TIME DEPENDENT CHEMICAL PROCESSES

With Special Reference to their Simulation and Optimisation

E. R. ROBINSON

TIME DEPENDENT CHEMICAL PROCESSES

With Special Reference to their Simulation and Optimisation

E. R. ROBINSON
M.A., Ph.D., M.I.Chem.E., C.Eng.
Principal Lecturer in Control and Computation,
Faculty of Engineering,
North East London Polytechnic

APPLIED SCIENCE PUBLISHERS LTD
LONDON

APPLIED SCIENCE PUBLISHERS LTD
RIPPLE ROAD, BARKING, ESSEX, ENGLAND

ISBN: 0 85334 608 9

WITH 21 TABLES AND 177 ILLUSTRATIONS

Printed in Great Britain by Galliard (Printers) Ltd Great Yarmouth

Preface

The technical literature covering theoretical aspects of chemical engineering simulation and optimisation is large in volume and continuously growing. The practical application of these simulation and optimisation techniques is, in contrast, very limited. The gulf between theoretical ideas and practical implementation is wide, despite the tremendous value of these techniques. In a world ever conscious of costs and profits, every technique which helps to improve efficiency must be considered; simulation and optimisation techniques provide some of the more important methods for achieving these objectives.

This book presents its material in a non-mathematical, and in some cases a non-fundamental manner. The emphasis throughout is on the presentation of the material in as simple a way as possible, with many complete examples. A rigorous presentation of mathematical techniques can be somewhat overpowering to an engineer who is merely seeking an efficient and effective technique. This book aims, therefore, to be a user guide and not a theoretical treatment.

The book will be valuable to the practising engineer who is anxious to apply techniques, but does not wish to become involved with rigorous theoretical derivations. The book will also provide useful ideas for chemical engineering degree students, and will be an introduction to the subject for post-graduate students.

The contents cover both analogue and digital simulation techniques, although the emphasis is on the use of digital computers. Many computer programmes are provided, these are written in the Fortran language used on the IBM 1130 computer. This system of Fortran is one of the simplest and the programmes should, therefore, be directly usable on most digital computers. Techniques are generally introduced by means of a very simple application followed by more realistic situations. This is particularly true in the optimisation area, where techniques are applied to simple algebraic expressions before being used for chemical engineering simulations.

I am indebted to many colleagues and friends at the North East London Polytechnic for their valuable help and advice during preparation of this

book. In particular I must thank Mr M. J. Young, Mr B. J. Hawkins and Dr B. L. Klemz for their many valuable ideas and for their assistance in proof reading. Finally I must mention my gratitude to my wife, without whose patience and assistance this book would never have been written.

E. R. ROBINSON

Contents

CHAPTER I

Dynamic Processes, Modelling and Simulation

SYMBOLS

A	Heat transfer area of heating coil
A_1	Heat transfer area for heat exchanger
A_2	Heat transfer area for heating coil
C_p	Specific heat of liquid
K	Constant
M	Mass of liquid
M_1, M_2	Boundary conditions for liquid mass
t	Time
t_1, t_2	Boundary conditions for time
U	Heat transfer coefficient for heating coil
U_1	Heat transfer coefficient for heat exchanger
U_2	Heat transfer coefficient for heating coil
W	Liquid charging rate
θ	Temperature of liquid
θ_0	Temperature of liquid charge
θ_1, θ_2	Boundary conditions of liquid temperature
θ'	Temperature of liquid leaving heat exchanger
θ_s	Steam temperature
θ_1'	Intermediate batch temperature

Chemical process engineers are most often concerned with the design and performance of continuously operated chemical plant under steady state conditions. There are, however, many occasions when a knowledge of the dynamic behaviour of a process is of great importance. The study of such situations has increased in recent years with the greater use of computing facilities, which has allowed investigations to be made of processes yielding dynamic equations which cannot be solved analytically.

The engineer's task in studying a time dependent situation firstly requires him to write down the equations which represent the process; these will

generally be a combination of algebraic and differential equations, with the latter being either ordinary or partial in nature. Having satisfied himself that the equations do truly represent the process under consideration he must seek a solution. Only in the case of very simple processes will an analytical solution be possible. The engineer must more often make use of computing facilities to obtain his answers.

