Concepts of Chemical Engineering 4 Chemists

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Preface

This book is meant as a handbook and resource guide for chemists (and other scientists) who either find themselves working alongside chemical engineers or who are undertaking chemical engineering-type projects and who wish to communicate with their colleagues and understand chemical engineering principles. The book has arisen out of the short course, Concepts of Chemical Engineering for Chemists, held annually at UCL since 1999 and the forerunner to the Royal Society of Chemistry's "4 Chemists" series of professional training courses, of which it is now part. It can be used as accompanying material for the course, or as a stand-alone reference book. The course itself is designed to provide basic information on the main aspects of chemical engineering in a relatively simple, but practical, manner. Hence, while this book tries to emulate this, it also includes worked examples, plus extensive reference lists and bibliographies in order that the reader can research elsewhere for more detail and for aspects that are not covered in the book.

This book aims to give chemists an insight into the world of chemical engineering, outlining the basic concepts and explaining the terminology of, and systems approach to, process design. It can be said that chemists create new molecules and compounds and chemical engineers manufacture these into useful products on a commercial scale, but, of course, the two disciplines do not work in isolation; chemistry and chemical engineering are intertwined. One only has to look at the history of chemical engineering and its origins in chemistry (or, more correctly, applied chemistry) to appreciate the close relationship between the two and their shared foundation in molecular behaviour. The reader is referred to Darton *et al.*'s collection of visionary essays on chemical engineering's role in society[1] and the Whitesides report, "Beyond the Molecular Frontier",[2] which reflect on the importance of chemists and chemical engineering working effectively together to tackle the enormous challenges facing the world today.

To work effectively together, chemists and chemical engineers need to know how to communicate. This was the premise for the short course mentioned above and is the basis on which this book is written. Hence, the book does not focus on the derivation of mathematical formulae, but rather on the use of the governing principles in process design. Before I describe what the book contains, it may be useful here to take a brief look at what a typical chemical engineering degree course involves.

WHAT CHEMICAL ENGINEERING INVOLVES

Chemical Engineers are responsible for the design and operation of processes and of products and their application. Since they must consider processes in their entirety, from raw materials to finished products, they use a "systems" approach, enabling the prediction of the behaviour of both the process as a whole and of the individual plant items. Once a plant has been designed, chemical engineers are involved in its construction, commissioning and subsequent operation. Hence, in terms of education, a chemical engineer will undertake courses in:

- Mathematics (the emphasis is on engineering, after all).
- Science (notably chemistry, biology, material science).
- Process analysis (defining the mass, momentum and energy balances for the entire process).
- Thermodynamics (determining the fundamental parameters on which the process can be analysed).

Once the process has been defined, attention can then be paid to the "unit operations", the reactors, separators, *etc.* that make up the process route, or flowsheet (Figure 1). This involves the study of:

- Reaction engineering (the manipulation of molecular behaviour to determine the reaction routes to a specified product).
- Transport processes (the physical manipulations that underlie the process).
- Separation processes (the manner in which products are separated and purified).

Interwoven with all these topics are the crucial areas of safety (see Figure 2), risk analysis, plant and equipment design, process control and process economics. A practising chemical engineer will often find that the data he/she requires is either unreliable or incomplete[3] and, hence, he/she must make sound judgements based on mathematics, physics and chemistry to determine appropriate simplifying assumptions, while at

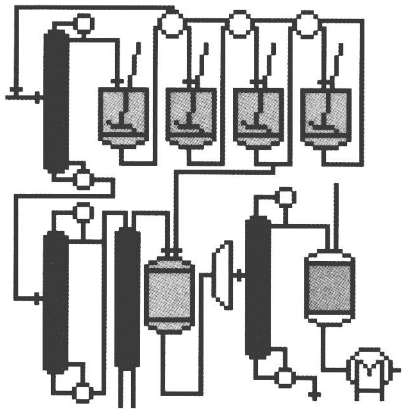

Figure 1 *Chemical engineers develop process flowsheets from mass and energy balances based on the conservation principle and using their knowledge of unit operations and thermodynamics*

Figure 2 *The explosion at the Buncefield oil depot in 2005 is a graphic example of how safety issues must always be paramount in chemical engineering (photo courtesy of Dr. Dave Otway, Department of Chemistry, University College Cork, taken by him from Ryanair flight FR903 STN-CORK at 11.40 am 11-12-05 10 min after take-off)*

the same time satisfying safety, environmental, operational and legal constraints.

Chemical Engineers are profoundly aware of their ethical and social responsibilities, encompassed in the notion of "sustainable development" which is becoming an increasing component of chemical engineering degree programmes. Often a chemical engineering student will supplement his or her degree programme with courses on environmental practice, law, management and entrepreneurship. In addition, a great deal of emphasis is placed on transferable skills training, in communication, teamworking and leadership.

The culmination of a degree programme in chemical engineering is the design project, in which the students work in teams to carry out the preliminary design of a complete process plant. This exercise involves the use of much of the material covered in the topic areas mentioned above, starting from the mass and energy balances and ending with a full economic appraisal, environmental impact and risk assessment (or, increasingly, a sustainability analysis on the socio-economic as well as environmental impacts) and safety analysis. Very often the teams will include MSc students with first degrees in chemistry, underlining the close relationship between the two disciplines and the need for mutual understanding in the development of effective and appropriate plant designs.

