tube-side.

Daily averages of plant data (inlet temperatures and volumetric flowrates) over a period of 1 year after a mechanical cleaning are reported in Figure 5.8(a,b) together with refinery calculations of the fouling resistance — based on the classic LMTD method (Figure 5.8(c)).

An underlying linear trend for the fouling resistance in Figure 5.8(c) is clear, although in the period around 60 to 100 days of operations a deviation is observed before the substantially linear behavior is restored. The sharp drop in tube-side flowrates (Figure 5.8(a)) could possibly be responsible for this large temporary increase in the fouling rate. A typical large non zero value of the fouling resistance calculated this way is evident, which should not be there when the

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tube length</td>
<td>$L$</td>
<td>6.1 m</td>
<td></td>
</tr>
<tr>
<td>Outer tube diameter</td>
<td>$d_o$</td>
<td>25.40 mm</td>
<td></td>
</tr>
<tr>
<td>Inner tube diameter</td>
<td>$d_i$</td>
<td>19.05 mm</td>
<td></td>
</tr>
<tr>
<td>Shell diameter</td>
<td>$D_s$</td>
<td>1.397 m</td>
<td></td>
</tr>
<tr>
<td>Tube count/shell</td>
<td>$N_t$</td>
<td>880</td>
<td>–</td>
</tr>
<tr>
<td>Pass number/shell</td>
<td>$N_p$</td>
<td>4</td>
<td>–</td>
</tr>
</tbody>
</table>
5.7 Analysis of unit RA–E01

Figure 5.7: Heat exchanger arrangement considered for unit RA–E01. The overall flow arrangement in the unit is co-current. Flow in first pass for shell A is co-current whereas in shell B is in counter-current with the shell-side fluid flow.

exchanger is clean. After just less than a year of operations (347 days) the exchanger underwent another (chemical) cleaning. On this basis, a time horizon of 347 days was chosen for the study.

The filtering procedure outlined in Section 5.4 was used to check the quality of measurements.

Figure 5.8: Inlet volumetric flowrates (a), terminal temperatures (b) for both tube-side and shell-side and fouling resistance calculated with refinery procedure (c) over a year after a mechanical cleaning for unit RA–E01.
Figure 5.9: Heat check $\phi$, calculated via Equation 5.49 from plant data, over a year after a mechanical cleaning for unit RA–E01. The dashed vertical line indicates the end of Period Ia whereas dotted line indicates the end of Period I.

Figure 5.9 shows the value of $\phi$ calculated via Equation 5.49 for all 347 days using typical physical properties values (i.e. $c_p$ and $\rho$ for tube–side and shell–side) provided by the refinery. This figure also introduces a notation used for all the following figures: data are reported as a clear dot if retained by the filtering procedure, as a dark dot if rejected. Also, two vertical dashed and dotted lines mark, respectively, the end of Period Ia (22 days in this case study) and Period I (60 days in this case study). For this unit, 30% of the data points were rejected in Period I. In the following prediction Period II (287 days or 9.5 months) 59 measurements (ca. 17%) were deemed unreliable, indicating a reasonable quality of the data used to test the simulation model in prediction mode.

5.7.1 Results and discussion

5.7.1.1 Estimation period

In all estimations, a constant measurement variance of 1°C was assumed for thermocouples. The parameter values obtained from the estimation procedure are reported in Table 5.4 for both parameter sets (A and B). The estimated crude API corresponds to a light crude, in line with indications by the refinery. The rather large fouling propensity of this oil — usually associated with heavier crudes — is reflected in the fouling parameters estimated in the subsequent step of
the estimation procedure (set B). Most parameters within each set are strongly correlated; this was not unexpected, given the empirical nature of the underlying physical properties and fouling models. As a result, statistical tests for individual parameter estimates indicate they have less than 95% statistical confidence. However, the model overall shows an adequate statistical fit to the plant data, within the variance specified, according to the standard $\chi^2$-test (Table 5.5). These tests show that, whilst individual parameters in the oil property and fouling/ageing models are not to be believed (probably due to attempting to model a range of oil slates for the former and some underlying mismatch in the model physics for the latter) the overall fit is very good. This is attributed to the model representing well the dominant aspects of thermal, hydraulic and fouling behavior in an integrated way.

Figure 5.10(a) and Figure 5.10(b) show overlay plots of model simulation results with, respectively, measured crude and residuum outlet temperatures for the whole estimation period (Period I). Each data point is reported with an error bar of ±1°C corresponding to the (assumed) variance of the temperature measurements. The model simulations fit well the measured plant data for all the data points for both shell-side and tube-side. In particular, for the tube (crude) side, all the points deemed 'reliable' by the filtering procedure are fitted within ±1°C. It is noteworthy that most of the data points which were filtered out and not used for parameter estimation turn out to be well simulated as well, indicating that, whilst they do not close the overall, steady-state, lumped thermal balance, they do close the more detailed, dynamic and distributed model developed here.

Table 5.4: Parameter set A and B estimates for unit RA–E01.

<table>
<thead>
<tr>
<th>Parameter set A</th>
<th>Optimal Estimate</th>
<th>Units</th>
<th>Parameter set B</th>
<th>Optimal Estimate</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resid. API</td>
<td>17.4 °API</td>
<td>RA–E01A α</td>
<td>0.00165</td>
<td>K m² W⁻¹ s⁻¹</td>
<td></td>
</tr>
<tr>
<td>Resid. ν₁₀₀°F</td>
<td>28.8 cSt</td>
<td>RA–E01A E</td>
<td>28.491</td>
<td>J mol⁻¹</td>
<td></td>
</tr>
<tr>
<td>Resid. MeABP</td>
<td>736.7 °C</td>
<td>RA–E01A γ</td>
<td>9.28×10⁻¹³</td>
<td>m⁴ K N⁻¹ J⁻¹</td>
<td></td>
</tr>
<tr>
<td>Crude API</td>
<td>37.5 °API</td>
<td>RA–E01B α</td>
<td>0.00165</td>
<td>K m² W⁻¹ s⁻¹</td>
<td></td>
</tr>
<tr>
<td>Crude ν₁₀₀°F</td>
<td>13.9 cSt</td>
<td>RA–E01B E</td>
<td>28.523</td>
<td>J mol⁻¹</td>
<td></td>
</tr>
<tr>
<td>Crude MeABP</td>
<td>350.2 °C</td>
<td>RA–E01B γ</td>
<td>9.35×10⁻¹³</td>
<td>m⁴ K N⁻¹ J⁻¹</td>
<td></td>
</tr>
</tbody>
</table>

Table 5.5: Weighted residuals and corresponding $\chi^2$-Values for unit RA–E01.

<table>
<thead>
<tr>
<th></th>
<th>Weighted residual</th>
<th>$\chi^2$-Value (95%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set A</td>
<td>10.902</td>
<td>21.026</td>
</tr>
<tr>
<td>Set B</td>
<td>59.651</td>
<td>92.808</td>
</tr>
</tbody>
</table>
Figure 5.10: Overlay plot of model simulations with crude (a) and residuum (b) outlet temperature over the estimation Period I for unit RA–E01. White data points show data filtered with the procedure developed, coloured data points show data deemed inaccurate. Error bars indicate ±1°C. The vertical dashed line shows the end of Period Ia.

5.7.1.2 Prediction period

To test whether the model can be used in a predictive mode (i.e. to extrapolate its results beyond the estimation period, without reestimating its parameters), the model was then used to simulate the exchanger for the rest of the year. Measured inlet temperatures and flowrates were input to the simulation, but all adjustable parameters (sets A and B) were kept fixed. The simulated
performance, in terms of output temperatures over the whole time horizon considered (347 days) is shown by the continuous lines in Figure 5.11 and Figure 5.12 for, respectively, tube–side and shell-side, together with all plant measurements. The outlet temperatures on both sides are predicted well over the entire period, even in the presence of rather major excursions, including the period between 60–100 days.

The contribution of fouling and ageing to the overall behavior of the unit is illustrated by the two extra lines plotted in the same figures:

- The dashed line was obtained using the same parameter set A as before but setting the fouling rate to 0 (i.e. \( \frac{dR_f}{dt} = 0 \)), corresponding to a case of no fouling.
- The dashed-dotted line was obtained using same parameter sets A and B but setting the pre-exponential term, \( A_a \), in the ageing to 0, corresponding to a case of fouling but with no deposit ageing.

In particular, from Figure 5.11 an insight can be gained on the opposite effects of fouling and ageing on the crude outlet temperature. Whilst fouling reduces the efficiency of the heat transfer thus decreasing the crude outlet temperature, ageing acts in the opposite way, by increasing the thermal conductivity of the deposits, thus enhancing the overall heat transfer. Temperature estimated without fouling or ageing in the model do not match the plant data, but do so when both phenomena are included.

A closer inspection of the accuracy of simulation results is made by considering the percentage residuals defined as:

\[
\varepsilon \equiv \left( \frac{\tilde{x}_i - x_i}{\tilde{x}_i} \right) \times 100\% \quad (5.52)
\]

where \( x_i \) is the simulated value of the variable considered at the \( i \)-th time step and \( \tilde{x}_i \) is the corresponding plant temperature measurement. Residuals of all data previously deemed ‘accurate’ on the tube-side (Figure 5.13(a)) lay between -1.2% and +0.6% (corresponding to absolute error values of -2.5°C and +1.5°C) over the 347 days of operation. Shell-side accuracy is somewhat lower as shown in Figure 5.13(b). In this case the residuals of all filtered data lay between -1% and +2% (-3°C and +6°C). The residuals show some systematic trend, as opposed to purely random scatter, indicating there is possibly some underlying model mismatch (not surprising, for example in view of likely oil slate changes over one year and shell-side assumptions). Even so, analysis of the parity plots (Figure 5.14) reveals that although the model tends to underestimate
Figure 5.11: Overlay plot of model simulations with crude outlet temperature measurements for unit RA–E01. Dashed line shows simulation run setting $R_f = 0$ whereas the dashed-dotted line shows simulation results with no ageing (i.e. $A_a = 0$). Void data points are reliable, filled ones are inaccurate. Vertical dashed line shows the end of Period Ia whereas vertical dotted line indicates the end of Period I and the beginning of Period II.
5.7 Analysis of unit RA–E01

![Graph showing overlay plot of model simulations with residuum outlet temperature measurements for unit RA–E01. Dashed line shows simulation run setting $R_f = 0$ whereas the dashed-dotted line shows simulation results with no ageing (i.e. $A_a = 0$). Void data points are reliable, filled ones are inaccurate. Vertical dashed line shows the end of Period Ia whereas vertical dotted line indicates the end of Period I and the beginning of Period II.](image)

Figure 5.12: Overlay plot of model simulations with residuum outlet temperature measurements for unit RA–E01. Dashed line shows simulation run setting $R_f = 0$ whereas the dashed-dotted line shows simulation results with no ageing (i.e. $A_a = 0$). Void data points are reliable, filled ones are inaccurate. Vertical dashed line shows the end of Period Ia whereas vertical dotted line indicates the end of Period I and the beginning of Period II.
the shell-side outlet temperature, over 85% of the points are within a ±1% error for both sides of the unit.

The effect of ageing was investigated in Figure 5.11 and Figure 5.12 by simply re-running simulations with the ageing parameter $A_a$ set to zero. However, the other fouling parameters used resulted from an estimation with ageing model included. To investigate whether this could mask the effect of ageing, and indeed whether it is necessary to include the ageing phenomena at all,
5.7 Analysis of unit RA–E01

Figure 5.14: Parity plot for tube–side (a) and shell–side (b) outlet temperatures for unit RA–E01. The dashed lines indicate ±1% deviation.

The parameter estimation procedure was performed again in Period Ib with $A_i$ set to zero. The results, reported in Figure 5.15 in the form of percentage residuals in the output temperatures, show that the error increases significantly. Moreover, a strong trend is introduced in the residuals, underling the structural importance of including ageing effects.

The contribution of each of the two shells, RA–E01A and RA–E01B to the overall average

Figure 5.15: Tube-side and shell-side percentage residuals when estimating parameters in Period Ib in case of no–ageing for unit RA–E01.
fouling resistance $R_f$, calculated from Equation 5.34, is shown in Figure 5.16. As expected for a clean exchanger, the value of the fouling resistance increases from an initial zero value. All variability present in the inlet temperatures and flowrates is smoothed out, to give a smooth curve. The rate of increase is high initially but tails off after about 150 days to an approximately constant value. Fouling in shell RA–E01A is slightly higher than in shell RA–E01B but the difference (in this case) is not large. Model outputs for $\bar{R}_f$ are also compared with refinery calculations. The latter shows a zero fouling resistance for the first few days, after which a sharp jump to an unexplained offset value of ca. $2 \times 10^{-3}$ m$^2$ K W$^{-1}$ occurs. The model results start from a zero fouling resistance for a clean heat exchanger.