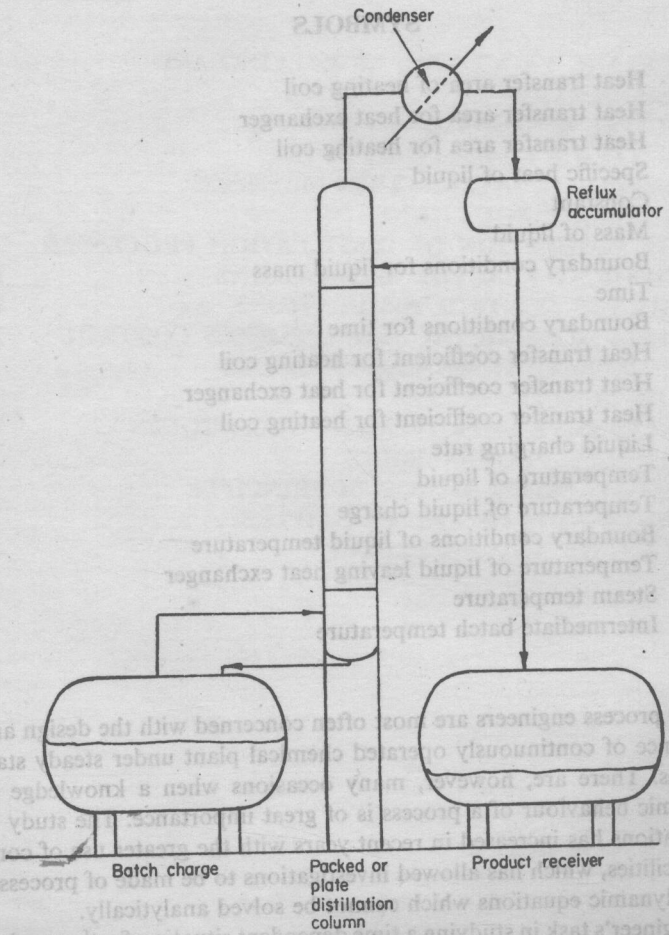

FIG. 1.1. Batch distillation process.

The stage of presenting the mathematics of a process in a manner which demonstrates a method of solution is known as 'modelling'. The next stage, the solution of the mathematics represented by the model, is known as 'simulation'. We shall be concerned with the modelling and simulation of chemical processes by analytical methods and by digital and analogue computer techniques.

Analogue computers allow combinations of algebraic and differential equations to be solved by establishing an analogous electrical circuit. Observations of voltages in this circuit show how various process parameters may be expected to vary with time. The electrical circuit is said to simulate the performance of the chemical process. Generally speaking the computer will simulate in a few minutes the operation of a chemical process over many hours.

Digital computers make use of a different approach, they will recognise and manipulate numbers only. Numerical methods must, therefore, be used in the solution of both algebraic and differential equations.

There are advantages and disadvantages in using both analogue and digital machines and these will be dealt with in the appropriate chapters. Briefly, however, it may be said that analogue machines will be more suited to small problems and digital to the larger processes.

The requirement that the chemical engineer should be able to solve, by computer means, the equations which he derives is becoming an essential of his profession. In the past, engineers have tended to be categorised into 'computer orientated' and 'non-computer orientated'. This division is rapidly disappearing, with all chemical engineers expected to be able to use computing facilities and to recognise the value and pitfalls in that use. Professional engineers are thus expected to be aware of computers but not dependent upon them. This book aims to develop this awareness in the specific field of time dependent chemical processes.

Consideration must now be given to areas of chemical engineering where dynamic processes are important. The following fields are all studies in process dynamics:

1. Batch processes
2. Continuous cyclic operations
3. Start up and shut down operations
4. Process control

Batch processes are by their very nature dynamic since operation is for a fixed time, during which many parameters, for example temperatures, masses and concentrations will change. Batch reactions will result in

changes in concentrations of the reactants and products, whilst batch distillation involves changes in product concentration and quantity with time.

Cyclic processes are those in which operation is carried out in distinct phases. Many catalytic chemical reactions result in a loss in catalyst efficiency with time. Such reactions are often carried out with two reactors in parallel, one being used for reaction whilst the catalyst of the other is being regenerated.

Another example of a similar cyclic process is the Wulff process for the production of acetylene. In this process acetylene is produced by the thermal decomposition of certain hydrocarbons. The cracking is carried out in a furnace containing hot brick checkerwork. The cracking is performed in a cyclic manner with the bricks being first heated by the burning of a gaseous fuel, followed by the cracking operation which reduces the checkerwork temperature. The complete cycle takes four minutes with the checkerwork being heated for one minute followed by one minute of cracking. These two operations are then repeated through the furnace in the reverse direction. Two furnaces, with staggered time cycles, are operated in parallel to maintain a continuous flow of hydrocarbon through the

