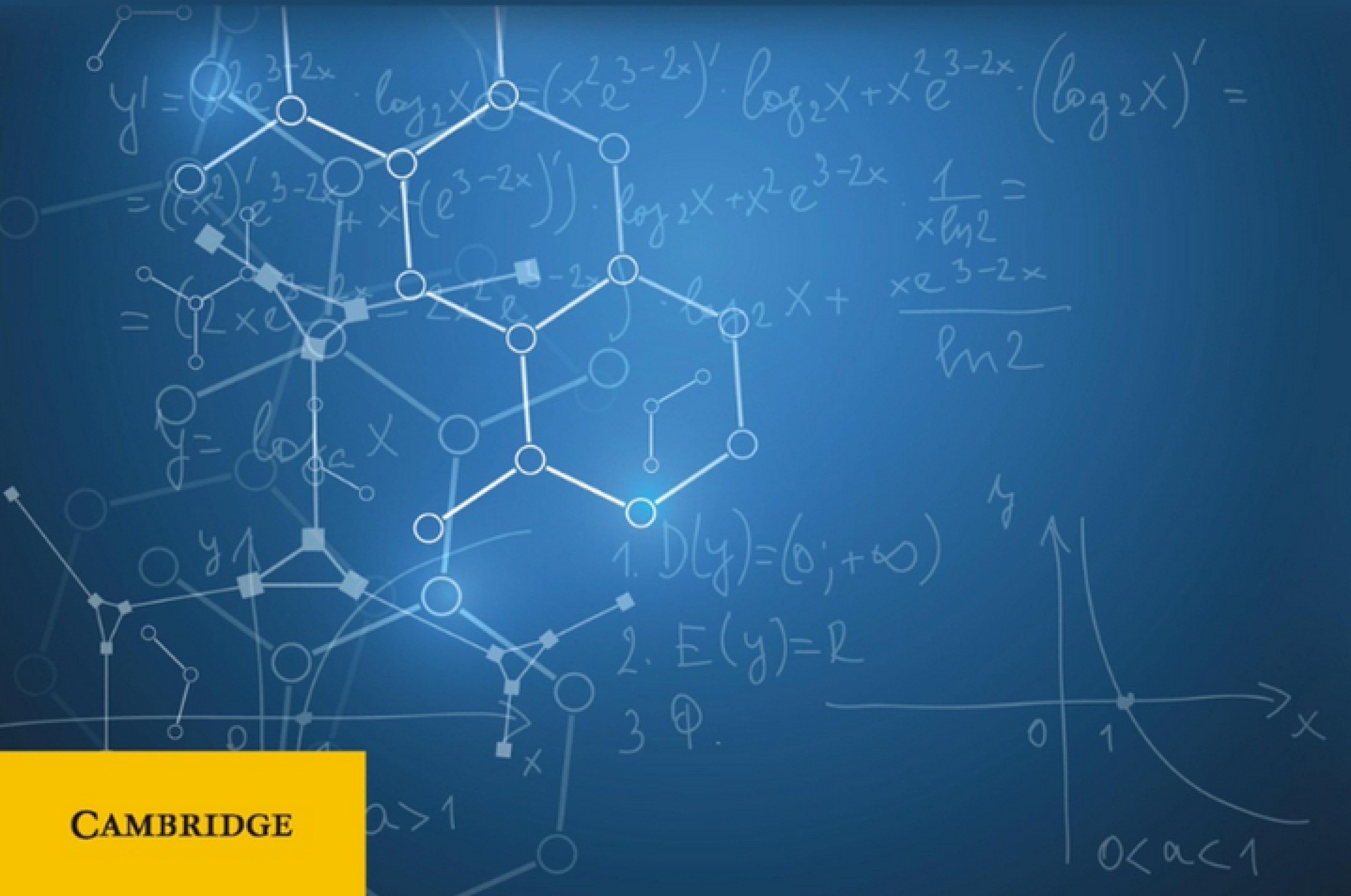
Mathematical Modelling and Simulation in Chemical Engineering

M. Chidambaram



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In order to model systems, understanding the basic principles and governing laws is essential for making suitable assumptions required to reduce the complexity of a system. Mathematical modelling and simulation tools provide a solid foundation for upgraded system performance. This book bridges the gap by elaborating the essential concepts, including differential equation models and development of model equations, useful for improved system functioning.