Given the high accuracy of the exit temperatures predicted by the model, it is likely that the overall fouling resistance calculated by the refinery merely reflects the gross approximations (e.g. in physical properties, lumped heat transfer coefficients etc.) used in its calculation. The difference between model and refinery-calculated fouling resistances in Figure 5.16 is not considered large by industrial refinery specialists, who acknowledge the approximate nature of their calculations and mostly consider just underlying trends anyway, not absolute values and would typically subtract from their curve the clean–exchanger offset. The overall trends shown substantially agree, and when the offset is subtracted, numerical values are also close. However, Figure 5.16 shows that the (perceived) sudden increase in fouling resistance around 80–100 days

**Figure 5.16:** Refinery calculated fouling resistance and model average $R_f$ for unit RA–E01. The dotted and dashed lines indicate average $R_f$ calculated for RA–E01A and RA–E01B respectively.
Figure 5.17: Variation over time of fluid density (a), specific heat capacity (b), dynamic viscosity (c) and thermal conductivity (d) at shell–side and tube–side outlet for each shell in unit RA–E01 with respect of inlet conditions.

can be fully explained by the measured changes in inlet flowrates, temperatures, and complex interactions arising, and is not a genuine increase in fouling rate.

The reason for the quality of model temperature predictions shown in previous figures may be explained by the fact that the model captures the essential physics in an appropriate way. It not only includes fouling and ageing (Figure 5.11 and Figure 5.12) but it also considers the effects of variation in physical properties over time and space (as function of temperature) on the heat transfer coefficient and key interactions between hydraulic and thermal aspects. Figure 5.17 shows that the variations of physical properties over the length of each shell in the unit and over time are, indeed, significant.

One of the main benefits of using a distributed model is that it is possible to track the effects of fouling along the heat exchanger over time for the same historical inlet temperature and flowrate profiles. Figure 5.18 shows the fouling layer thickness along the four passes of each shell at
the end of period II (347 days after the previous cleaning). A first observation is that in the counter-current passes, owing to a larger film temperature, the increase in fouling thickness along the tubes is much larger compared to the passes in parallel flow. This difference is particularly evident in the colder shell (RA–E01A) where the driving force (i.e. temperature difference) is larger. Figure 5.18 corroborates the speculations by Polley et al. (2002b) regarding the effect of flow arrangement on fouling. The model predicts a larger thickness of the fouling layer at the tube outlet of shell RA–E01A than at the inlet of shell RA–E01B. This is counter-intuitive as the latter shell is the one at higher crude bulk temperature. However, the film temperature (on which fouling depends according to Equation 5.30) is, on average, more than 2.5°C higher at the inlet of shell RA–E01B than the outlet of E01A. It is noted that the deposits accumulated over the 347 days of operations amount to ca. 3 mm, which corresponds to a large reduction (over 40%) in cross-sectional area available to the crude flow and has a strong impact on the unit’s hydraulics. It also confirms that the thin-layer assumption often used in fouling models cannot be applied.

The effects of fouling on energy recovery is drastic. Figure 5.19(a) reports the heat duty from model simulations in case of fouling and no fouling over time. It can be noted that the two curves diverge significantly over time. The difference between the two heat duties shown in Figure 5.19(b), represents the energy lost instantly due to fouling. Figure 5.19(b) also shows the integral of the heat duty loss over time, which represents the cumulative energy loss, calculated in 22.4 GWh (8.064 × 10^{13} J) after 347 days of operations. If this loss were to be compensated entirely at the furnace (i.e. no dumping effects given by the interaction with other exchangers in
5.7 Analysis of unit RA–E01

Figure 5.19: Heat duty from model simulations in case of fouling and no fouling over time in unit RA–E01 (a). The energy lost due to fouling, represented by the shaded area, and the cumulative energy loss over time are given in (b).

the network, the cost in extra fuel burnt would be in excess of US$670,000 (at a cost of US$27 MWh$^{-1}$ and with 90% efficiency of the furnace).

Finally, it is possible to appreciate the effects of fouling on the hydraulics of the exchangers in Figure 5.20 where the pressure drops are reported for the tube–side of the 2 shells as dotted (RA–E01A) and dashed lines (RA–E01B), and the sum of the two. As the two shells are geometrically identical, for the first few days after the cleaning pressures drops are the same whereas, when fouling becomes significant, the contribution to the total pressure drops given by RA–E01B is more important than that given by RA–E01A. The overall increasing trend shown in Figure 5.20 unveils the large impact of fouling on the unit. It should be noted that the hydraulic model has not been validated against plant data as pressure drop measurements are usually not logged by

Figure 5.20: Pressure drops in unit RA–E01.
Table 5.6: Summary of data for the four units considered. Temperature ranges refer to the minimum coldest and the maximum hottest temperature on record for a given side each unit. Run length is the period of time considered between two cleanings.

<table>
<thead>
<tr>
<th>HEX name</th>
<th>No shells</th>
<th>Shell-side T</th>
<th>Tube-side T</th>
<th>Tube-side design v</th>
<th>Run length</th>
</tr>
</thead>
<tbody>
<tr>
<td>RA–E01</td>
<td>2</td>
<td>220–350</td>
<td>190–250</td>
<td>2.5</td>
<td>349</td>
</tr>
<tr>
<td>RA–E02</td>
<td>2</td>
<td>220–320</td>
<td>170–250</td>
<td>1</td>
<td>162</td>
</tr>
<tr>
<td>RB–E01</td>
<td>1</td>
<td>240–300</td>
<td>180–210</td>
<td>1.7</td>
<td>550</td>
</tr>
<tr>
<td>RB–E02</td>
<td>1</td>
<td>155–270</td>
<td>130–160</td>
<td>2.7</td>
<td>310</td>
</tr>
</tbody>
</table>

refineries and are virtually not available. Nonetheless, the capability of predicting pressure drops represents another important feature of the model that can assist the refiners in monitoring the performance of the PHT.

5.8 Analysis of other units

The same procedure described for RA–E01 was applied to the other three units summarised in Table 5.6. Table 5.7 reports for each case the estimates of the physical property and the fouling model parameters obtained. The values obtained for the oil gravity varies between 27–37 API. The estimated fouling activation energy, \( E_f \), shows a remarkable consistency, varying between 28.5 and 32.1 kJ mol\(^{-1}\) and compares well with typical values (21–33 kJ mol\(^{-1}\)) reported in literature for crude oil reaction fouling (Crittenden et al., 1992). The values for \( E_f \) and \( \alpha \) also compare well with those reported by Yeap et al. (2004) and used in Chapter 4 (see Table 4.2) to build the fouling model. The suppression constant, \( \gamma \), is somewhat lower (about one order of magnitude) than the value indicated by Table 4.2 but in line with other estimations by Yeap et al. (2004) (for one of the data sets used they estimated \( 8.38 \times 10^{-13} \) m\(^4\) K N\(^{-1}\) J\(^{-1}\)).

Table 5.7: Summary of parameter set A and set B estimates for all units considered.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Units</th>
<th>RA–E01</th>
<th>RA–E02</th>
<th>RB–E01</th>
<th>RB–E02</th>
</tr>
</thead>
<tbody>
<tr>
<td>Shell API</td>
<td>[°API]</td>
<td>17.4</td>
<td>1.3</td>
<td>24.4</td>
<td>22.4</td>
</tr>
<tr>
<td>( \mu_{\text{00/F}} ) [cSt]</td>
<td>28.8</td>
<td>2356.7</td>
<td>3.6</td>
<td>1.7</td>
<td></td>
</tr>
<tr>
<td>MeABP [°C]</td>
<td>736.7</td>
<td>778.1</td>
<td>500</td>
<td>612</td>
<td></td>
</tr>
<tr>
<td>API [°API]</td>
<td>37.5</td>
<td>27.6</td>
<td>31</td>
<td>31</td>
<td></td>
</tr>
<tr>
<td>( \mu_{\text{00/F}} ) [cSt]</td>
<td>13.9</td>
<td>28.3</td>
<td>1.6</td>
<td>1.6</td>
<td></td>
</tr>
<tr>
<td>MeABP [°C]</td>
<td>350.2</td>
<td>434.1</td>
<td>250</td>
<td>250</td>
<td></td>
</tr>
<tr>
<td>( \alpha ) [m(^2) K J(^{-1})]</td>
<td>0.0016</td>
<td>0.0014</td>
<td>0.0014</td>
<td>0.0014</td>
<td>0.0015</td>
</tr>
<tr>
<td>( E_f ) [kJ mol(^{-1})]</td>
<td>28.49</td>
<td>30.47</td>
<td>30.39</td>
<td>32.13</td>
<td>30.35</td>
</tr>
<tr>
<td>( \gamma ) [m(^3) K N(^{-1}) J(^{-1})]</td>
<td>(9.28 \times 10^{-13}), (9.35 \times 10^{-13}), (10.31 \times 10^{-13}), (10.29 \times 10^{-13}), (7.76 \times 10^{-13}), (9.42 \times 10^{-13}),</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
5.8 Analysis of other units

5.8.1 Results and discussion

Overlay diagrams of measured vs. estimated temperatures similar to Figure 5.11 and Figure 5.12 have been produced for all the 4 units considered, reporting the predictive performance of the model, but are not shown for confidentiality reasons. Here, to facilitate an overall comparison, results are shown in Figure 5.21(a) and Figure 5.21(b) for all exchangers in terms of percent residuals for, respectively, tube–side and shell–side outlet temperatures.

![Error vs. Time (a)](image1)

![Error vs. Time (b)](image2)

**Figure 5.21:** Percentage residuals of fluid outlet temperature with model simulations on the tube–side (a) and shell–side (b) for all units examined.
In Figure 5.21, residuals for each unit are represented by markers of different shape. The end of the estimation period, Period I (fixed to 60 days for all units) is indicated with the vertical dotted line. As already mentioned, the duration of Period Ia was different for each unit as it depends on the quality of the measurements and is not indicated in the figure. The residuals for each individual heat exchanger show some weak systematic trend, as opposed to purely random scatter, indicating there is possibly some underlying model mismatch (not surprising, for example in view of the many oils slate changes over the long periods of time considered). Even so, 93\% of all data are within ±2\% error on the shell–side and ±1\% on the tube–side. The major deviation is given by RB–E02 which is expected as this is the lowest temperature unit and small absolute errors reflect in large percentage errors. It is interesting to note that the quality of model predictions remains good (within a narrow error band) over extended periods of time (up to 16 months). These are industrially relevant time horizons as required for planning of cleanings to optimize a refinery economic performance.

Finally, Figure 5.22 reports parity plots of the predicted vs. measured temperatures for the shell (a) and tube (b) sides, for all four units, thus covering a wide temperature range. Analysis of these plots reveals that over 80\% of all the points (i.e. including clearly erroneous measurements, such as the previously noted flat plant temperatures at ca. 235°C, evident in Figure 5.22(b)) are within a ±1\% error (indicated by the dashed lines) for both sides of the unit.

![Figure 5.22: Parity plot of fluid outlet temperature on the tube–side (a) and shell–side (b) for all units examined. Dashed lines indicate ±1% deviation from parity (diagonal line).](image)
5.9 Retrofit of unit RA–E01

The model validation with plant data performed in the previous section, gives the necessary confidence to exploit its capabilities to assess alternative design that mitigate fouling and reduce energy losses. The detailed analysis carried out in Section 5.7 has unveiled that energy losses produced by fouling in unit RA–E01 add up to 22.4 GWh after 347 days of operation. In this section, a simple retrofit option is considered with the aim of reducing these losses.

Increasing velocity — thus wall shear stress — has a beneficial effect on fouling and it is the process variable on which the designer has most control (Section 2.4.4.4). It seems reasonable therefore to choose this variable first to improve the unit’s performance. For a given flowrate, a way of achieving larger velocities within the tubes is to increase the number of tube–side pass, \( N_p \). This is relatively an inexpensive option to be implemented in existing units as it requires only to replace the heat exchanger headers, leaving in place existing tube bundle and shell.

In the case considered here, the retrofit of unit RA–E01 was performed by increasing the number of tube–side pass of the existing configuration from 4 to 6. All other geometric parameters (e.g. flow arrangement, number of tubes, etc.) were kept at the original values reported in Table 5.3. Values for physical properties and the fouling model parameters were fixed at the values estimated with the procedure described in Section 5.4 and reported in Table 5.4. Simulations were then performed under the same plant conditions (Figure 5.8(a,b)), over 347 days after a mechanical cleaning, used for the 4 pass unit. This allowed for testing how the retrofitted unit would have performed in the refinery if the proposed design were actually used at the process conditions experienced in the plant. Comparison with simulation results reported in Section 5.7 for the existing exchanger allows to assess potential saving achievable with the new configuration.

5.9.1 Results and discussion

Figure 5.23(a) shows the beneficial effects on the fouling resistance produced by the higher velocities within the 6 pass exchanger. The value of the overall fouling resistance is reduced by ca. 25% after a year of operation at the expenses of the increased pumping power required to counteract the larger pressure drop (Figure 5.23(b)). Whilst the extra pressure drop generated by the new configuration, ca. 0.5 bar (50,000 Pa), seems acceptable in clean conditions, at the
Figure 5.23: Fouling resistance (a) and pressure drops (b) in the existing design compared with the retrofit configuration proposed.

End of the operating period, it reaches ca. 3 bar which may be still be accepted, depending on the hydraulic flexibility of the refinery (considerations on mechanical design are excluded in this preliminary analysis).

Figure 5.24(a) shows that difference in outlet temperatures of the tube–side fluid (crude) between operations with the existing unit and the retrofitted one can be as large as 4°C. Cumulative energy savings are estimated to add up to almost 5 GWh (Figure 5.24). This is equivalent to a 22% reduction of the losses generated by fouling in the 347 days of operation of unit RA–E01 (Figure 5.19), equivalent to ca. US$150,000 in furnace fuel alone.

