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ENERGY AND PROCESS INTEGRATION

by

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FOREWORD

Optimisation of the use of energy is of fundamental importance, particularly in view of the increasing tensions between energy supply and demand which the world now faces. Chemical processes in general, and distillation processes in particular, account for a significant fraction of the world's energy usage. For example, distillation processes account for around 3% of the energy utilisation in the US. There is thus a significant incentive to so design systems that energy utilisation is minimised. Much progress has been made by the application of simple methods such as pinch technology (see for instance B. Linnhoff and R. Smith, Section 1.7 of the Heat Exchanger Design Handbook, also published by Begell House), but the problems encountered in complex distillation systems are such that a much higher level approach is needed.

It is therefore very timely for Begell House to publish this monograph by Michael Georgiadis and Efstratios Pistikopoulos both of whom are from the Centre for Process Systems Engineering (CPSE) at Imperial College. CPSE is an international leader in the areas of process simulation, optimisation and control. One can confidently expect that the application of techniques of the type described in this volume will make an important contribution to making the best use of mankind's increasing scarce energy resources.

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Chapter 1

Introduction

Process synthesis, when first emerged as a separate research area, was defined as *"the act of determining the optimal interconnection of processing units as well as the optimal unit type and design of the units within a process system"* (Nishida *et al.*, 1981). Optimality has been determined mainly from the economic performance of a process system, with one of the major factors of the economic viability of a chemical plant being traditionally its energy consumption. Hence, in parallel with synthesis efforts for overall processes, the heat recovery problem formed on its own an active research field. Following the general synthesis trends, evolutionary methods were developed in parallel, independently or even in conjunction with algorithmic techniques. Heat integration possibilities have been explored after the chemical plant structure and design have been determined or simultaneously, with the synthesis of separation systems, reaction networks etc. In the last decade, increasing environmental awareness, in chemical plant design as well as in other areas, has drawn attention to another type of plant integration, towards waste minimization and minimum environmental impact. Integration of waste treatment technologies has led towards "mass" integrated processes, which comply more efficiently with environmental specifications. Heat and mass integration have evolved to being two major directives in the synthesis and design of chemical processes that perform efficiently with low operating, capital and environmental cost.

In the context of process synthesis distillation is a highly utilized and at the same time one of the most energy intensive unit operations in the chemical process industry. Mix indicated in 1978 (Mix *et al.*, 1978) that distillation consumed about *3%* of the US energy and that *10%* savings in distillation energy could amount to savings of about *$500* million in the national energy cost. Today, the expense of distillation-related energy consumption has reached even higher levels, considering the expansion of the use of distillation in industry and the higher cost of utilities. These economic-nature reasons have imposed the treatment of energy efficiency as the main design target in distillation.

Due to its importance, distillation has received particular attention in Chemical Engineering, with publications about the operation and design of countercurrent separation cascades dating as early as 1889 (Sorel, 1889). Moreover, since multicomponent separations require the use of sequences of distillation columns, significant research efforts have concentrated on the synthesis of these systems aiming at energy efficiency. Research on this subject has been further powered by the fact that extensive energy savings can be achieved through the selection of the most energy efficient sequence, amongst a large number of available candidates. This is an explicit consequence of the

dependence of distillation systems' energy consumption on the feed mixture and on the order in which its components are separated.

Technological breakthroughs are constantly called in to propose new techniques for energy efficiency that would compensate for the ever increasing energy related distillation expenses. Two of the most promising techniques are the Heat Integration and the Thermal Coupling of distillation columns. The former is based on the energy savings that can be achieved by heat integrating two distillation columns, that is, by using the heat generated in a column's condenser for the heat required in another column's reboiler, while satisfying appropriate temperature difference conditions. This technique can lead to substantial energy savings, which could reach the order of *50%*, when compared to non-heat integrated arrangements. Similar energy savings have been reported through the use of Thermal Coupling techniques in distillation, where heat units and their associated utilities are eliminated through the use of two-way liquid and vapour interconnections between columns, the latter being characterized as complex columns. These energy savings are the direct result of the elimination of heat units and the increase of thermodynamic efficiency, due to the minimization of remixing effects, which are generally associated with non-Thermally Coupled arrangements.

However, in order to apply the aforementioned synthesis techniques for energy efficiency, certain complicating issues need to be addressed, which are mainly of structural and physical nature. The structural complications are related to the large number of alternative arrangements that need to be considered. Even in the simplest case from a structural perspective, where sequences of simple columns are examined (columns with a single feed and two products), the extensive connectivity possibilities between columns lead to the generation of a large number of alternative column sequences, which are increased with the number of components to be separated. Moreover, these structural complications become even more intense through the incorporation of structural possibilities associated with Heat Integration and Thermal Coupling.