Sustainable development is defined as "development that meets the needs of the present without compromising the ability of future generation to meet their own needs". As stated in Ref. 4, technological change must be at the heart of sustainable development. In order to achieve a sustainable future, the basic principles that should guide technological (and societal) development are that consumption of resources should be minimised while that of non-renewable materials should cease, with preference given to renewable materials and energy sources. It is chemical engineers, together with chemists and other scientific disciplines, who will lead this technological revolution.[5] Although beyond the scope of this book, these issues must be at the forefront of all process and product developments and the concepts covered here are the bases on which to found this progress.

WHAT THIS BOOK CONTAINS

The book begins in Chapter 1 with the cornerstone of any process design, the development of mass and energy balances, based on the simple conservation principle. From such balances a chemical engineer will then go on to add more detail in order to come up with a fully optimised process flowsheet, providing the most efficient, safe and economic route to the production of the specified chemicals within the constraints of thermodynamics, material properties and environmental regulations. All chemical processes are dynamic in nature, involving the flow of material (fluid flow or momentum transfer) and the transfer of heat and mass across physical and chemical interfaces. The central part of any chemical process is the reactor, in which chemicals are brought together to produce the precursors to the eventual products. A chemical engineer must be able to predict and manipulate chemical reaction kinetics to be able to design such reactors. Hence, the concepts of chemical reaction engineering in relation to reactor design are considered in Chapter 2. The equally important principles behind momentum, heat and mass transfer are then covered in the following three chapters. Moving often huge quantities of material around a plant, through pipelines and in and out of vessels, requires a knowledge of fluid mechanics and its use in the design of the appropriate pumps and measurement equipment (Chapter 3). Maintaining rates of reactions and product quality requires the transfer of heat to and from chemicals, often through physical boundaries (*e.g.* pipe and vessel walls), and heat exchangers are a common means in which this transfer is achieved. The formulation of heat-transfer rate equations is described in Chapter 4 and their use demonstrated in the design of shell and tube heat exchangers. Mass transfer typically occurs in the separation of chemical components to remove impurities from the desired product. Distillation is a common separation technique employed in chemical plants and is described in Chapter 5.

Often, chemical plant design is informed by laboratory and pilot-scale experimentation. While the initial chapters in this book will inform the reader of the most important design parameters that need to be measured and determined from such experiments, how to then ensure that these parameters perform in the same way in a large-scale plant is the subject of Chapter 6. Although it is desirable to conduct the experimental work in the system for which the results are required, this is not always easy. The system of interest may be hazardous or expensive to build and run, while the fluids involved may be corrosive or toxic. In this case scale models are used, which overcome the above problems and allow extensive experimentation. In the majority of cases the model will be smaller in size than the actual, desired plant, but sometimes, due to the nature of the materials to be handled, the fluids involved may also be different. Scale-up is only possible if the model and plant are physically similar and, hence, the procedure is based on dimensionless groups. How to develop and use these groups is described in Chapter 6.

Many chemicals at some stage in a process (*i.e.* whether as raw materials, intermediates, products and by-products) are in powder form. Often, the handling of powders is mistakenly assumed to be relatively straight forward, leading to disastrous consequences (*e.g.* clogging of storage vessels, dust explosions, *etc.*). The characterisation and handling of powders is described in Chapter 7, with particular emphasis given to fluidisation as a common process operation. Particle science and technology is a rapidly maturing field but, surprisingly, there is still much reliance on empiricism in chemical engineering practice.

Throughout the design of a chemical plant, issues relating to safety, economics and environmental impact must be considered. By doing so, the risks associated with the plant can be minimised before actual construction. The same principle applies whatever the scale of the process. The field of process control (Chapter 8) considers all these issues and is, indeed, informed by the type of hazard analyses described in Chapter 10. The objectives of an effective control system are the safe and economic operation of a process plant within the constraints of environmental regulations, stakeholder requirements and what is physically possible. Processes require control in the first place because they are dynamic systems, so the concepts covered in the earlier chapters of this book are central to process control (*i.e.* control models are based on mass, energy and momentum balances derived with respect to time). Chapter 8 focuses on the key aspects of control systems.

The economic assessment of a proposed plant, known as project appraisal, is necessary at the design stage in order to determine its viability, the capital requirements and the expected return on investment. Such an analysis can kill a project at any stage in the design. Chapter 9 discusses how the planning for profitable operation is undertaken.

Last, but not least, safety is considered in terms of the analysis of the risks associated with potential hazards identified by detailed consideration of the proposed process flowsheet. Safety is the number one concern for chemical engineers and the reader should not confuse the fact that it is the focus of the final chapter in this book with its order of importance. However, in order to carry out a hazard study and risk assessment, one must understand the concepts on which a process flowsheet is developed, and these are covered in the preceding chapters. The procedure describe in Chapter 10 is recognised as best practice in the process industry sector.

The chapter authors of this book have tried to keep mathematical derivations to a minimum and have assumed that their readers have background knowledge of thermodynamics, since the latter is ubiquitous to both chemistry as well as chemical engineering. The authors are all either full time members of academic staff at UCL or, in the cases of Robert Thornton and Ken Sutherland, are retired industrialists who have extensive experience in their respective fields and have taught undergraduate courses on crucial aspects of chemical engineering practice. My thanks are due to them for their hard work in not only preparing the contents of this book but also in the development and delivery of the lectures and practical sessions of the "Concepts of Chemical Engineering for Chemists" course. Without their efforts, there would be neither.

Stef Simons
UCL

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