Figure 5.24: Difference in tube–side outlet temperature between the existing and the retrofitted unit (a) and cumulative energy savings, with respect to the existing unit, achieved using the 6 pass design (b) using the plant operating conditions.
5.10 Concluding remarks

A novel dynamic, distributed model for a multi-pass shell–and–tube heat exchanger has been developed for use in refinery pre–heat trains, where fouling deposition results in severe energy inefficiency. The model accounts for the geometry of the heat exchanger and captures the variation of physical properties with temperature, over time and space thus achieving accurate predictions of the local heat transfer coefficients. It also considers several aspects of the fouling phenomena such as its dependence on process conditions, the fouling propensity of the crude and the ageing mechanism. The formulation in cylindrical coordinates makes it possible to overcome the thin slab approximation — often used in the past — accounting for curvature effects in the heat flux. Interactions between the growth of the fouling layer and the crude oil flowing inside the tubes are captured by solving a moving boundary problem.

As a result, it is possible to perform a detailed analysis of the related spatial and temporal effects on the thermal and hydraulic performance of the heat exchanger unit. Contributions of different shells in the same unit can be unveiled and critical zones identified. This goes well beyond current practice which relies on the use of averaged thermo–hydraulic models and/or very aggregate, highly empirical fouling factors.

A formal validation of the model has been performed despite the well known difficulties in collecting and analysing industrial data on fouling behaviour. Primary plant measurements rather than derived fouling resistances were used to estimate model parameters. This avoids incorporating in the analysis errors produced not from plant measurements but from assumptions in calculations. Data for 4 units (comprising 6 shells in total) in 2 different refinery sites, covering a range of conditions (i.e. temperatures, flowrates, etc.) have been used. Coupled with a suitable estimation procedure that adapts a small number of parameters (9 for each unit), the model has been proven sufficiently flexible to cope with the different process conditions, heat exchanger geometries and crude fouling behavior.

The case studies shown have highlighted the fact that a 2 months estimation period (starting from clean conditions) with daily data is sufficient to generate the necessary model parameters, yielding an excellent representation of the outlet temperatures during the estimation period itself. Subsequently, the model with the adjusted parameters could be used in a predictive way for another 4–16 months to predict outlet temperatures with accuracy within 1% on the tube–side and 2% on the shell–side.
In the model presented, fouling is limited to the tube-side. The results presented here indicate that (at least for the cases considered) the potential under-prediction of shell-side heat transfer resistance does not have a significant effect. This may not always be true. Indeed, a large mismatch between this model and plant measurements can indicate (indirectly) that shell-side fouling may be important. Of course, in the presence of very large shell-side fouling rates the model may not be applicable and, for generality, it would be useful to also include shell-side fouling.

The accuracy achieved for the predicted outlet temperatures, and the smooth profiles of the overall fouling resistance curves obtained over several months are judged to be satisfactory for use in refinery applications and time horizons of industrial relevance. It is concluded that the model and approach can be used with confidence to predict fouling trends, and consequential losses of thermal, hydraulic and energy performance in oil preheat trains. It has been shown that the model can be used to propose retrofit designs of individual units and test them in real plant conditions. In the particular case considered, a 22% reduction in energy losses was achieved by using a simple retrofit option (increased number of tube–side pass). This opens the possibility to optimize the design and operation of heat exchanger networks which minimize fouling and, ultimately, maximise operability and profits.

Benefits of using the approach proposed are twofold: on one hand the model can be used in refineries as an enhanced monitoring tool, on the other it is possible to incorporate fouling at the design stage. The use of the model for monitoring activities would allow:

- Early detection of problems when there is a change in crude slate.
- Calculation of energy losses, thus extra costs, due to fouling.
- Informing operational decisions such as cleaning scheduling.

At the design stage, the model would enable to:

- Explore different retrofit options to mitigate fouling.
- Assess the economic impact of a chosen design on overall refinery costs and CO₂ emissions.

The model of the single heat exchanger allows therefore a detailed analysis of each unit in a PHT independently. However, important dynamic interactions amongst units (e.g. the variation of outlet temperatures and flowrates in one exchanger affects the driving force in downstream units) can only be appreciated through a complete network simulation. This would allow predicting
important operating variables (e.g. CIT, CIP), assessing costs produced by fouling in the PHT and guide the retrofit of possible network structures that maximise energy efficiency over time. The set–up of a network simulation and the development of a set of key indicators to systematically assess impact of fouling will be the focus of the next chapter.
Chapter 6

Crude pre–heat train undergoing fouling: network simulation

Synopsis

The single shell–and–tube heat exchanger model developed thus far is used here as a building block for the simulation of refinery pre–heat trains. Such a network is easily built up within a commercial simulation system. To systematically assess the impact of fouling at the network level, several key performance indicators (KPIs) are proposed. These take into account energy losses and GHG emissions at the furnace, pumping power and throughput reduction as well as the respective economic impact. Analysis of network simulation results, assisted by the KPIs, is then presented for two case studies. The first case study focuses on assessing the impact of fouling on the hot–end of a refinery PHT. The second case study illustrates how the model can be used to effectively account for fouling dynamics in the retrofit of PHTs. In the latter case, simulation results show that network designs that maximize energy recovery in clean conditions (following traditional pinch rules) may not be best when fouling occurs. It is concluded that a proper retrofit design must consider time varying fouling effects.
6.1 Introduction

The detailed dynamic model developed in Chapter 5 is for a single shell-and-tube heat exchanger. However, in a PHT, no heat exchanger exists on its own (Figure 6.1) and the distinct fouling behaviour of each heat exchanger affects the overall performance of the network. Complex interactions amongst the units can only be unveiled by a simulation of the entire network.

The implementation of model equations in gPROMS greatly facilitate the set-up of a network simulation. All necessary equations that govern the single heat exchanger model were wrapped in an object that can be easily instantiated through a graphic user interface and readily replicated in a flowsheet environment to generate the topology of a specific network. Figure 6.2 shows a screenshot of a typical network.

The operation of the network is simulated via the simultaneous solution of equations for all exchangers. Each exchanger in the network is represented using the detailed dynamic model with suitably instantiated parameters for geometry, fouling, ageing etc. Simulating each unit at this level of detail allows gaining insights on how each heat exchanger individually contributes to the overall network performance.

A network starts with a source model where the properties of the material flow streams, used to interconnect units, are specified. Each material flow streams provides the following

![Figure 6.1: Multi-scale model of a typical pre-heat train undergoing crude oil fouling.](image-url)
information:

- Temperature
- Mass or volumetric flowrate
- Pressure
- Composition in terms of °API, MeABP and $\mu_{100^\circ F}$

In the source model, basic physical properties are computed by the API relationships (Riazi, 2005) at the specified conditions. The outlet of each unit is interconnected to the inlet of the following one via a material stream that passes all the input information listed above. The network is terminated by the use of a sink model for each stream which collects all the information of outlet streams.

Other units included in the CDU such as the desalter and the furnace are modelled in a simple way to account only for their thermal effects on the network (i.e. no variation in composition, phase, etc.). The pre–flash drum is not included in the two case studies considered here and therefore not modelled. Simple heat and mass balances are used for flow splits and junctions.
6.2 Assessment of network performance: key performance indicators

Variable flow conditions, temperatures, crude slates as well as geometry of single HEXs and structure of the network affect in different ways the fouling behaviour of a PHT, thus the energy recovered and, ultimately, the refinery bottom line. However, given the large number of variables involved, it may be difficult to isolate causes of inefficiencies and identify different contributors to the overall performance. The task of identifying dynamic interactions amongst units is particularly challenging when considering different structures for network retrofit.

To assess in a consistent way the performance of a PHT network undergoing fouling and to be able to evaluate potential benefits in restructuring the network, a set of key performance indicators is proposed here.

Given that the phenomena involved are intrinsically dynamic, some of the KPIs presented in the following sections (and summarised in Table 6.1) are referred to a reference time, \( t_{KPI} \) and used to provide a snapshot of network conditions and history up to that point in time. Some of these indicators refer to clean conditions which can be easily calculated at time 0 if all the heat exchangers in the network can be assumed clean at that time and the inputs (flowrate, temperature and pressure) are kept constant. However, if real plant data are to be used as input, it is not easy

<table>
<thead>
<tr>
<th>KPI</th>
<th>Description</th>
<th>Units</th>
<th>Equation</th>
<th>Evaluate</th>
</tr>
</thead>
<tbody>
<tr>
<td>01</td>
<td>Decline in CIT with respect of clean conditions at time ( t_{KPI} ).</td>
<td>˚C</td>
<td>6.1</td>
<td>Thermal performance.</td>
</tr>
<tr>
<td>02</td>
<td>Cumulative cost at ( t_{KPI} ) associated to extra fuel burnt in furnace.</td>
<td>US$</td>
<td>6.5</td>
<td>Thermal performance.</td>
</tr>
<tr>
<td>02r</td>
<td>Cumulative cost at ( t_{KPI} ) associated to different energy recovery at the furnace vs. reference HEN configuration.</td>
<td>US$</td>
<td>6.8</td>
<td>Thermal performance.</td>
</tr>
<tr>
<td>03</td>
<td>Cumulative cost at ( t_{KPI} ) of extra CO(_2) released because of fouling.</td>
<td>US$</td>
<td>6.11</td>
<td>Environmental impact.</td>
</tr>
<tr>
<td>03r</td>
<td>Cumulative cost difference at ( t_{KPI} ) of extra CO(_2) released because of fouling vs. reference HEN configuration.</td>
<td>US$</td>
<td>6.13</td>
<td>Environmental impact.</td>
</tr>
<tr>
<td>04</td>
<td>Time at which the furnace firing limit is reached.</td>
<td>days</td>
<td>6.15</td>
<td>When production loss starts.</td>
</tr>
<tr>
<td>05</td>
<td>Cumulative cost of production loss at ( t_{KPI} ).</td>
<td>US$</td>
<td>6.18</td>
<td>Production loss.</td>
</tr>
<tr>
<td>05r</td>
<td>Cumulative difference of cost of production loss vs. reference HEN configuration at ( t_{KPI} ).</td>
<td>US$</td>
<td>6.20</td>
<td>Production loss.</td>
</tr>
<tr>
<td>06</td>
<td>Increase in CIP at ( t_{KPI} ).</td>
<td>bar</td>
<td>6.21</td>
<td>Hydraulic performance.</td>
</tr>
<tr>
<td>07</td>
<td>Cumulative cost at ( t_{KPI} ) of energy losses at the pump due to fouling.</td>
<td>US$</td>
<td>6.24</td>
<td>Hydraulic performance.</td>
</tr>
<tr>
<td>07r</td>
<td>Cumulative cost at ( t_{KPI} ) of energy losses at the pump due to fouling vs. reference HEN configuration at ( t_{KPI} ).</td>
<td>US$</td>
<td>6.26</td>
<td>Hydraulic performance.</td>
</tr>
<tr>
<td>08</td>
<td>Cumulative total extra costs at ( t_{KPI} ) due to fouling.</td>
<td>US$</td>
<td>6.27</td>
<td>Overall economic performance.</td>
</tr>
</tbody>
</table>
to determine a reference clean conditions performance. In this case model simulations can be exploited to provide reference clean conditions by setting $R_f = 0$ in each unit.

### 6.2.1 Assessment of thermal efficiency

To maintain the temperature at the inlet of the crude distillation column at a desired value while the CIT declines because of fouling in the PHT, extra fuel must be burnt at the furnace which is not necessary when the train is clean. The decline in CIT with respect to clean conditions over time can therefore be used as a measure of the overall thermal performance of the network:

$$\Delta \text{CIT}(t) = \text{CIT}^{\text{clean}} - \text{CIT}$$

(6.1)

Equation 6.1, evaluated at $t = t_{\text{KPI}}$ provides KPI–01 the first key performance indicator considered here. Energy loss at the furnace, $E_{Q_{\text{loss}}}$, associated with $\Delta \text{CIT}$ is calculated as the integral over time of the difference between the total actual heat supplied by the furnace to the crude, $Q_{\text{fuir}}$, and the total heat duty in clean conditions, $Q_{\text{fuir}}^{\text{clean}}$:

$$E_{Q_{\text{loss}}}(t) = \int_0^t (Q_{\text{fuir}} - Q_{\text{fuir}}^{\text{clean}}) \, dt$$

(6.2)

However, depending on the overall efficiency of the furnace, $\eta_{\text{fuir}}$:

$$\eta_{\text{fuir}} = \frac{\text{kWh uptake by oil}}{\text{kWh of furnace fuel}}$$

(6.3)

the actual fuel consumption is higher than that calculated in Equation 6.2 and the increased energy requirements, $E_{\text{fuel}}$, caused by the decline in CIT, met by burning the additional fuel, are:

$$E_{\text{fuel}}(t) = \frac{E_{Q_{\text{loss}}}}{\eta_{\text{fuir}}}$$

(6.4)

The energy cost is the energy of the fuel that must be supplied to compensate for fouling times its price, $P_{\text{fuel}}$ (in US$ MWh\text{ }^{-1}$):

$$C_{\text{fuir}}(t) = E_{\text{fuel}} \times P_{\text{fuel}}$$

(6.5)
6.2 Assessment of network performance: key performance indicators

$C_{fur}$ evaluated at time $t = t_{KPI}$ provides KPI–02. In case of a retrofit, however, it is useful to compare this cost for a given network structure, configuration $C_j$, with that in the reference configuration, $C_1$. Do this, first it is necessary to calculate the total (cumulative) energy required for each configuration considered:

$$E^{C_j}(t) = \int_{0}^{t} \dot{m}c_p(COT - CIT_j) \, dt; \text{ for } j = 1, \ldots, N_c$$

(6.6)

where $N_c$ denotes the number of retrofit configurations explored whilst $CIT_j$ is the coil inlet temperature in each configuration $j$ and $COT$ the fixed coil outlet temperature, required for distillation. The difference in performance (extra energy recovered at the furnace) of each retrofit provides the comparison between the different configurations considered:

$$\Delta E^{C_1-C_j}(t) = E^{C_1} - E^{C_j}; \text{ for } j = 2, \ldots, N_c$$

(6.7)

In economic terms, the fuel savings, $S_{v_{fuel}}$, associated with $\Delta E^{C_1-C_j}$ are:

$$S_{v_{fuel}}(t) = \Delta E^{C_1-C_j} \frac{P_{fuel}}{\eta_{fur}}; \text{ for } j = 2, \ldots, N_c$$

(6.8)

The cumulative fuel savings up to time $t = t_{KPI}$ provide the KPI–02r indicator for network retrofit.