The physical complications are related to the complexity of the underlying physical phenomena, which involve simultaneous mass and heat exchange between liquid and vapour streams at the tray cascades. Furthermore, the physics of the problem are such, that the choice of the optimal configuration is largely dependent on the feed mixture to be separated (its components' relative volatilities and composition). It has been reported (Tedder and Rudd (1978), Agrawal and Fidkowski (1998)) that, for a particular separation, column configurations which are generally regarded as highly energy efficient (for instance, fully thermally coupled columns), can, in fact, have larger energy consumptions than sequences of more conventional columns. Consequently, in order to evaluate efficiently the energy consumption of a particular column sequence and the energy savings that can potentially be achieved through its heat integration or thermal coupling, the aforementioned physical phenomena need to be accurately captured.

Summarizing, it is not an exaggeration to state that the economic importance and associated complications, have made the distillation column sequencing problem for energy efficiency, one of the most challenging synthesis problems in chemical engineering, with numerous approaches proposed for its solution. One of the earliest attempts was based on total enumeration. This approach, though, is limited to problems with only a few alternatives. Other main approaches are the heuristic and physical insight ones. The former relies on rules of thumb derived by engineering knowledge and/or by the use of short-cut models, while the latter is based on the exploitation of basic physical principles which are also based, to a certain extent, on simplified models and on graphical represen-

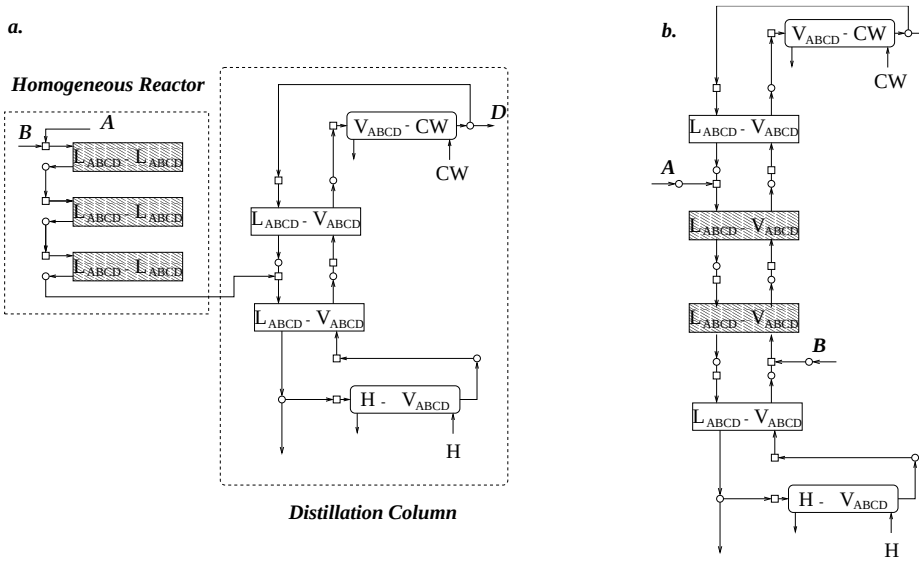

Figure 1.1: GMF Reactive and Separating System Representation (Ismail *et al*, 2001)

tations of the problem. These approaches generally enable quick and inexpensive calculations for the alternatives' physical evaluation. However, the fact that they are derived based on simplifying assumptions, which are valid only for certain cases, places a major limitation on their accuracy, validity and applicability. Furthermore, more complications arise when the developed heuristics are conflicting, suggest more than one possible solutions, or do not cover the details of the examined problem.

Finally, the most recent approach addressing this problem is the mathematical programming (algorithmic) approach, where the synthesis of column sequences is formulated as an optimization problem. Based on mathematical programming, one of the most important systematic approaches, which has been receiving increased attention over the last years, is superstructure optimization. Superstructures are, in general, superset flowsheets incorporating every feasible realization of the process in question. The generation and evaluation of each alternative realization takes place with the solution of an optimization problem, which usually involves the use of continuous and binary *(0-1)* variables, rendering the problem a Mixed Integer Programming (MIP) problem. However, most of these methods either use simplifying assumptions, limiting the validity and accuracy of the results, or treat the problem rigorously but at an expense of computational effort.