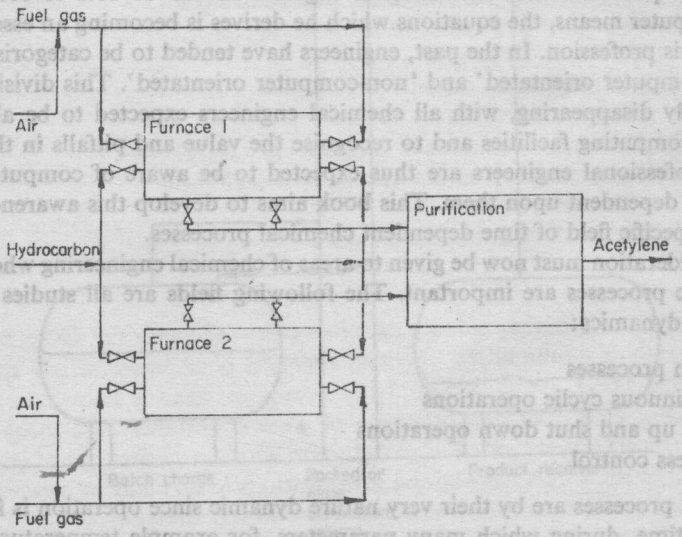

FIG. 1.2. Wulff process for the production of acetylene.

process. During the cracking operation the extent of cracking will be a function of the brickwork temperature, which will be greater at the beginning of the operation than at the end. Within each cycle the process is dynamic with variations in product concentration, it is of value to be able to predict this concentration variation in order to calculate optimum cycle times.

Recent suggestions (Cannon, 1961, Schrodt, 1967) have been made that the process of distillation should be operated in a cyclic manner with the reflux being sent to the column in pulses. Thus the concentrations of low boiling components will increase at the top of the column during periods when reflux is being applied, and decreased when it is not.

The start-up and shut-down periods of chemical plant operation are non-productive in nature and should, therefore, be reduced in time to a minimum. Simulations of these periods are generally carried out with this aim in mind.

The subject of process control is intimately tied up with a study in process dynamics. It is necessary to be able to describe a process in equation form and to use these equations in a process simulation which will predict the performance of any given control scheme. It is the field of process control which has largely been responsible for the impetus which has developed for process simulation in recent years.

Having seen that dynamic processes are of importance in present day chemical engineering, and may assume even more importance in the future, we must look at the derivation of the equations which will form the basis of our simulations.

DERIVATION OF EQUATIONS

Consider the heating of a well stirred batch of liquid by use of an isothermal heating coil as shown in Fig. 1.3.

Provided that there are no heat losses the rate at which heat is gained by the mass of liquid is equal to the rate at which heat is transferred from the coil.

$$MC_p \frac{d\theta}{dt} = UA(\theta_s - \theta) \tag{1.1}$$

If the specific heat of the liquid and the heat transfer coefficient are assumed constant the equation may be rewritten as

$$\frac{d\theta}{dt} = K(\theta_s - \theta) \tag{1.2}$$

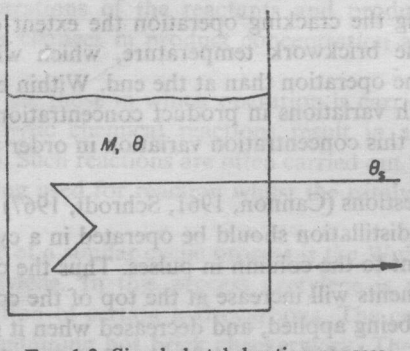

FIG. 1.3. Simple batch heating process.

where

$$K = \frac{UA}{MC_p} \tag{1.3}$$

Integration is then possible from the initial temperature θ_1, when $t = 0$, to a new value θ_2 when $t = t_2$ to give

$$\ln\left(\frac{\theta_s - \theta_1}{\theta_s - \theta_2}\right) = Kt_2 \tag{1.4}$$

The time required to heat the batch from an initial temperature θ_1 to a new temperature θ_2 may be calculated from eqn (1.4) and the repeated solution of this equation for different values of θ_2 may be regarded as a simulation of the process.

Reference to eqn (1.1) shows that the process equation was derived from the expression:

rate of heat accumulation = rate of heat inflow

For a more general case with heat outflow the relationship should be written as:

rate of accumulation = inflow rate − outflow rate

This equation applies to heat or mass, but is applicable only when chemical reactions are not present. When reactions are present component concentrations are produced and heat is usually liberated or absorbed, resulting in an extra reaction term in the above relationship. The equation, however, holds for all non-reacting systems and will be much used in the simulation of distillation columns.