6.2.2 Assessment of environmental impact

The combustion of extra fuel at the furnace also produces the release of greenhouse gases to the environment for which fouling is responsible. The extra tons of carbon dioxide emitted up to time $t$ caused by thermal inefficiencies, $M_{CO_2}$, can be calculated as:

$$M_{CO_2}(t) = E_{fuel} \times m_{CO_2}$$

(6.9)

where $m_{CO_2}$ denotes the carbon emission per Joule of energy produced in the combustion of a given fuel assumed to be constant. This is calculated dividing the carbon content of the fuel, $C_C$ (in kgC kg$^{-1}$fuel), by its energy content, $F_E$ (in kWh kg$^{-1}$fuel):

$$m_{CO_2} = \frac{C_C \times MW_{CO_2}/MW_{C}}{F_E}$$

(6.10)
where MW\(_{\text{CO}_2}\) and MW\(_C\) denote, respectively, the molecular weight of CO\(_2\) and carbon.

Under environmental laws (e.g. the Emissions Trading Scheme in Europe), the extra release of greenhouse gases to the environment adds economic penalties to the operations. In this study it is assumed that in clean PHT conditions the refinery is just within its allocated allowance and that any extra ton of carbon dioxide caused by fouling, \(M_{\text{CO}_2}\), has to be paid for. This may not be the case depending on the allowances allocations to and within the refinery. The costs associated with the extra CO\(_2\) emissions are:

\[
C_{\text{emiss}}(t) = M_{\text{CO}_2} \times P_{\text{CO}_2}
\]  

(6.11)

where \(P_{\text{CO}_2}\) is the price per kg of CO\(_2\) (in US$ kg\(^{-1}\), assumed constant) and \(C_{\text{emiss}}\) at \(t = t_{\text{KPI}}\) provides KPI–03.

If network retrofit is considered, the savings in CO\(_2\) emissions for each configuration \(C_j\) with respect to the reference configuration \(C_1\) are calculated from the fuel energy savings in Equation 6.7:

\[
\Delta M_{\text{CO}_2}^{C_1-C_j}(t) = \Delta E^{C_1-C_j} \times \frac{m_{\text{CO}_2}}{\eta_{\text{fur}}}
\]  

(6.12)

The CO\(_2\) savings associated with \(\Delta M_{\text{CO}_2}^{C_1-C_j}\) are:

\[
S_{\text{emiss}}(t) = \Delta M_{\text{CO}_2}^{C_1-C_j} \times P_{\text{CO}_2}; \text{ for } j = 2, \ldots, N_c
\]  

(6.13)

The cumulative CO\(_2\) savings up to time \(t = t_{\text{KPI}}\) provide KPI–03r for network retrofit.

### 6.2.3 Assessment of production loss

The reduction in thermal efficiency caused by fouling is paid not only at the furnace as extra energy and emission costs but also as loss of production. As seen in Section 2.3.2.2, a furnace has a maximum heat duty achievable, \(Q_{\text{fur}}^{\text{max}}\):

\[
Q_{\text{fur}}^{\text{max}} = \dot{m}^{\text{max}} c_p (\text{COT} - \text{CIT})
\]  

(6.14)

where \(\dot{m}\) denotes the crude mass flowrate in the furnace and \(c_p\), its specific heat capacity, calculated as a function of the average temperature between CIT and COT. With a large decline in CIT due
to fouling, the furnace may hit its firing limit (FFL). The time when this happens, \( t_{\text{FFL}} \), provides a key performance indicator, KPI–04, and is defined as:

\[
    t_{\text{FFL}} = t\big|_{Q=Q^{\text{max}}}
\]  

(6.15)

At this point, the throughput must be reduced causing loss of production. When constrained by the furnace firing limit, \( \dot{m} \) is calculated from Equation [6.14]

\[
    \dot{m}^{\text{max}} = \frac{Q^{\text{max}}_{\text{fur}}}{c_p (\text{COT} - \text{CIT})}
\]  

(6.16)

The mass lost in production, \( M_{\text{prod}} \), is given by:

\[
    M_{\text{prod}}(t) = \int_0^t \left( \dot{m}^{\text{clean}} - \dot{m} \right) dt
\]  

(6.17)

where \( \dot{m}^{\text{clean}} \) is the mass flowrate in clean condition and \( \dot{m} \) the actual throughput. The cost associated the production loss, \( C_{\text{prod}} \) is then calculated as:

\[
    C_{\text{prod}}(t) = \frac{M_{\text{prod}}}{0.1569 \rho} \times P_{\text{bbl}}
\]  

(6.18)

where \( P_{\text{bbl}} \) is the operating margin per bbl of crude (US$ bbl^{-1}). \( C_{\text{prod}} \) as calculated in Equation [6.18] at time \( t = t_{\text{KPI}} \) provides KPI–05.

To assess network retrofit performance with respect to production loss, the difference (excess) production achieved by each configuration \( C_j \) with respect to the reference configuration \( C_1 \) is calculated from the difference in massflowrate over time:

\[
    \Delta M_{\text{CO}_2}^{C_1-C_j}(t) = \int_0^t (\dot{m}^{C_j} - \dot{m}^{C_1}) dt; \text{ for } j = 2, \ldots, N_c
\]  

(6.19)

The savings associated with \( \Delta M_{\text{CO}_2}^{C_1-C_j} \) are:

\[
    S_{\text{v prod}}(t) = \frac{\Delta M_{\text{CO}_2}^{C_1-C_j}}{0.1569 \rho} \times P_{\text{bbl}}; \text{ for } j = 2, \ldots, N_c
\]  

(6.20)

\( S_{\text{v prod}} \) evaluated at \( t = t_{\text{KPI}} \) denotes KPI–05r.
6.2 Assessment of network performance: key performance indicators

6.2.4 Assessment of hydraulic efficiency

The reduction in tubes cross-sectional area produces an increase in pressure drops that must be countered by increasing the energy supplied to the pump to maintain the largest throughput achievable within the FFL constraint. Pressure drops, shear stress and velocity within individual heat exchangers can be used to evaluate the hydraulic impact of fouling. However, the hydraulic performance of the whole network can be assessed via the increase in coil inlet pressure (CIP) over time with respect to clean conditions:

\[ \Delta \text{CIP}(t) = \text{CIP} - \text{CIP}^{\text{clean}} \] (6.21)

The value of \( \Delta \text{CIP} \) at \( t = t_{\text{KPI}} \) provides KPI–06. The cost of energy loss associated with the increase in pumping power required to counter the hydraulic effects of fouling is another useful indicator of the network performance. The integral over time of the difference between pumping power in clean conditions, \( W^{\text{clean}} \), and the actual pumping power (i.e. in fouled conditions), \( W \), gives the energy losses at the pump due to fouling, \( E_{\text{pump}} \):

\[ E_{\text{pump}}(t) = \int_{0}^{t} \left( W^{\text{clean}} - W \right) dt \] (6.22)

Where the pumping power, \( W \), is calculated via Equation 5.26. The energy losses \( E_{\text{pump}} \) calculated in Equation 6.22 translate in electric energy requirements, \( E_{\text{elec}} \), which depends on the efficiency of the pump, \( \eta_{\text{pump}} \):

\[ E_{\text{elec}}(t) = \frac{E_{\text{pump}}}{\eta_{\text{pump}}} \] (6.23)

Pumping costs are calculated as:

\[ C_{\text{pump}}(t) = E_{\text{elec}} \times P_{\text{elec}} \] (6.24)

where \( P_{\text{elec}} \) is the price of electricity in US$ kWh\(^{-1}\). \( C_{\text{pump}} \) evaluated at \( t = t_{\text{KPI}} \) provides KPI–07.

In case of a retrofit, the CIP in a given configuration \( C_j \), is compared to that in a reference configuration, \( C1 \). The total (cumulative) electric energy required for each configuration \( C_j \), is defined as:

\[ \Delta E_{\text{elec}}^{C1-C_j}(t) = E_{\text{elec}}^{C_j} - E_{\text{elec}}^{C1} ; \text{ for } j = 2, ..., N_c \] (6.25)
6.2 Assessment of network performance: key performance indicators

Savings associated with $\Delta E_{\text{elec}}^{C_1-C_j}$ are:

$$S_{\text{elec}}(t) = \Delta E_{\text{elec}}^{C_1-C_j} \times \frac{P_{\text{elec}}}{\eta_{\text{pump}}}; \text{ for } j = 2, .., N_c$$ (6.26)

which, calculated at $t = t_{KPI}$ indicates KPI–07r for network retrofit.

6.2.5 Overall fouling costs

The sum of all costs previously considered provides the cumulative total cost up to time $t$ due to fouling:

$$C_{\text{fouling}}(t) = C_{\text{fur}} + C_{\text{emiss}} + C_{\text{prod}} + C_{\text{pump}}$$ (6.27)

where, in summary, $C_{\text{fur}}$ is the cost of the additional energy that must be provided by burning extra fuel in the furnace to counter the decline over time in CIT, $C_{\text{emiss}}$ is the costs associated to the extra emission of CO$_2$ due to fouling, $C_{\text{prod}}$ is the cost associated with the reduction in throughput, and $C_{\text{pump}}$ is the electricity cost due increase in pumping power required to maintain a constant throughput. The cumulative cost of fouling, $C_{\text{fouling}}$, evaluated at $t = t_{KPI}$ denotes KPI–08 which comprehensively summarises the economic impact of fouling in the CDU. For network retrofit, KPI–08r is the sum of KPI-02r, KPI-03r, KPI-05r, KPI-07r.

The prices of fuel, electricity, CO$_2$, and parameter values in Equation (6.10) used in the following case studies are reported in Table 6.2. Refining margins vary substantially with time and a number of factors (e.g. location of the refinery, types of crude processed etc.). The range for $P_{\text{bbl}}$ in Table 6.2 refers to the refining margins reported by Polley et al. (2009a). In Table 6.2 the price of CO$_2$ under ETS is assumed to be US$30 t^{-1}$.

It should be pointed out that the assessment of the costs is based on no action been taken to

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Symbol</th>
<th>Units</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon content in fuel</td>
<td>CC</td>
<td>kgC (kg fuel)$^{-1}$</td>
<td>0.7</td>
</tr>
<tr>
<td>Energy content of fuel</td>
<td>$F_E$</td>
<td>kWh (kg fuel)$^{-1}$</td>
<td>11.7</td>
</tr>
<tr>
<td>Price of CO$_2$ under ETS</td>
<td>$P_{\text{CO}_2}$</td>
<td>US$ t^{-1}$</td>
<td>30</td>
</tr>
<tr>
<td>Price of electricity</td>
<td>$P_{\text{elec}}$</td>
<td>US$ MWh^{-1}$</td>
<td>50</td>
</tr>
<tr>
<td>Fuel price</td>
<td>$P_{\text{fuel}}$</td>
<td>US$ MWh^{-1}$</td>
<td>27</td>
</tr>
<tr>
<td>Profit margin per bbl</td>
<td>$P_{\text{bbl}}$</td>
<td>US$ bbl^{-1}$</td>
<td>2$\div$10</td>
</tr>
<tr>
<td>Furnace efficiency</td>
<td>$\eta$</td>
<td>–</td>
<td>90%</td>
</tr>
<tr>
<td>Pump efficiency</td>
<td>$\eta_{\text{pump}}$</td>
<td>–</td>
<td>80%</td>
</tr>
</tbody>
</table>
clean any unit as cleaning and shut down costs are not considered here.

6.3 Network simulation and retrofit: case studies

Two case studies are presented for two different networks:

HEN1: the hot–end of a refinery is simulated (Section 6.3.1) to illustrate the detailed analysis made possible by the use of the model developed in Chapter 5 assisted by the techno–economic analysis proposed in the previous section.

HEN2: the PHT of a small refinery is analysed and retrofit options, aimed at increasing overall energy recovery, are assessed.

6.3.1 HEN1: Analysis of fouling impact on economics

Figure 6.3 shows the section of the network considered which starts downstream of the pre–flash drum (D–01) and comprises 5 shell–and–tube heat exchanger units before the furnace (F–01). Crude oil flows on the tube–side in all units. Of the 5 exchanger units, 4 are double shells and one, E–04, is a single shell. The units’ main geometrical parameters are reported in Table 6.3. Downstream of the first unit, the crude stream splits in two branches, namely B1 and B2, rejoining just before the furnace. The former branch, B1, comprises units E–02 and E–03 whereas the latter branch, B2, comprises units E–04 and E–05.