The analytical and numerical techniques for solving various mathematical model equations, including nonlinear algebraic equations, initial value ordinary differential equations (ODEs) and boundary value ODEs are discussed here. There is a detailed discussion on optimization methods and sensitivity analysis. In addition, numerous MATLAB/ Scilab applications are interspersed throughout the text and several case studies involving full details of simulation are presented. The accompanying website will host additional MATLAB/ Scilab problems, model question papers, simulation exercises, tutorials and projects. This book will be useful for students of chemical engineering, mechanical engineering, instrumentation engineering and mathematics.

M. Chidambaram was Professor at the Department of Chemical Engineering, Indian Institute of Technology, Chennai. He also served as Director, National Institute of Technology, Tiruchirappalli during 2005–10. He taught for more than 25 years, and has written several books. His areas of interest include instrumentation and process control, computer control of processes, process analysis and simulation. Professor Chidambaram is the co-author of *Relay Autotuning for Identification and Control* (Cambridge University Press, 2014).

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Preface

This course book on mathematical modelling and simulation has been structured for undergraduate and postgraduate students of Chemical Engineering. It can also be used as a reference book for Instrumentation and Control Engineering, Mechanical Engineering, and Mathematics.

The requirements for modelling a system are: first, an understanding of the underlying physics of the systems and the laws governing it; second, an ability to make suitable assumptions to analyze the system while retaining the valid and realistic description of its behaviour. The aim of this text is to provide readers such practice through several simple examples for setting up model equations followed by their solutions by either analytical or numerical techniques. Wherever possible, analytical methods are provided. For the numerical solution, Matlab/Scilab routines are used.

The first chapter introduces the basic steps in mathematical modelling. Chapter 2 presents the development of mathematical models for simple systems. It provides discussions through several examples making use of mass balance, energy balance or momentum balance equations. In addition, one example for a transport reactor is also given to analyze the problem in detail. The development of partial differential equation with the associated boundary conditions is given for an isothermal tubular reactor with the axial dispersion model.

Chapter 3 provides several examples illustrating the modelling of systems with complex behaviour. Systems exhibiting output multiplicity behaviour, input multiplicity behaviour, and oscillatory behaviour, etc., are discussed.

Chapter 4 presents commonly occurring linear differential equation models and the analytical solution of such equations. The series solutions are given for variable coefficient linear ODEs. Application of the Laplace transform method to solve linear partial differential equation is presented. The solution of a linear partial differential equation (PDE), by the method of separation variable, is also discussed with examples.

Chapter 5 presents the basics of the numerical solution of nonlinear algebraic equations, IVP nonlinear ODEs, BVP nonlinear ODEs, and nonlinear PDE model equations with examples.

Chapter 6 provides case studies involving variable coefficient ODEs, and PDEs with the details on the simulation of such systems.

Chapter 7 poses the problem of discriminating model equations for systems. The use of the periodic operation, to discriminate the model equations, is proposed with the simulation results.

Chapter 8 elucidates the sensitivity analysis of model equations. The direct differentiation method and the finite difference method are discussed.

Chapter 9 provides an overview of optimization methods by analytical methods and numerical methods. Several examples are given for the optimization problems. An introduction is given to the multi-objective optimization methods and the random search optimization method. The importance of estimating model parameters from the output of the system is brought out with examples.

In Chapter 10, the use of Matlab and Scilab routines is discussed to solve the mathematical model equations with several examples.

Chapter 11 provides an introduction to transfer function models, the development of simple model equations and the mathematical methods required to design PI/PID controllers for stable and unstable systems with examples.

Chapters 1, 2, 4, 5, a part of chapter 8, and a part of chapter 10 can be used for an undergraduate level course in any engineering discipline, and Chapters 3, 5, 7, 9 and 11 can be used for a post graduate level course in the Chemical Engineering program. Chapters 2, 3, 5, 9 and 11 can be considered at the postgraduate level for students from Mechanical Engineering, Instrumentation and Control Engineering, and Mathematics. For all the above disciplines, Chapter 10 can be marked for self-study, with two hours for demonstrating the simulation examples.