It has been seen that provided constant values can be assigned to two process parameters the equation representing the heating of an agitated batch can be solved analytically. A study of the literature of heat transfer will show however that the coil to fluid heat transfer coefficient may be calculated from a complex relationship involving the fluid physical properties and the overall temperature difference. The simulation of the process is now the solution of eqn (1.1) with U a function of temperature and fluid properties. The problem cannot now be solved analytically, if allowance for variations in physical properties is made, and a different approach is required. The accurate simulation of perhaps the simplest dynamic process which may be envisaged has thus led to a single differential equation which cannot be solved analytically.

Methods for the solution of combinations of equations will be dealt with later; at present we will concentrate on the derivation of equations for simple dynamic processes.

Consider now the process of simultaneous heating and charging of a batch of liquid as shown in Fig. 1.4. Before we consider the changes in temperature and mass of the batch of liquid, it will be necessary to determine the temperature of the liquid entering the batch. If we assume that the time taken for the external exchanger to reach equilibrium is very small compared with the total heating time, we may carry out a heat balance around the heat exchanger to give:

$$WC_p(\theta' - \theta_0) = U_1A_1\frac{\theta' - \theta_0}{\ln\dfrac{\theta_s - \theta_0}{\theta_s - \theta'}} \tag{1.5}$$

Rearranging this gives

$$\theta' = \theta_s - \frac{\theta_s - \theta_0}{e^{U_1A_1/WC_p}} \tag{1.6}$$

Expressions may now be written down for the rate of accumulation of both mass and heat within the batch. For mass we have

$$\frac{dM}{dt} = W \tag{1.7}$$

For heat

$$\frac{d}{dt}(MC_p\theta) = U_2A_2(\theta_s - \theta) + WC_p\theta' \tag{1.8}$$

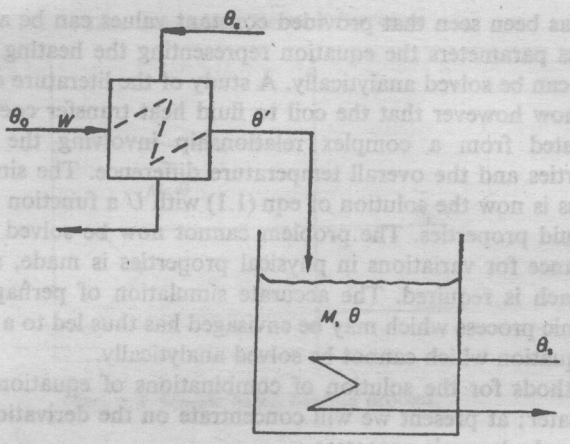

FIG. 1.4. Batch heating/charging process.

Expanding the left hand side of eqn (1.8) as the differential of a product, treating C_p as a constant, and using eqn (1.7) yields

$$MC_p \frac{d\theta}{dt} = U_2A_2(\theta_s - \theta) + WC_p(\theta' - \theta) \tag{1.9}$$

A model of the process is shown in Fig. 1.5 in which the similarities between the mathematical model and the physical situation are apparent. The entries to each box represent the information needed for the calculations at each stage. It should be noted that the equations may be either algebraic or differential and we shall consider, in later chapters, methods for solving both types.

Our process simulation is now given by the simultaneous solution of eqns (1.6), (1.7) and (1.9). If both heat transfer coefficients are assumed constant and provided that the charging rate is kept constant an analytical solution of these equations is possible. The solution will calculate the time required to bring the process from its initial conditions at $t = 0$ of $M = M_1$ and $\theta = \theta_1$ to terminal conditions of $M = M_2$ and $\theta = \theta_2$.

A brief consideration of this problem will show that if the value of the charging rate, W, is very low it will be possible to achieve the required terminal temperature θ_2 as the liquid leaves the external heat exchanger. As the value of the charging rate is increased the temperature of the liquid leaving the exchanger will decrease and the value of $M = M_2$ may be reached before the batch temperature reaches θ_2. In this case the time required will be calculated in two stages, the first will determine the time

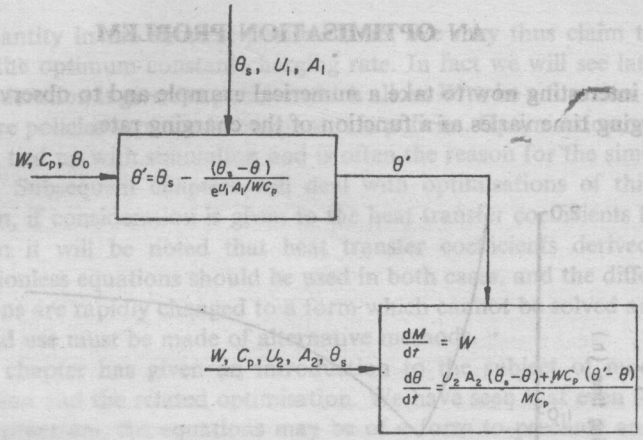

FIG. 1.5. Model of heater/charger problem.