Inputs such as temperatures, flowrates, and fluid characteristics of all inlet streams (S1–S5), were set to typical values for this refinery (not reported here for confidentiality reasons) and

![Figure 6.3: HEN1 hot–end structure of the crude pre–heat.](image)
Table 6.3: Summary of exchangers’ main geometrical parameters in HEN1. Counter-current arrangement in multiple shells is indicated with cc, parallel flow with p.

<table>
<thead>
<tr>
<th>Branch</th>
<th>E–01A</th>
<th>E–01B</th>
<th>E–02</th>
<th>E–03</th>
<th>E–04</th>
<th>E–05</th>
</tr>
</thead>
<tbody>
<tr>
<td>No. shells</td>
<td>–</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Arrang.</td>
<td>–</td>
<td>cc</td>
<td>p</td>
<td>cc</td>
<td>–</td>
<td>p</td>
</tr>
<tr>
<td>Pass</td>
<td>2</td>
<td>2</td>
<td>4</td>
<td>2</td>
<td>4</td>
<td></td>
</tr>
<tr>
<td>$D_S$ [mm]</td>
<td>1245</td>
<td>1194</td>
<td>1397</td>
<td>990</td>
<td>1270</td>
<td>1397</td>
</tr>
<tr>
<td>$d_i$ [mm]</td>
<td>19.86</td>
<td>19.86</td>
<td>19.86</td>
<td>13.51</td>
<td>19.86</td>
<td>19.86</td>
</tr>
<tr>
<td>$d_o$ [mm]</td>
<td>25.40</td>
<td>25.40</td>
<td>25.40</td>
<td>19.05</td>
<td>25.40</td>
<td>25.40</td>
</tr>
<tr>
<td>$N_t$</td>
<td>–</td>
<td>764</td>
<td>850</td>
<td>880</td>
<td>630</td>
<td>890</td>
</tr>
</tbody>
</table>

kept constant throughout the simulations. Initial conditions assume that all heat exchangers are clean (no fouling deposit) at time $t=0$ and the evolution of fouling and performance indicators is simulated for one year of operation, with no cleaning.

Values of the fouling model parameters (Equation 4.37) were estimated from actual plant data for one of the heat exchangers as described in Section 5.4 and used for all the other units. In this way it is assumed that the pre–exponential factor, $\alpha$, the activation energy, $E_f$, and the suppression constant, $\gamma$, depend on the average crude properties processed in the refinery. It is acknowledged that an estimation of the parameters for each heat exchanger may provide more accurate predictions of the fouling behavior. However, this goes beyond the purpose of this study where no attempt is made to compare simulation results with (confidential) plant data.

6.3.1.1 Results and discussion

Simulation results include the temperatures, flowrates and pressures in all streams in the network, the flowrate split in the two branches B1 and B2, the CIT and the heat load at the furnace in addition to the detailed behavior of each unit.

Whilst one of the strength of the model developed in Chapter 5 is its distributed nature, it is difficult to assess network performance of a PHT that comprises several units. Thermal efficiency in each unit of the network is instead assessed at first by using its average fouling resistance over time, $\bar{R}_{fi}$ (calculated via Equation 5.34) for $i = 1, \ldots, N_u$, where $N_u$ denotes the number of units in the network. This is helpful to identify critical units in the network that exhibit severe fouling. For these units a more in–depth analysis can then be performed (e.g. determining local fouling resistance, thickness of the deposit layer etc.). Individual average fouling resistances, for each shell over one year are reported in Figure 6.4. Units in branch B1 show the largest values for the
fouling resistance in the network. In particular, whilst E–03 is at higher temperature, the velocity is higher than in unit E–02. As a result, the combination of temperatures and wall shear stress in E–03 are such that the fouling rate is lower than that in E–02.

Figure 6.5 reports the temperature field plot of the network. This plot, introduced by Wilson et al. (2002) shows on the y axis the temperature of the hot fluid (shell–side) and on the x axis the temperature of the cold one (crude) and is very useful to assess at a glance the status of the network. The impact of fouling on the thermal performance of the network can be assessed by comparing the black segments (at initial clean conditions) with the red ones (at fouled conditions after one year of operation). There is an evident, large and not uniform shift of the outlet temperatures of units E–01, and the two units in branch B2 (E–04 and E–05) due to fouling whilst a better performance overtime of units in branch B1 (E–02 and E–03) is seen. Counter–intuitively, these are also the exchangers with higher fouling rate (Figure 6.4). An explanation for this can be found by considering that units E–05AB and E–02AB are interconnected on the shell–side by stream S5 (Figure 6.3). A decrease in heat duty over time caused by fouling in E–05AB results in an increase of the inlet temperature in the shell–side of E–02AB. Therefore, for this unit, the decrease in duty due to fouling is countered by an increasingly higher shell–side
temperature. As a result, the two branches, thermally balanced in clean conditions (crude outlet temperatures of E–03B and E–05B differ by 0.7°C), become heavily unbalanced in fouled conditions. After a year, the difference in the crude outlet temperatures of the two branches is over 65°C.

An inspection of the pressure drops across the units (Figure 6.6(a)), shows that the hydraulic performance of the network over time is the result of rather distinct fouling effects in the different units. Surprisingly, however, E–02, the unit experiencing the highest fouling rate, seems to be the least affected by fouling from an hydraulic point of view. This is due to the thermo–hydraulic interactions of fouling within two parallel branches. In clean conditions, 40% of the total mass flowrate flows through branch B1 and 60% through branch B2. From Figure 6.6(b) it can be noted that the difference between the two flowrates increased significantly over time, reaching 10% of the total in B1 and 90% in B2 after a year of operation. The oil flow split (Figure 6.6(b)) is defined for branch B1 as:

\[ S_p = \frac{\dot{m}_{B1}}{\dot{m}_{B1} + \dot{m}_{B2}} \times 100 \]  \hspace{1cm} (6.28)
6.3 Network simulation and retrofit: case studies

Figure 6.6: Evolution of tube–side pressure drop across each shell (a) and flow split between the two branches as percentage of the total flowrate (b) in HEN1.

Lower flowrates mean lower velocities across the exchangers in branch B1 which can explain the higher fouling rate in this branch. As also noted by other authors (Ishiyama et al. 2008; de Oliveira Filho et al. 2009), it is therefore important to control flow splits to avoid hydraulic unbalances in the network. The effects of controlling the flow split ratio between branches B1 and B2 is discussed in Section 6.3.1.2.

Figure 6.7 shows the thickness of the fouling layer deposited in the two hottest units of the train (E–03 and E–05) after one year. The different arrangements of the two units show a noticeable difference. Shells in unit E–03 (Figure 6.7(a)) are arranged so that the shell–side fluid flows in counter–current to the tube side fluid. This results in a large difference in deposit

Figure 6.7: Thickness of the fouling layer, after one year of operation, in units E–03 (a) and E–05 (b) in HEN1. Arrows indicate the direction of the crude flow in each pass.
thickness between the two shells in the same unit, with a smaller value (ca. 3.8 mm) at the tube–side inlet of shell E–03A and a larger one (ca. 4.65 mm) at the outlet of the tube–side of shell E–03B. However, there is no noticeable gap in thickness between the two shells in unit E–05 (Figure 6.7(b)) which are in parallel flow. The overlap that can be noticed between the last pass of unit E–05A and the first two passes of E–05B is due to the difference in film temperature, $T_f$, produced by the internal arrangement in E–05B.

The combined performance of all units in the network is reflected in the progressive decline of the CIT and increase in CIP over time (Figure 6.8(a)). After one year ($t_{KPI}=365d$), KPI–01 = -43.20°C and KPI–06=2.44 bar. These are sizable reductions that would be prevented in real refinery operations with periodic cleaning actions to avoid the large costs that will be shown later. The increase in heat duty associated with this decline is reported in Figure 6.8(b). The maximum heat duty $Q_{max}^{furn} = 90$MW (Equation 6.14) is reached after ca. $t_{FFL}=239$ days (KPI–04=135d). An assessment of the individual contribution of all losses considered in Equation 6.27 is reported in Figure 6.9(a). From an environmental point of view, an extra release at the furnace of ca. 3.2 t h$^{-1}$ of CO$_2$ on average is responsible for more than US$840,000 in one year of operation (KPI–03). An order of magnitude smaller (KPI–07=US$38,000) is the pumping cost over a year due to extra electric energy needed to counter the increase in pressure drops across the network. The fuel energy cost is larger and adds up to almost US$3.5M (KPI–02). It is quite evident that the cumulative costs surge as soon as production has to be throttled back after 239 days when the furnace limit is reached. If a smaller furnace (85MW) was used (Figure 6.9(b)), its firing limit is
Figure 6.9: Cumulative costs over time for different refinery margins ($P_{bbl}=\text{US}$2±10$bbl^{-1}$) in HEN1 for $Q_{faw}^{\text{max}}=90\text{MW}$ (a) and $Q_{faw}^{\text{max}}=85\text{MW}$ (b).

reached 131 days sooner ($t_{FFL}=108\text{d}$) and these costs are expected to increase significantly (up to ca. US$15.4M).

6.3.1.2 Flow split ratio control

To assess the importance of controlling the crude flow split ratio between the two branches B1 and B2, the network was simulated by controlling the flowrate in each branch to be constant at a fixed flow split ratio (40% in branch B1 and 60% in branch B2 as in clean conditions). The average fouling resistance for each shell in the network with fixed flow split is shown in Figure 6.10. The mass flowrate flowing in the two branches remains unaltered over time (until the FFL is reached) thus avoiding thermo–hydraulic channelling due to fouling in the branch at lower hydraulic resistance. Because of the higher flowrates compared to the uncontrolled case, the fouling rates are significantly lower in branch B1 and show an asymptotic behaviour previously not shown in Figure 6.4. However, units E–04 and E–05 in branch B2 show a larger value of the average fouling resistance compared to the uncontrolled case. Forcing the flow split to remain constant, the pressure drops are increased with a CIP 0.8 bar larger than in the base case after a year of operations with an increase of cumulative costs for pumping power almost US$10,000 larger than the base case.

The overall beneficial effect of controlling the flow split at a constant ratio can be appreciated in Figure 6.11(a) which shows that the drop in CIT after a year is over 4°C less than the base case in which the flow split ratio is not controlled. The two branches are now thermally more
balanced with only a small difference in outlet temperatures of ca. 2.5°C seen after a year of operation. As a result of the better thermal performance, at the expense of the pressure drops, $t_{FFL}$ is delayed by 33 days (KPI–04=266d) compared to the base case (Figure 6.11(b)) and the total costs are reduced by almost US$1.4M over a year of operation.

Figure 6.10: Averaged fouling resistance over time in each shell of HEN1 with fixed flow split.

Figure 6.11: Effect of controlling the flow split ratio on HEN1 thermal performance and costs. CIT predictions (a) and cumulative costs (b) for the base case with uncontrolled flow split ratio are compared with the fixed split ratio case.
6.3 Network simulation and retrofit: case studies

6.3.1.3 The cost of getting it wrong

The benefit of the multi-scale approach undertaken in this thesis can be appreciated by examining, for example, the contribution of ageing to the network performance. The importance of using the ageing model was already highlighted in Section 5.7.1.2 where it was concluded that, if ageing is not included in the model, the outlet temperatures would have been estimated with a significant less accuracy. At this stage it is interesting to know how much this difference would affect the accuracy of predictions at the network level and the economic analysis. Figure 6.12(a) shows the CIT value over time for the base case \( (P_{\text{bbl}} = \text{US}$10 bbl}^{-1}, Q_{\text{max}}^{\text{fur}} = 90 \text{ MW}) \) and a no-ageing case. The latter has been obtained by considering the same process conditions, fouling and cost parameters as in the base-case with the only difference that the pre-exponential term, \( A_a \), in Equation 4.14 set to zero in all units. After a year of operation, a difference of 15°C in CIT for the two cases is estimated. As previously noted, ageing has a beneficial effect on heat transfer as it increases the value of the thermal conductivity of the deposit layer. As a result, not only the outlet temperature of the individual units in the no-ageing solution are lower that predicted in the base-case, but the furnace firing limit is reached at \( t_{\text{FFL}} = 101 \text{ days} \), 138 days earlier than the base-case. Figure 6.12(b) shows in economic terms the cost of getting such prediction wrong. After a year of operation, the difference in the estimation of total cumulative cost, KPI–08, in the two cases is over US$16M.

![Figure 6.12: Impact of ageing on HEN1. CIT loss (a) and total cumulative costs (b) for the base case are compared with the no-ageing case.](image-url)
Table 6.4: KPI summary at $t_{KPI}=365$ d with refinery margins at US$10$ bbl$^{-1}$ for HEN1.