It is a pleasure to acknowledge the contributions of the people who helped the author in writing this book. The book owes much to the numerous authors of original research papers and textbooks. The author gratefully acknowledges the assistance provided by his students Thanga Mani, Peela V. V. K. S. Ganesh, E. Rajeshkannan, Vivek Shankar Pinnamaraju, the course assistance for the course processes analysis and simulation, and Aditya Sarkar Kantha (NIT-Warangal), an internee. The author thanks his research scholars Chandrasekhar Besta, S. Nikita, C. Sankar Rao, V. Dhanya Ram and Simi Santosh for their assistance.

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1

Introduction to Mathematical Modelling

The definitions of mathematical modelling of systems, along with analysis, synthesis and compensation of a system are given in this chapter. The basic steps in the development of model equations are given. The classification of model equations and the types of mathematical equations encountered are given. The need for the black box modelling and grey box modelling and their limitations are given.

1.1 MATHEMATICAL MODEL

Description of a system by mathematical equations is called mathematical modelling. It is important to capture the essential features of a system to describe (design), forecast (predict), optimize the operating conditions and to design a suitable controller. Some of the application areas of model equations are in process design, process control, process safety, operating training simulators, and environmental impact assessment, etc. Each application area may require different form of mathematical model equations. Mathematical modelling method involves analysis, numerical simulation, followed by experimental tests. Development of mathematical model needs general laws and constitutive relations. The general laws are the conservation or balance equations of mass, momentum and energy. Some of the terms or variables in the general conservation equation are to be obtained by the constitutive equation(s).

The constitutive relations are experimental in nature and strongly depend on the phenomenon under consideration. Some examples include Fourier's laws of heat conduction, Fick's law of diffusion of a substance, reaction rates, equilibrium relations and equation of state, Newton's law of viscosity, isotherms for adsorption, hold up of catalyst, etc. This is also known as phenomenological law, i.e., a law which is arrived at by observing natural phenomena and not derived from the basic principles. The mathematical equations are algebraic equations, ordinary differential equations, partial differential equations, etc. A detailed physical insight has to be gained before the mathematical description can be formulated.

In general, the development of a completely exact model is rather difficult. Sometimes the theory of the phenomenon is not completely known; sometimes the experimental facts are not available; sometimes there is no need to include all details—often we simply look for the trends. Oftentimes, the analytical solution of differential equations is rather difficult or impossible because the equations are nonlinear or several coupled equations constitute the model. In such cases, the use of the numerical solutions using computers, or specifically designed software package (as standard subroutines) is desirable to get the solution.

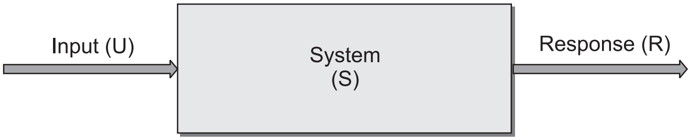


Fig. 1.1 Input, system and response

The three general problems we face with respect to any system (Fig. 1.1) are:

Synthesis: given the input U and desired response (R) find S (design the system to get the desired output for the given input). The synthesis problem is known as the *design problem.*

Analysis: Given U and S, find R (given the system and the input find the output). The analysis problem is known as the *prediction* problem.

Compensation: given S and R, find U (given the system and the desired output, find the input). This problem is called *control problem*.

If we are good at the analysis problem, then the other two problems (synthesis and compensator) can be solved by reformulating the problem as an analysis problem. For example, in the synthesis problem, we assume the system and for the given input, by the analysis we can find the output. If this output is matching with the given output, then the assumed system is correct. Otherwise, we have to modify the system and repeat the problem. Similarly, for the compensator problem, we assume the input and by analysis problem calculate the output. If this output matches well with the given output, then the assumed input value is correct. Otherwise, the input value is to be changed, and the procedure is repeated. How to change the input depends on how good we are at the analysis problem.