1.1 Book Objectives

Synthesis Target: *Find energy efficient process flowsheets such as simple, heat integrated and complex distillation column sequences, by systematically generating and evaluating the structural alternatives in an unified and compact way.*

In this work the approach proposed for addressing this problem is based on the Generalized Modular Framework (GMF) (Papalexandri and Pistikopoulos, 1996) (Proios, 2004). The GMF is

an aggregation superstructure optimization method for process synthesis at the conceptual level. It provides an alternative approach to the superstructure methods mentioned above, by using multipurpose building blocks of adequate abstraction and structural possibilities in the potential structural combinations, where the represented units and their connectivities are not *rigidly* predefined. An illustration of the GMF for the representation of reactive separating and reactive distillation systems is given in Figure 1.1. However, the GMF goes beyond simply generating the structural alternatives, since it can also evaluate them physically with respect to their energy consumption. This is possible since the GMF building blocks are accompanied by aggregated physical models, which can capture the underlying physical phenomena based on fundamental mass and heat exchange principles. Moreover, due to aggregation, the generated physical problems are of a compact size, thus reducing considerably the computational effort required for their solution.

In order to efficiently and systematically obtain the superstructure-based synthesis target set in this book, the following objectives need to be met:

Distillation Column Physical Representation

The GMF Physical Model will be modified appropriately in order to capture efficiently the physical phenomena taking place in a simple distillation column and consequently its energy consumption levels. The structural representation of the column will be realized by appropriately fixing the structural components of the GMF. Then a comparison to an accurate rigorous tray-by-tray distillation model will aim at the validation of the GMF physical representation. This physical representation and validation is of particular importance as it will provide the basis for the proposed GMF distillation column sequencing methods.

Simple Distillation Column Sequences

The objective is to develop a GMF Structural Model for the systematic generation of all the structural alternatives for the simple distillation column sequencing problem, using an adequate number of building blocks and appropriate interconnection rules between them. This structural model will be coupled to the GMF Physical Model and to a formal optimization solution procedure, in order to address the full synthesis problem, that is, the systematic generation *and* evaluation of simple column sequences, with the view of finding the most energy efficient column arrangement.

Heat Integrated (HI) Simple Distillation Column Sequences

Based on the GMF simple column sequencing method proposed, the aim is to extend the GMF for the incorporation of HI possibilities, in order to obtain more energy efficient distillation column designs. The HI problem will be formally addressed through the introduction of a Heat Integration (HI) block. The GMF Structural Model will be appropriately modified in order to incorporate structurally the HI block and the potential presence of heat units. Furthermore, the GMF Physical Model will also incorporate physically the HI block, while focusing on the heat integration feasibility conditions and the pressure effects on the represented columns' operation.

Complex Distillation Column Sequences

The objective is to propose a synthesis methodology which will allow the incorporation of Thermal Coupling techniques for energy efficiency in the distillation sequences. A GMF Structural Model will be proposed incorporating, in a unified way, complex columns, such as the Petlyuk sequence (Fully Thermally Coupled column), along with simple column sequences. The GMF Physical Model will then be applied in order to capture the underlying physical phenomena and the potential thermodynamic efficiency of thermal coupling.

GMF Physical Representation Enhancement

The GMF is an aggregation superstructure optimization method for process synthesis at the conceptual level, capturing efficiently the *general* trends in the underlying mass and heat transfer phenomena. The objective at this point is the increase of the levels of the GMF physical representation. This is proposed through the enhancement of the GMF Physical Model, by being appropriately coupled with formal discretization techniques, used for the order reduction of distillation column models. In doing so, principles of a simulation tool will be incorporated in the GMF conceptual design tool, while preserving and enhancing the latter's representational advantages.

1.1.1 Book Outline

This Book is structured as follows. In Chapter 2 an overview of the GMF is given, focusing on the latter's basic structural and physical principles. The GMF is modified through the incorporation of appropriately defined Auxiliary blocks in order to enhance its physical representation. The GMF Physical Model is then presented with a special focus on distillation. The GMF distillation representation is then validated through a comparison to a rigorous distillation model over a distillation column optimization case study.

Chapter 3 extends the ideas presented in Chapter 2, for the synthesis of simple distillation sequences using the GMF. A systematic method is proposed for the mathematical representation of superstructures, based on propositional logic expressions. The proposed methodology is applied to case studies for the first two members of multicomponent distillation. The GMF Structural Model generates the structural alternatives and the GMF Physical Model evaluates them with respect to their energy consumption using a formal optimization solution procedure, until the most energy efficient sequence is obtained.

In Chapter 4 the GMF simple column sequencing method is modified for the formal incorporation of heat integration possibilities, through the introduction of a Heat Integration block. The HI column sequencing method proposed, captures the structural possibilities and the physical phenomena, with particular focus on the effects of pressure, which is explicitly considered in the GMF Physical Model. The simple column sequencing case studies are revisited and new HI designs are obtained leading to higher energy savings.

Chapter 5 addresses the problem of complex column sequencing through the GMF. A systematic structural model is used for the mathematical representation of a superstructure incorporating simple and complex column arrangements. The GMF Physical Model is then coupled to the structural

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