<table>
<thead>
<tr>
<th>KPI</th>
<th>Units</th>
<th>$Q_{fuer}=85$ MW (Base case)</th>
<th>$Q_{fuer}=90$ MW (Fixed split ratio)</th>
<th>$Q_{fuer}=95$ MW (no ageing)</th>
</tr>
</thead>
<tbody>
<tr>
<td>01-CIT drop</td>
<td>°C</td>
<td>-42.74</td>
<td>-43.20</td>
<td>-44.39</td>
</tr>
<tr>
<td>02-Fuel cost</td>
<td>US$</td>
<td>2,746,892</td>
<td>3,454,188</td>
<td>3,631,168</td>
</tr>
<tr>
<td>03-$CO_2$ cost</td>
<td>US$</td>
<td>669,701</td>
<td>842,143</td>
<td>885,291</td>
</tr>
<tr>
<td>04-$t_{FFL}$</td>
<td>day</td>
<td>108</td>
<td>239</td>
<td>&gt;365</td>
</tr>
<tr>
<td>05-Production loss</td>
<td>US$</td>
<td>11,955,230</td>
<td>2,326,874</td>
<td>0</td>
</tr>
<tr>
<td>06-CIP increase</td>
<td>bar</td>
<td>35,915</td>
<td>38,464</td>
<td>39,531</td>
</tr>
<tr>
<td>08-Total costs</td>
<td>US$</td>
<td>15,407,740</td>
<td>6,661,668</td>
<td>4,555,990</td>
</tr>
</tbody>
</table>

6.3.1.4 Summary of HEN1 performance in the different cases

The use of the key performance indicators is useful to compare the different cases considered so far for network HEN1. Table 6.4 summarises the KPIs for the different cases investigated. It can be seen that the overall costs are dominated by the size of the furnace. The smaller the capacity of the furnace, the smaller $t_{FFL}$ and the larger the total extra costs associated to fouling. It can also be seen how controlling the flow split ratio to a constant value would be a cost effective solution to reduce total costs and that not considering ageing would result in a large over-estimation of production loss caused by fouling.

6.3.2 HEN2: Analysis of retrofit options

The objective of this second case study is to show that using high fidelity thermo-hydraulic simulations that capture complex dynamic interactions in the network provides a better way to analyse alternative PHT retrofit options than currently available. For this purpose, first a network is modelled based on an industrial case study of a small refinery (ca. 20,000 bbl day$^{-1}$) serving a state island and is used as base-case. Parameters that characterise the fouling behaviour in each unit are estimated so as to fit the performance of this base-case. Once the fouling behaviour is captured, the same values are used to assess alternative network retrofit configurations, with the goal of increasing overall energy recovery.

Three network retrofit structures are proposed. The first follows pinch rules to maximize energy recovery based on clean exchanger performance whilst the remaining two seek to improve the energy recovery while also taking into account the fouling behaviour. The results for the proposed retrofit designs are analysed with particular regard to the CIT achieved and the heat load at the furnace over the entire period.
6.3 Network simulation and retrofit: case studies

6.3.2.1 Base–case: existing network

In order to protect proprietary information, the heat and mass balance for the existing network comprising 7 exchangers (Figure 6.13) have been adjusted and some features of the plant (reported in Table 6.5) have been changed. Nonetheless, these changes do not affect the validity of the conclusions. This network structure will be referred to as configuration C1 and represents the base–case for the study. The performance of the pre–heat train was monitored at start–up (after cleaning) and after 8000 hours of operation (Table 6.5). Units E–01, E–02 and E–04 did not change significantly their performance over the operating period whereas the other four units exhibited severe fouling. The observations of the refinery operators were that fouling in units E–05 and E–06 occurred mainly on the tube–side (the crude oil flowed through the tubes) and this was the only side of these units which was periodically cleaned. Unit E–03 fouled on the shell–side (which handled column residues) but not on the tube–side. Unit E–07 fouled heavily on both sides. For the following analysis it is assumed that:

- The desalter temperature is optimally controlled and that its performance does not affect the fouling behaviour of the network.
- Crude is on the tube–side and hot fluids flow on the shell–side in all units.

Table 6.5: HEN2 heat exchanger geometries and performance in clean conditions ($T_{in}^0, T_{out}^0$) and after 8000 hours ($T_{in}^*, T_{out}^*$). For all units $L=20$ ft (6.1 m) and $d_o=3/4$ in (19.05 mm).

<table>
<thead>
<tr>
<th>Unit</th>
<th>$N_t$</th>
<th>$N_p$</th>
<th>$B_r$</th>
<th>$L_{nc}$</th>
<th>$N_0$</th>
<th>$D_t$</th>
<th>Flow [kg h$^{-1}$]</th>
<th>$T_{in}^0$ [°C]</th>
<th>$T_{out}^0$ [°C]</th>
<th>$T_{in}^*$ [°C]</th>
<th>$T_{out}^*$ [°C]</th>
<th>Flow [kg h$^{-1}$]</th>
<th>$T_{in}^0$ [°C]</th>
<th>$T_{out}^0$ [°C]</th>
<th>$T_{in}^*$ [°C]</th>
<th>$T_{out}^*$ [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>E–01</td>
<td>152</td>
<td>6</td>
<td>22</td>
<td>178</td>
<td>32</td>
<td>444</td>
<td>10000.00</td>
<td>205.00</td>
<td>44.00</td>
<td>205.00</td>
<td>44.10</td>
<td>100000.00</td>
<td>32.00</td>
<td>51.30</td>
<td>32.00</td>
<td>51.30</td>
</tr>
<tr>
<td>E–02</td>
<td>308</td>
<td>8</td>
<td>17</td>
<td>146</td>
<td>40</td>
<td>584</td>
<td>20000.00</td>
<td>290.00</td>
<td>83.00</td>
<td>290.00</td>
<td>83.00</td>
<td>100000.00</td>
<td>51.30</td>
<td>96.50</td>
<td>51.30</td>
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<tr>
<td>E–03</td>
<td>336</td>
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<td>17</td>
<td>130</td>
<td>43</td>
<td>584</td>
<td>50000.00</td>
<td>254.60</td>
<td>295.40</td>
<td>246.10</td>
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<td>100000.00</td>
<td>120.50</td>
<td>121.20</td>
<td>120.50</td>
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<tr>
<td>E–04</td>
<td>620</td>
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<td>17</td>
<td>153</td>
<td>37</td>
<td>798</td>
<td>40000.00</td>
<td>220.00</td>
<td>147.50</td>
<td>220.00</td>
<td>147.50</td>
<td>100000.00</td>
<td>116.70</td>
<td>147.50</td>
<td>116.70</td>
<td>147.50</td>
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<tr>
<td>E–05</td>
<td>1130</td>
<td>6</td>
<td>17</td>
<td>136</td>
<td>41</td>
<td>1100</td>
<td>60000.00</td>
<td>280.00</td>
<td>207.20</td>
<td>280.00</td>
<td>207.20</td>
<td>100000.00</td>
<td>200.50</td>
<td>221.30</td>
<td>200.50</td>
<td>221.30</td>
</tr>
<tr>
<td>E–06</td>
<td>240</td>
<td>2</td>
<td>17</td>
<td>138</td>
<td>41</td>
<td>520</td>
<td>10000.00</td>
<td>280.00</td>
<td>208.50</td>
<td>280.00</td>
<td>208.50</td>
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<td>193.40</td>
<td>193.40</td>
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<tr>
<td>E–07</td>
<td>968</td>
<td>4</td>
<td>17</td>
<td>137</td>
<td>41</td>
<td>740</td>
<td>50000.00</td>
<td>360.00</td>
<td>295.40</td>
<td>360.00</td>
<td>295.40</td>
<td>100000.00</td>
<td>200.50</td>
<td>221.30</td>
<td>200.50</td>
<td>221.30</td>
</tr>
</tbody>
</table>

Figure 6.13: HEN2 structure in the base–case configuration.
- Given the small throughput, the furnace firing limit is never reached (i.e. $Q_{fur} << Q_{fur}^{max}$).

### 6.3.2.2 Proposed network revamps

By analysing the stream temperatures reported in Table 6.5 it is clear that more energy can be recovered from the residue stream. If pinch rules for maximum energy recovery are applied, the area of E–07 would be increased. This can be done, for example, by adding an extra unit E–07x, identical to E–07 in geometry. The resulting network structure, referred to as configuration C2, is shown in Figure 6.14(a). In this design, the hot residue stream is matched with the crude at its highest temperature. Whilst this ensures maximum heat recovery in clean conditions, over time fouling is expected to penalize the overall heat recovery of the network as the wall temperatures, on which fouling depends, are also maximized.

![Diagram](image)

**Figure 6.14:** HEN2 network retrofit configurations C2 (a), C3 (b) and C4 (c).
To increase the performance over time, we analyse an alternative network retrofit, configuration C3 in Figure 6.14(b). This goes against traditional pinch rules by matching the hot residue stream with the crude at an intermediate temperature (at the exit of E–05). In his configuration, the residue stream enters the extra unit E–07x, placed between units E–05 and E–06 and subsequently enters E–07 and E–03. As a result, heat recovery in clean conditions is expected to be less than that achievable with configuration C3, however, the crude at the highest temperature exchanges heat with a lower temperature residue stream.

A third alternative configuration, C4 in Figure 6.14(c) considers the residue entering first unit E–07 as in the base–case structure and then unit E–07x which is placed between E–05 and E–06 as in structure C3. The additional area and new exchanger design could also be optimised for each configuration, but this was not done to provide a more direct comparison of the effect of adding the same area in different positions. The performance given by the different designs is assessed by considering the value of the CIT achieved over time and the total energy required by the furnace to maintain a constant value of the coil outlet temperature of 360°C. Equation 6.7 is used to assess the performance of the three retrofit configurations proposed over the base–case. As the same additional heat exchanger E–07x is used in all three retrofit options, the capital costs will be the same.

### Results and discussion

Figure 6.15 shows the CIT for the base–case and the three retrofit options. It can be seen that in clean conditions (i.e. \( t=0 \)), for configurations C2 and C4 the CIT is over 13°C larger than that achieved in C1, indicating a good extra energy recovery. Despite the extra heat transfer area available in configuration C3 compared with C1, the initial CIT in configuration C3 is 3.5°C lower than in the base–case. This is because the performance of existing units E6 and E7 falls due to reduced temperature driving force.

Over time, however, things change significantly because of fouling. Fouling rates in E–07 are highest for configurations C3 and C4, and lowest for C1 and C2 (Figure 6.16(a)). Unit E–07x fouls more in C2 then in C3 and C4 (Figure 6.16(b)). As a result, after less than a month of operations, the CIT in C3 is maintained at a higher value compared to that of the base–case C1. After 150 days C3 starts recovering more energy than C2. The structure generated according to pinch rules, C2, results in the worst performance over long time. After ca. 300 days, the CIT in
the retrofit structure C4 also falls below that of C3.

Figure 6.17 (a) shows that the drop in CIT over time is drastic for C1 and C2 whilst C4 performs better. Configuration C3 in particular is the one that suffers the least from the decrease in CIT ($KPI_{01}|_{C_1,t=600d} = -20.8^\circ C$).

The networks perform very much differently also from an hydraulic point of view. Figure 6.17 (b) shows the increase in pressure drops with respect to clean conditions for each configuration.

Figure 6.16: Average fouling resistance calculated over time for exchangers E–07 (a) and E–07x (b) in HEN2.
ration considered ($\Delta CIP$, calculated in Equation 6.21). Since the existing network C1 has one unit less (E–07x), it has a lower total pressure drop and a lower $\Delta CIP$ compared to the others ($KPI–06|_{C1,t_{KPI}=600d}=5.4$ bar). Among the three proposed retrofits, C4 performs the worst, with $KPI–06|_{C1,t_{KPI}=600d}=22.3$ bar.

Whilst the analysis of the CIT and CIP highlights the importance of considering fouling
6.3 Network simulation and retrofit: case studies

Figure 6.18: Extra energy recovered each the network with respect to the base–case in the three retrofit cases considered for HEN2. The right axis shows the equivalent economic savings in terms of fuel burnt at the furnace (i.e. not including CO$_2$) costs.

dynamics in the retrofit of PHT networks, it is not sufficient to assess which structure, amongst those proposed, provides the largest overall amount of energy recovered over time.

Figure 6.18 shows the (cumulative) amount of extra energy recovered by the network through one of the three proposed retrofits, as variation in the energy required in the furnace, with respect to the base–case (Equation 6.7). Although barely appreciable in Figure 6.18, given the scale of the graph, it should be noted that $\Delta E_{C1-C3}$ is negative for ca. the first 50 days of operations, confirming that at clean conditions, configuration C3 has a negative impact on the overall energy recovery. However, after roughly a year of operations configuration C3 starts performing better than C2, the configuration proposed following pinch rules. By analysing Figure 6.18 another important aspect can be unveiled. Whilst the CIT in configuration C3 becomes larger than that in C4 after ca. 300 days, the cumulative extra energy recovered by the latter is constantly larger than that recovered by the former. In configuration C4, the fouling resistance in E–07 increases with respect to the base–case (the tube side temperatures are higher) but it results in the lowest fouling resistance in E–07x. Clearly, the position of the extra unit and its fouling behaviour is paramount for the overall performance of the network. In economic terms, savings in fuel costs alone are shown on the right axis of Figure 6.18.