In many cases, theoretical treatments are available for models for which there is no perfect physical realization is available. In this case, the only possible test for an appropriate theoretical solution is to compare with the ‘data’ generated from a computer simulation. An important advantage of the simulations is that different physical effects, which are present simultaneously in real systems, may be isolated and, through separate consideration by simulation, may provide a much better understanding. Simulations of the simplified models can ‘switch off’ or ’switch on’ these effects and thus determine the particular consequences of each contributing factor. We wish to emphasize that the aim of simulations is not to provide better ‘curve fitting’ to experimental data than does by the analytic theory.

The goal is to create an understanding of the physical properties and processes which is as complete as possible, making use of the perfect control of ‘experimental’ conditions in the ‘computer experiment' and of the possibility to examine every aspect of system configuration in detail. The desired result is then the elucidation of the physical mechanisms that are responsible for the observed phenomena. The relationship among the theory, experiment and simulation is similar to those of vertices of a triangle, each is distinct, but each is strongly connected to the other two.

Empirical models: The method is easy to develop. The idea is to fit a curve through a set of data and use this curve in order to predict the outcome. We may not be confident that the method is applicable outside the range (extrapolation) .

Stochastic model: ('stochastic' in Greek means to guess). We try to estimate the probability of certain outcomes based on the available data.

1.2 DEVELOPMENT OF MATHEMATICAL MODEL

$$\text{Knowledge of the system} + \text{Mathematics} \rightarrow \text{Modelling} \tag{1.1}$$

To develop a mathematical model of a system, we must know both the subject knowledge and mathematics. Subject knowledge must both precede and follow the mathematical modelling to ensure that the essential features of the system are taken into account and to check the mathematical model solution gives a meaningful solution.

Mathematical modelling is an art. It requires experience, insight and understanding. Teaching this art is also another art. Criteria for a successful model include a good agreement between the prediction and the observations, of drawing valid conclusions and simplicity of the model . Modelling forces us to think clearly about the system. We may need different models for explaining different aspects of the same situation or even for different ranges of the variables. The search for a unified model continues. Sticking to one model may prevent the insight. Comparison of the prediction with the observations reveals the need for new experiments to collect the needed data. Mathematical models can also lead to the development of new concepts. Every model contains some parameters, which are to be estimated. The model must itself suggest experiments. The parameter, if possible, is to be calculated independently. Sometimes, new mathematical methods have to be developed. If the model is oversimplified, it may not represent the reality. If the model is overambitious, then the mathematical model equations may need very complicated methods of solutions. Mathematical models are constantly updated (or improved), to make them more realistic. Thus, we need to develop hierarchy of models, each of which is applicable to increased complex situation.

The modelling process starts (Fig. 1.2) with the analysis of the problem for idealization and for various assumptions. Once the idealized model is formulated, it can be then translated into the corresponding mathematical model in terms of differential equations. The modelling step involves idealization and simplification of the real world problem, to develop a simple model to extract the essential features of the system. From the physical model, we can use the first principles such as the conservation of mass, energy and momentum to translate in to mathematical equations. Then, the model equations will be solved to find the prediction under appropriate conditions. This step will involve in solving the model equations analytically or numerically by appropriate techniques. The process is known as the simulation. The predictions will be validated against the existing models, or well established bench-mark and the experimental data.

If the results are satisfactory (rare at first attempt), then the mathematical model can be accepted. If not, both the assumptions and idealization of the physical model and mathematical modelling will be modified based on the feedback and then the new simulation and prediction will be carried out.

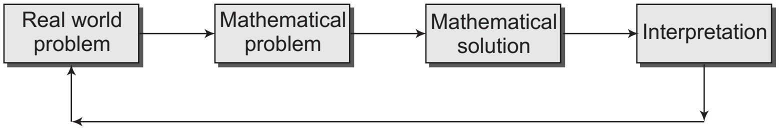


Fig. 1.2 Principle of mathematical modelling (Bender, 1978)

The mathematical model equations must be verified. This is done using a prototype and an experimental verification of the model behaviour. It is also desirable to consider special limiting cases to ensure that the model has the proper behaviour. Every term in the mathematical model must have the same units as in every other term. The algebraic sign of the term makes sense in the overall context of the equation. The resources available consist of available man-power, time, the availability of computing resources, and the software programs. It is valuable to start with a simple model having a limited purpose, and then to improve upon it as required. Table 1.1 gives the classification of the model and Table 1.2 gives the forms of model equations encountered.