required to bring the mass from M_1 to M_2 whilst the temperature is raised from θ_1 to some new value θ_1', such that $\theta_1 < \theta_1' \leq \theta_2$. The second period will be that required to raise the temperature from θ_1' to θ_2 using the internal heating coil only. Using eqn (1.7) in (1.9) we may write

$$WMC_p \frac{d\theta}{dM} = (U_2A_2\theta_s + WC_p\theta') - (U_2A_2 + WC_p)\theta \qquad (1.10)$$

integrating this equation gives

$$\frac{WC_p}{(U_2A_2 + WC_p)} \ln \frac{\{(U_2A_2\theta_s + WC_p\theta') - (U_2A_2 + WC_p)\theta_1\}}{\{(U_2A_2\theta_s + WC_p\theta') - (U_2A_2 + WC_p)\theta_1'\}} = \ln \frac{M_2}{M_1} \qquad (1.11)$$

which will enable a value for θ_1' to be calculated. The time, t, required for this period is obtained, by integrating eqn (1.7), as

$$t_1 = \frac{M_2 - M_1}{W} \qquad (1.12)$$

The period, t_2, required to bring the batch from θ_1' to θ_2 using the internal coil only is obtained from eqn (1.4), i.e.

$$t_2 = \frac{M_2C_p}{U_2A_2} \ln \left(\frac{\theta_s - \theta_1'}{\theta_s - \theta_2}\right) \qquad (1.13)$$

giving a total charge period

$$t = t_1 + t_2 \qquad (1.14)$$

AN OPTIMISATION PROBLEM

It is interesting now to take a numerical example and to observe how the charging time varies as a function of the charging rate.

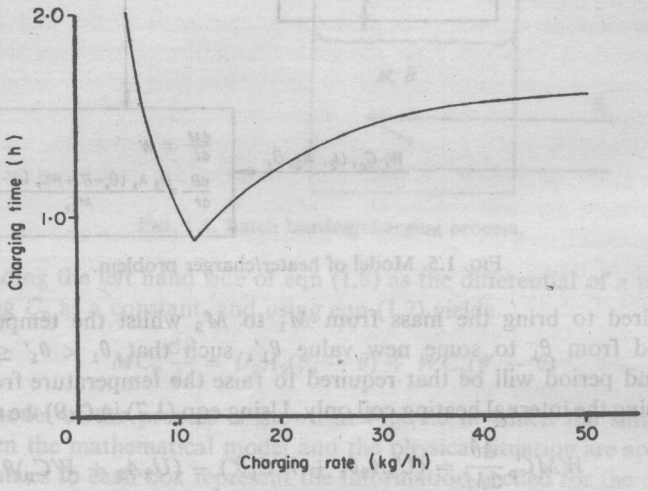

FIG. 1.6. Charge time as a function of charge rate.

Figure 1.6 shows how the time varies for different values of the constant charging rate W, for the parameter values of Table 1.1.

It will be seen that the charging period required goes through a minimum. This is clearly the best constant charging rate to use, since the objective in the process will be to bring the batch to its required temperature

TABLE 1.1

PARAMETER VALUES FOR HEATER/CHARGER PROCESS

U_1A_1	= 10 kcal/h °C
U_2A_2	= 10 kcal/h °C
θ_0	= 0°C
θ_1	= 50°C
θ_2	= 70°C
θ_s	= 100°C
M_1	= 10 kg
M_2	= 20 kg

and quantity in the shortest possible time. We may thus claim to have found the optimum constant charging rate. In fact we will see later that if consideration is given to policies which allow W to be a function of time there are policies superior to constant rate policies. Optimisation, we have seen, is tied up with simulation and is often the reason for the simulation studies. Subsequent chapters will deal with optimisations of this type.

Again, if consideration is given to the heat transfer coefficients for this problem it will be noted that heat transfer coefficients derived from dimensionless equations should be used in both cases, and the differential equations are rapidly changed to a form which cannot be solved analytically, and use must be made of alternative methods.

This chapter has given an introduction to the subject of modelling, simulation and the related optimisation. We have seen that even for very simple processes, the equations may be of a form to preclude analytical solution, and alternative methods, based upon computers, may be necessary.