Table 6.6 reports summary of the KPIs used to comprehensively assess the fouling behaviour of the different configurations at $t_{KPI}$=600. With respect to CIT drop, network C2 is the worst
6.4 Concluding remarks

**Table 6.6**: KPI summary at $t_{KPI}=600$ days for HEN2 and the three proposed retrofits.

<table>
<thead>
<tr>
<th>KPI label</th>
<th>Unit</th>
<th>C1</th>
<th>C2</th>
<th>C3</th>
<th>C4</th>
</tr>
</thead>
<tbody>
<tr>
<td>KPI–01</td>
<td>°C</td>
<td>-49.0</td>
<td>-52.2</td>
<td>-20.9</td>
<td>-41.7</td>
</tr>
<tr>
<td>KPI–02r</td>
<td>US$</td>
<td>451,000</td>
<td>616,000</td>
<td>691,000</td>
<td></td>
</tr>
<tr>
<td>KPI–03r</td>
<td>US$</td>
<td>110,000</td>
<td>150,000</td>
<td>168,000</td>
<td></td>
</tr>
<tr>
<td>KPI–04</td>
<td>days</td>
<td>∞</td>
<td>∞</td>
<td>∞</td>
<td>∞</td>
</tr>
<tr>
<td>KPI–05r</td>
<td>US$</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>KPI–06</td>
<td>bar</td>
<td>5.4</td>
<td>16.7</td>
<td>20.2</td>
<td>22.3</td>
</tr>
<tr>
<td>KPI–07r</td>
<td>US$</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
<td>&lt;1000</td>
</tr>
<tr>
<td>KPI–08r</td>
<td>US$</td>
<td>561,000</td>
<td>766,000</td>
<td>859,000</td>
<td></td>
</tr>
</tbody>
</table>

performer (KPI-01$_{C2}$=-52°C). KPI-02r estimated for the different configurations shows that of over US$450,000 in fuel savings can be achieved by using configuration C2 whilst ca. US$600,000 using C3 and ca. US$680,000 using configuration C4. The extra economic benefit of C4 vs. C2 is ca. 50%. Whilst after 300 days of operation, the energy recovered in retrofit ranks options as C4>C2>C3, after 600 days the ranking becomes C4>C3>C2. In fuel costs alone, these differences translate in ca. US$230,000 over 600 days between a network structure designed accordingly to pinch rules and one that takes into account fouling. Of course, other factors such as reduction in throughput, which were not included in this second case study, could play a crucial role (as shown for HEN1) in the choice of the arrangement. In absolute energy and monetary terms, benefits are expected to be much higher for larger refineries.

### 6.4 Concluding remarks

The gPROMS simulation environment used allows the easy modelling, solution and analysis of different configurations of single units and/or network layouts as function of process conditions, while using the sophisticated thermo–hydraulic model presented for all units.

In the first case study presented, the network analysed comprised 9 shells arranged in a typical hot–end configuration and showed the counter–intuitive behavior of some of the units over time due to fouling. In particular, coupling of the thermal and hydraulic aspects of the network allowed capturing the substantial change in mass flowrate split between the two branches of the network as fouling progresses and establishing how this in turn affects the fouling behavior of each unit. If this split is not calculated correctly, it may lead to inaccurate estimation of the fouling rate and misleading decisions about which unit to clean. It has also been highlighted the importance of including detailed phenomena at the micro–scale, such as ageing of the deposits,
as they can affect estimations of the costs associated with fouling. Model simulations show that this could be a very costly mistake. The large costs involved with energy consumption but also with loss in production and CO₂ emission, confirm the need for accurate monitoring of fouling.

The second case study presented in this chapter, highlighted that in the design of heat exchanger networks rules aiming at maximising energy recovery alone based on clean conditions may not give the best strategy to pursue in retrofitting PHTs networks. In particular it has been shown that energy recovery differences in three alternative retrofit solutions can be large and that fouling plays a major role in the energy recovery which is not captured if steady state conditions alone are considered at the design stage.

The approach presented is a powerful tool for the analysis of fouling behavior of a network and estimation of its impact on costs. From the two case studies shown here, some key conclusions can already be drawn:

1. It is feasible to simulate multi–unit networks using detailed, high fidelity dynamic models. This analysis captures complex time–varying interactions, are not revealed by simpler models.
2. Uncontrolled flow splits may lead to unbalanced performance of different branches, exacerbating fouling. Accurate estimation of the local fouling effects is required for flow split control.
3. Network designs based merely on energy integration concepts which use simplified models which neglect fouling dynamics may lead to uneconomic layouts. Fouling behavior should be included in the analysis.
4. A trade–off exists between maximum energy recovery and fouling behaviour.
5. A detailed mathematical model is required to accurately assess energy losses and, ultimately, refinery costs related to fouling.

With a detailed model on hand, a number of options to mitigate fouling can be investigated, from monitoring of fouling behaviour and its economic impact, to the retrofit of a single unit, to re–shaping the network layout, to the control of flow split and analysis of cleaning schedules. Finally, other units could be integrated in the simulation and analysis, for example the pre–flash drum or the crude distillation column.
Chapter 7

Conclusions

Synopsis

This thesis was concerned with fouling in pre–heat trains of refinery crude distillation units. The main goal was to develop a high fidelity model for shell–and–tube heat exchangers capable of capturing thermo–hydraulic effects of tube–side fouling. In this final chapter, the main features of the model are summarised and key conclusions from model predictions are drawn. The contributions and achievements of the research undertaken are also highlighted. Finally, suggestions for future directions are presented.
7.1 Summary

This thesis has highlighted that fouling in crude pre–heat trains has a tremendous impact on refinery efficiency, operability, costs and health & safety of personnel and equipment. A survey of relevant literature, presented in Chapter 2, has highlighted that chemical reaction fouling in general is a complex problem that has challenged researchers for decades. Crude oil fouling presents even more challenges because of the several uncertainties related to the number of species involved and the variability of the composition. Nonetheless, it was possible to identify key process variables, namely velocity and temperature, that are correlated to the fouling rate.

In Chapter 3 limitations of current heat exchanger and heat exchanger network design methodologies in dealing with fouling were exposed. It has been discussed how the use of such methodologies may lead to design solutions that exacerbate fouling and produce significant losses in the long run. The need to develop improved tools that capture the dependence of fouling on process conditions and time has also been identified. It has been shown that existing models for crude oil fouling in refinery heat exchangers are subject to a number of assumptions that limit their accuracy. To overcome these limitations, a systems approach has been undertaken in this thesis.

A multi–scale modelling approach has been proposed to include the interactions of several phenomena at different scales of investigations. The thesis structure unfolded by following the same logic. Micro–scale phenomena (e.g. local fouling rate, ageing and surface roughness dynamics) have been modelled at the tube level which is representative of lab–scale apparatuses. The tube model has been subsequently incorporated at the macro–scale in the model of an industrial shell–and–tube heat exchanger. The interconnections of several units, according to specific PHT topologies, allowed simulation of entire networks to assess the impact of fouling at the plant scale and ultimately on the refinery bottom–line.

In Chapter 4, the interactions between local operating conditions and fouling deposition are captured at the tube level by coupling the solution of a moving boundary problem with the use of the fouling rate model by Ebert–Panchal, used in a distributed way. This distinctive feature of the model, allows calculating the thermal resistance and thickness of the fouling layer along the tube as well as its interactions with heat transfer and fluid–dynamics. Two models that capture important phenomena, namely surface roughness dynamics and ageing of the deposits, which are often neglected in literature, have been proposed. The first model captures the effects of the
increase in surface roughness due to fouling deposition on the convective heat transfer coefficient. The second describes the change in thermal conductivity caused by the exposure of the deposit layer to high temperatures for a long time.

In Chapter 5 the single tube model has been used as building block to simulate, at unit level, multi-pass shell–and–tube heat exchangers. The distributed nature of the model allows identifying critical zones where deposition is particularly severe and proposing geometries that mitigate fouling. The multi–pass model was implemented in a commercial process simulator (gPROMS) and validated using data from two different refineries operated by major oil companies. A procedure to analyse refinery data and support the estimation of a set of model parameters has also been established. It has been shown that there is an excellent agreement (less than 2% error) between model predictions and primary plant measurements (i.e. temperatures) even when the model is tested for its predictive capabilities over long periods (i.e. 16 months). The model has been used to precisely quantify energy losses caused by fouling and propose retrofit options to minimise them.

Lastly, in Chapter 6 the high fidelity exchanger model was used to simulate entire networks of different configurations. The network models have been easily built in a flowsheeting environment by linking unit–level models, suitably instantiated with geometric parameters, via appropriate stream connections. A set of key performance indicators (KPIs) has been proposed and used to systematically assess the impact of fouling on refinery operability and economics (e.g. reduction in throughput, extra furnace fuel, etc.) on two case studies of pre–heat networks. In the first case study, the simultaneous solution of equations for all exchangers allowed calculation of energy losses for each unit, assessment of the impact of fouling on the overall thermo–hydraulic performance of the network and unveiled the complex interactions between several units. It has been shown that the implementation of a simple control scheme (i.e. flow ratio control in two parallel branches of the network) can save ca. US$1.3M over a year of operation. Moreover, it has been shown that phenomena occurring at the micro–scale, such as ageing of the deposits, can largely affect estimations of the costs associated with fouling at the plant level. A second case study has been presented to assess energy losses and the effectiveness of network retrofits aimed at minimising them. In this case the model has been proven useful to identify network structures that increase energy savings by mitigating fouling in the long run, over and above networks generated following traditional pinch rules for maximum energy recovery in a clean network.
7.2 Contributions and Achievements

The innovative contribution of this work should be seen in the context of a field that has not progressed much beyond the use of the so called ‘fouling factors’ in over 40 years of research. Key contributions of this work are:

- A mathematical model that, given exchanger geometries, inlet temperatures and flowrates, is capable of calculating the exchanger’s outlet temperatures within a 2% error, even when the model is tested for its predictive capabilities over extended periods (up to 16 months of operations) (Coletti and Macchietto, 2010a,c).
- A procedure to analyse refinery plant data discarding gross errors, produced by unreliable measurements, which may compromise the success of the parameter estimation procedure used and hence the quality of model predictions.
- The combined use of a dynamic and distributed thermo–hydraulic model with a fouling rate model. This allowed the calculation of key quantities (e.g. fouling resistance, heat flux, heat transfer coefficient, etc.) as a function of time and space across the unit considered. Such an approach increased model accuracy with respect to the previous standard, which involved the use of lumped fouling resistances and heat transfer coefficients in the calculations (Coletti and Macchietto, 2010a).
- The use of cylindrical coordinates in the heat balance equations and a moving boundary approach to calculate temperature and thermal conductivity profiles across the radial direction of the fouling layer allowed overcoming the thin–slab approximation used in previous attempts, thus removing the limitation in accuracy for large thicknesses (i.e. > 10% of the tube diameter) (Coletti and Macchietto, 2010a).
- The use of primary plant measurements (rather than derived fouling resistances) in conjunction with state–of–the–art model–based parameter estimation techniques to estimate values for the model parameters. This allowed avoiding errors in the analysis of fouling data resulting from simplifying assumptions in earlier calculations (Coletti and Macchietto, 2010a).
- For the first time in open literature, an attempt has been made to model surface roughness dynamics due to chemical reaction fouling. The proposed model explains some otherwise puzzling phenomena such as an (apparent) initial negative fouling resistance (Coletti et al., 2010b).
7.3 Future work

- The development of an ageing model, in collaboration with the University of Cambridge, to describe the structural changes of the fouling deposits over time which was previously simply neglected (Ishiyama et al., 2009b), and its use within the distributed heat exchanger model (Coletti et al., 2010b).

- The use of the advanced dynamic model to simulate dynamic behaviour of networks and the development of a set of KPIs to systematically analyse fouling behaviour and its techno–economic impact on different PHTs (Coletti and Macchietto, 2009c, 2010b).

The above features led to the development of a method that exceeds current industrial practices, which relies heavily on heuristic and past experiences for design and operational decision making. The benefits that this approach offers are:

- The possibility of accurately predicting crude oil fouling behaviour in existing refinery heat exchangers allows enhanced monitoring capabilities. Although demonstrated with historical data, these can be implemented on–line to assess energy and economic losses due to fouling and prevent them with adequate strategies (e.g. control of flow splits). (Coletti and Macchietto, 2009b,c).

- Retrofit options aimed at maximising performance while accounting for fouling in both heat exchangers and heat exchanger networks can be assessed and their effectiveness over long period of times tested. (Coletti et al., 2010a).

- Fouling can be accounted for at the design stage of single units and networks of heat exchangers (Coletti and Macchietto, 2008, 2009a).

This research effort led to the publication of 5 journal articles, 1 invited article in a specialised magazine and 6 papers in edited conference proceedings. The results were also disseminated at several international conferences and 3 industrial invited talks.

7.3 Future work

The model developed in this thesis has proven highly flexible and capable of being readily adapted to different geometric configurations to simulate pilot plants, heat exchangers and networks. It should be pointed out that capabilities of the model have yet to be fully exploited. For example, the dynamic nature of the model would allow real–time model based predictive
control of flow splits between different branches in the network to prevent thermo–hydraulic channeling.

Future improvements and extensions of the model may include:

- The model has been validated only from a thermal point of view but not from an hydraulic one as direct measurements of pressure drops were not available. The value used for the thermal conductivity of the initial deposit (i.e. $\lambda_0$), affects the calculations of the fouling layer thickness which, in turn, affects pressure drops, velocity and shear stress within the tubes. The value used here is considered conservative as it is the lowest in the literature range. For given value of $R_f$, the calculated thickness is in fact smaller for small values of $\lambda_0$. However, only the use of pressure drop measurements can validate the hydraulic predictions of the model. This could be pursued in conjunction with the experimental programme scheduled on the high pressure test rig built as a part of the CROF project by other sub–projects (Macchietto et al., 2009).

- The parameter estimation methodology used here relies on the first 60 days of refinery measurements to capture the fouling behaviour of a given unit. It would be useful to explore the possibility of reducing this time in order to find the minimum number of days required to reliably predict future fouling trends.