Table 1.1 *Model classification (Hangos and Cameron, 2001)*

Group of models	Classification	Criterion of classification
I	Mechanistic	Based on mechanism/underlying phenomena
	Empirical	Based on input-output, trials or experiments
II	Stochastic	Contains model elements that are probabilistic nature
	Deterministic	Based on cause effect analysis
III	Lumped parameters	Dependent variables not function of special position
	Distributed parameter	Dependent variables are a function of special position
IV	Linear	Super position principle applies
	Nonlinear	Super position principle does not apply (occurrence of product of dependent variables and/or its derivatives)
V	Continuous	Dependent variables defined over continuous space time
	Discrete	Only defined for discrete values of time/ or space
	Hybrid	Containing continuous and discrete behaviour

Table 1.2 *Forms of model equations (Hangos and Cameron, 2001)*

Type of model	Equation Types	
	Steady state problem	**Dynamic problem**
Deterministic	Nonlinear algebraic	ODEs/PDEs
Stochastic	Algebraic/difference equation	
Lumped parameter	Algebraic equation	ODEs
Distributed parameter	Elliptic PDEs	Parabolic PDEs
Linear	Linear algebraic equations	Linear ODEs
Nonlinear	Nonlinear algebraic equations	Nonlinear ODEs
Continuous	Algebraic equations	ODEs
Discrete	Difference equations	Difference equations

ODEs: Ordinary Differential Equations; PDEs: Partial Differential Equations

1.3 SIMULATION

Simulation is the process of analyzing a whole process or a part of it, using the model equations. The purpose of simulation is to find the optimal operating conditions/parameters, analyzing the effect of the input variables on the performance of the system and design of controllers, Simulation is defined as experimentation with the mathematical equations/models. Solving the mathematical model equations to understand the behaviour of the system is called simulation.

1.3.1 Nonlinear differential equations

Whenever there is a product of dependent and/or its derivative terms present in the equation, then the system is called nonlinear. Examples are:

$$[dy/dx]^2 + y = 0 \tag{1.2}$$

$$y[d^2 y/dx^2] + dy/dx + y = 0 \tag{1.3}$$

$$[d^2y/dx^2] + dy/dx + \exp(y) = 0 \tag{1.4}$$

The boundary conditions are usually linear.

The nonlinearity is with respect to the dependent variable (and its derivative). If any term present in the right side of equation [as a function of independent variable], then it is called a non-homogeneous equation. If the coefficient is nonlinear in the independent variable then the equation is called as a variable coefficient equation:

$$(d^2y/dx^2) + (x^2+x)(dy/dx) + y = 0 \tag{1.5}$$

We have considered here the ordinary differential equations. Similarly, we can write the partial differential equations.

Autonomous system:

$$dy_i/dt = f_i\,(y_{1,}\, y_2,\, y_3),\ i = 1, 2, 3 \tag{1.6}$$

The above model equation, without the appearance of independent variable in the function f, is called an autonomous system (also known as a time invariant system).

1.4 CONSERVATION OF MASS/ENERGY/MOMENTUM

Input – output = accumulation (transient condition) (1.7)

Input – output = 0 (steady state condition) (1.8)

The input terms represent the mass entering the system and the mass generated by the reaction or mass transferred from other phase to the phase under consideration. Similarly, the output term consists of mass leaving out, mass consumed by the reaction, mass transported from this phase to another phase. Total mass balance and the component mass balance in each phase are to be written. The conservation equation for the mass of the i-th chemical species at steady state condition is given by

Rate of mass of the i-th species in – rate of mass of the i-th species out + rate of generation of mass of the i-th species in the system = 0 (1.9)

The mass of i-th species may enter or leave the system by two means: (1) by inlet or outlet stream; and (2) by exchange of mass between the system and its surroundings through the boundaries of the system, i.e., inter-phase mass transfer. If it is a reacting system, we need to know the reaction kinetics for the reactions.

The conservation statement for total energy under steady state condition takes the form

Rate of energy in – rate of energy out + rate of energy generated in the system = 0 (1.10)

Energy must enter or leave the system by two means: (i) by inlet or outlet steams; (ii) by exchange of energy between the system and its surroundings through the boundaries of the system in the form of heat and work.