- To be completely predictive (i.e. do not rely on past measurements), fouling behaviour could be captured with the use of thermodynamic packages (e.g. using the approach by Edmonds et al. (1999)) that can predict onset of fouling as a function of process conditions and composition. This however, would require information that are often non readily available (when at all) to refineries such as the exact composition of the crude blend processed and how this changes over time. Moreover, the necessary thermodynamic models to accomplish this in a reliable way do not appear to be available in the near future.

- The heat exchanger and network retrofits proposed, respectively, in Section 5.9 and Section 6.3.2 are mostly concerned with assessing the effect of fouling by simulation of specific heat exchanger geometries and network structures. However, a combination of enhanced heat transfer and reduced fouling can be achieved via a dynamic optimisation that targets maximum energy recovery or, more generally, economic performance over time. Targets for operating time could also be introduced. In this case, a design would not guarantee the maximum energy recovery but it would favour a longer run to avoid costly maintenance
action within refinery turn–arounds. Overall a dynamic optimisation which takes into account all costs associated with fouling (i.e. reduction in throughput, energy loss including fuel at the furnace and pumping power, GHG emissions and maintenance) is envisaged. The model is already implemented in a process simulator with optimisation capabilities.

- Issues regarding the control of flow split in parallel branches of networks have been discussed in a simple way by using an ideal controller in Section 6.3.1.2 to keep the flow ratio to a fixed value. More realistic control structures and/or different targets (e.g. maximum CIT) can be considered. The dynamic formulation of the model lends itself very well for this type of study and an online implementation for model predictive control is envisaged.

- Optimisation of cleaning scheduling. Where fouling cannot be prevented by the use of well designed heat exchangers, cleaning in–between refinery turn–arounds is unavoidable. This is very costly for operators and there is scope for the development of tools that help them to plan cleaning schedules. A shift from basic heuristic with limited predictive capabilities to more advanced ‘model–based maintenance planning’ approach which takes advantage of sophisticated optimisation techniques would be required. Optimisation approaches have been already attempted in this area, however they either rely on simplified models (i.e. linear fouling models) or on very basic optimization algorithms which do not guarantee a global optimum. An implementation of the accurate fouling model proposed in this thesis in a MINLP model would be of great value to reliably minimise overall costs and plan effective cleaning scheduling of PHT.

The model could also be extended to different areas of fouling in refinery heat exchangers and other application areas:

- Fouling in reboilers. This also accounts for a large portion of energy inefficiencies in an oil refinery. The challenge here will be to modify the model to account for a two phase flow.

- Fouling in fired heaters. This is usually experienced by refineries which are not particularly affected by fouling in the pre–heat train. In this case modification of the model will involve implementing a different underlying heat transfer mechanisms (i.e. radiation).

- Cooling water fouling. The growth of biological organisms on heat transfer surfaces is a major problem in cooling systems. Here, it would be required to identify modelling methodologies to capture a different fouling mechanism.
Appendix A

Sensitivity analysis of the Ebert–Panchal model

To assess the importance of the different contributions to the fouling resistance calculated through the Ebert–Panchal model, a sensitivity analysis has been performed on Equation 4.37. Parameter and variables in Equation 4.37 have been fixed at the average value indicated in Table A.1 and let vary, one at the time, by assigning 1000 random values sampled from a normal distribution around the mean value and standard deviation reported in Table A.1.

Figure A.1 shows the value of the fouling resistance, $R_f$, as a function of the variation of parameter $\alpha$ (a), $\beta$ (b), $E_f$ (c), $\gamma$ (d) and variables $T_f$ (e), $\nu$ (f), $Re$ (g), $Pr$ (h). Although the velocity does not appear explicitly in Equation 4.37 in this sensitivity analysis it is preferred to the shear stress, $\tau$, as it enables an easier physical interpretation. Whilst the response of $R_f$ is essentially linear for $\alpha$, $\gamma$ and $Pr$, the responses to the the variation of the other quantities is non linear with the largest variation given by $E_f$.

The relative contribution to the fouling resistance, after a year of operation, of each parameter

Table A.1: Average parameter and standard deviation values used for the sensitivity analysis.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Average value</th>
<th>Standard deviation</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>0.0015</td>
<td>0.0005</td>
<td>m$^2$W$^{-1}$s$^{-1}$</td>
</tr>
<tr>
<td>$\beta$</td>
<td>0.66</td>
<td>0.1</td>
<td>–</td>
</tr>
<tr>
<td>$E_f$</td>
<td>28,000</td>
<td>5,000</td>
<td>J mol$^{-1}$</td>
</tr>
<tr>
<td>$\gamma$</td>
<td>$7.3\times10^{-12}$</td>
<td>$5\times10^{-12}$</td>
<td>m$^2$K W$^{-1}$s$^{-1}$Pa$^{-1}$</td>
</tr>
<tr>
<td>$\nu$</td>
<td>2</td>
<td>0.5</td>
<td>m s$^{-1}$</td>
</tr>
<tr>
<td>$T_f$</td>
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<td>40</td>
<td>ºC</td>
</tr>
<tr>
<td>$Re$</td>
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<td>5,000</td>
<td>–</td>
</tr>
<tr>
<td>$Pr$</td>
<td>8</td>
<td>0.5</td>
<td>–</td>
</tr>
</tbody>
</table>
Figure A.1: Sensitivity analysis for the Ebert–Panchal model. Response of $R_f$, after one year of operation, to the individual variation $\alpha$ (a), $\beta$ (b), $E_f$ (c), $\gamma$ (d), $T_f$ (e), $v$ (f), Re (g), Pr (h) in Equation 4.37.
Figure A.2: Sensitivity analysis for the Ebert–Panchal model. Response of $R_f$, after one year of operation, to the variation of the different quantities in Equation 4.37 (a) and the response of $R_f$, after one year of operation, normalised between its minimum and maximum value to the variation of the same quantities, normalised between the minimum and maximum value of each quantity. Note the axis break after 0.01 K m$^2$ W$^{-1}$ (a) and 0.01 (b).

and variable considered is shown in Figure A.2. The variation of parameters $E_f$ and $\beta$ are the two top contributors whilst among the variables, $T_f$ has the largest influence on the final value of $R_f$ (Figure A.2 a)). This is not surprising given the exponential nature of the response to these specific quantities (Figure A.1). Figure A.2 b) reports the same response of $R_f$, after one year of operation, normalised between its minimum and maximum value to the variation of the various quantities in Equation 4.37, each normalised between its minimum and maximum value.
Appendix B

Computational fluid dynamics in fouling research

In the open literature computational fluid dynamics (CFD) is beginning to be applied to the design of heat exchanger equipment to describe in particular the shell–side flow (Andrews and Master, 2005; Vessakosol and Charoensuk, 2010) and to assess the effects of baffle spacing (Mohammadi et al., 2009) and the benefits of helical baffles (Wang et al., 2009; Zhang et al., 2009). Most articles that use a CFD approach to study fouling behaviour focus their attention on flat plate heat exchangers, commonly used in the food industry (Kho and Müller-Steinhagen, 1999; Zettler and Müller-Steinhagen, 2001; Jun, 2005). Brahim et al. (2003b,a) integrate a model for the fouling layer deposition and suppression with a CFD (Fluent) analysis of the parallel flow across flat plates. The authors used a mechanistic model for fouling of calcium sulphate. Using a structured grid for the calculations of the flow between parallel flat plates, they considered both the velocity and the heat flux distribution as a function of the time–dependent total thickness of the layer. To avoid the need for a moving boundaries approach, they considered a “fictitious crystal growth model”. This consist in varying the inlet velocity as a function of the thickness of the layer, which is calculated through the deposit mass (given by the deposition/suppression model) by its density.

Various other uses of CFD in fouling research include the method of Saghatooslam et al. (2010) who used a commercial package (Fluent) to calculate the thickness of the fouling layer in a crystal; Al-Anizi and Al-Otaibi (2009) who used CFD to design enhanced impingement plates subject to fouling; Bergeles et al. (1997) who predicted particle deposition in lignite utility...
boilers and Bouris et al. (2005) who studied the effects of a novel tube cross–sectional area on the fouling behaviour of a gas.

Unlike other areas mentioned above, CFD has not often been applied to fouling analysis in heat exchangers processing crude oil. Clarke and Nicolas (2000) explored the effects of shell–side crude oil fouling in a 14–baffle unit. The shell volume was modelled as a porous medium and the tube bundle was represented by a reduction in porosity. This is a method commonly used to reduce the computational effort (Tierney, 1992). Impermeable surfaces were used for the baffles. The Ebert–Panchal model (the exact form of the equation used is not specified) was then used on the shell–side to take into account the formation of deposits on the outer surface of the tubes. To represent deposition, the model artificially increases the fluid viscosity, as the deposit thickness increases, in the cells around the tubes. This seems to be a very crude approach which is limited by a number of assumptions (e.g. the interactions between tube and shell–side are neglected by setting an arbitrary fixed linear temperature profile on the tub–side). However, it seems that attempts in literature to simulate fouling on the shell–side of a heat exchangers are limited to this one paper.

Very recently Yang et al. (2009b) showed that a CFD approach can be used to interpret crude oil fouling data in a batch stirred vessel.
Appendix C

Commercially available software for heat exchanger design

The main software commercially available to design heat exchanger are reviewed here with emphasis on how fouling is accounted for. The review is limited to software capable of perform thermo–hydraulic design. Software for the detailed mechanical design is not considered here.

The industry standard software for the thermo–hydraulic design of heat exchangers appears to be *Xchanger Suite* by Heat Transfer Research, Inc. (HTRI), a company leader in process heat transfer and heat exchanger technology located in College Station, Texas (USA). Recently (September 2009), HTRI has entered into a strategic alliance with Honeywell (who acquired research, technical documents, and source code from Aspen Technology, Inc.) to utilize data and codes originally generated by Heat Transfer and Fluid Flow Services (HTFS). Fouling dynamics is not taken into account and the usual TEMA fouling factors are used. HTRI recently released another software, *R–trend*, that calculates and trends the fouling resistance for shell–and–tube heat exchangers. Unfortunately, no information on the model used for the calculations is available. HTRI not only develops software but have also experimental facilities for treating a wide variety of fluids, including gas oils and crude oils which can provide information for the validation of the design programs.

KBC has recently acquired *Persimmon* from Veritech Inc., a dedicated software for ‘crude unit monitoring and simulation’. The simulation program includes a network rating and simulation program and a comprehensive cleaning cycle analysis. The software performance relies on the ability to look at alternate network structures so that process designers can optimize existing
structures or design new ones for unit debottlenecking or for unit expansion studies. Few indications on the fouling model used in the calculations are available, but they claim id that “the fouling model for each heat exchanger can be user specified according to analytical models or from plant operating records and experience”.

Aspen Shell & Tube Exchanger is the thermo–hydraulic desig software by AspenTech. It has the advantage that can be interfaced with two of the most popular process simulators (Aspen Plus and HYSYS) which enables to rigorously model heat exchanger operation and identify capital savings opportunities within the context of the overall process. The software is also bi–directional integrated with Aspen Shell & Tube Mechanical whcih allows for efficient optimization to thermal and mechanical constraints. Fouling factors based approach is used.

SPRINT is a software developed by the Centre for Process Integration (founded by BP, ExxonMobil and Hydra) at Manchester University (UMIST). Its approach to heat exchanger network retrofit is based on the Network Pinch concept.

A comprehensive heat transfer simulation program is HEXTRAN (SimSci–Esscor) that allows for single exchanger and network designs, pinch analysis, exchanger zone analysis, split flow, and cleaning cycle optimizations. One of the main strength of this software is the large physical properties database and the thermodynamic models implemented. Another software of the same company is ARPM (Automated Rigorous Performance Monitoring) that uses real–time plant data and rigorous simulation models to highlight optimal operations targets and equipment degradation due to fouling. The TEMA fouling factors for the design.

Express Plus is a software for the rating, design, and retrofit of heat exchanges developed by IHS ESDU. The sofware is based on the design space concept (ESDU 2000 reviewed in Section 3.2.2) and allows the generation of plots useful to quickly assess the effect of main geometric parameters on the fouling behaviour of the unit under scrutiny. Design factors included in such plots include overall thermal duty, tube–side pressure drop, shell–side pressure drop and maximum and minimum tube–side velocities. Express Plus also allows the designer to determine the effects on pressure drops and heat transfer coefficients that a range of tube inserts would have on the design. Fouling is accounted for by the use of the modified Ebert–Panchal model (Panchal et al. 1999) and the software provides a simple way of fitting fouling trends to plant data to calculate the fouling threshold. A similar approach was developed by Butterworth (2002), in the educational software DEVIZE that has the advantage that can be interfaced with the
mode established Xchanger Suite by HTRI. Table C.1 summarises the software reviewed. It is highlighted that IHS ESDU Express and KBC Persimmon are the only commercial software that account, somehow, for the dynamics of fouling. They all seem to be based on lumped models and do no take into account the variation of fouling resistance and thickness within the unit (IHS ESDU express Plus does calculates the fouling rate at inlet and outlet of the exchanger but averages out the informations for the design purposes).
Appendix D

Dissemination record

**Journal Articles**


**Refereed Conference Papers in Edited Books**


**Refereed Conference Papers**

**Other Conference Contributions (not refereed)**


Invited talks and seminars


References


References


References


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