Depending upon the situation, the modelling may require only the mass balance and/or energy balance and /or momentum balance.

Rate of momentum in – rate of momentum out + rate of momentum generation = 0 (1.11)

Rate of momentum generation is equal to the summation of forcing on the system. The basic steps in the development of the balance equations are given by:

Define the system: if possible, draw the sketch; list the suitable assumptions made; write down the mass balance and /or energy balance and/or momentum balance equations.

Use the appropriate correlation to calculate the mass transfer/energy transfer coefficients relevant to the problem at hand: write the initial conditions and solve the ordinary differential equations.

Let us discuss on the classification of models given in Table 1.1

(1) First principle modelling versus empirical modelling

The first principles modelling (or white box or mechanistic modelling) is based on the conservation laws (of mass/energy/momentum). For the transport coefficient and the reaction kinetics, we use the empirical relationships. The mechanistic models have an advantage of preserving the physical insight into the process as the model variables coincide with the process variables. A major drawback of the physical modelling is that it is time demanding approach.

In empirical modelling (or black box modelling), an input–output relationships is constructed using the experimental data of the process. Whenever there is a lack of knowledge of the process and /or time limitation to develop a model, the empirical modelling is desirable. A disadvantage of this approach is that it may require extensive experimentation to obtain the input–output data of sufficient quality for a newly developed process or a process under development. Extrapolation to outside the experimental data condition is not recommended. Mathematical representation include time series models such as Auto Regressive Moving Average (ARMA), Auto Regressive with eXogenous input (ARX), Output Error Model (OE) models; artificial neural network (ANN) models; Fuzzy models and partial least square (PLS) models, etc. The model parameters have no direct relationship to that of the first principles.

2) Lumped versus distributed parameters models

The model equations should be as simple as possible. Hence, the lumped parameter models are preferred over the distributed parameter models (described by partial differential equations) as they are simple and computationally less demanding. However if the variable (say, temperature) is varying along the spatial coordination, it may be desirable to develop a DPS (Distributed Parameters System) models. For controller design purposes, the DPS model should be converted in to a set of LPM and hence the number of equations is larger for the design of the control systems.

3) Linear versus nonlinear models

For analysis of the processes and optimization of the systems, appropriate nonlinear model is required. For purpose of designing controllers, a linear model may be adequate. Sometimes, switching over linear models, for tuning the controllers, is recommended. For a highly nonlinear process such as pH process, a nonlinear model based control law is required. The nonlinear models may be difficult to solve analytically.

4) Steady-state versus dynamic models

For continuous time processes, to design a process or optimization of the operating variables we require steady state models. For analyzing the oscillatory behaviour, we may need the unsteady state models. For design of the controller also we need dynamic models. For batch processes, the dynamic model is required.

5) Continuous versus discrete-time models

Usually the continuous time modelling is required to analyze the behaviour of the process. For design of controllers, particularly adaptive control or optimal control, etc., we may need discrete time models. Some numerical solution of ODE models may require discrete models.

6) Deterministic models versus stochastic models

It is traditional to model the nature in the deterministic terms. However, neither the nature nor the engineered systems behave in a precisely predictable fashion. Systems are almost always inherently 'noisy'. Therefore, in order to model a system realistically, a degree of randomness is to be considered in the model. Even though one cannot precisely predict a next event, one can predict how next events will be distributed. Unlike the traditional data analysis, where the statistics (such as mean, standard deviation, and the like) are calculated from the given data, we can generate here a set of data having pre specified statistics. The actual input signal will never be replaced, but its statistics will most likely still be stationary.

1.5 RANDOM PROCESSES

In simulating dynamic processes, it is important to model not only the system itself but also the input data that drives the system. Input signals are rarely deterministic. In such cases, we call them random processes because the input signals have an inherent fluctuation built around the underlying unpredictable processes.

In most stochastic models, the system *per se* is fixed and deterministic. Even though they might vary with time, systems are usually well behaved and not subjected to erratic fluctuations. In contrast, the signals that drive the system often appear somewhat random and noisy. Signals are in essence time series of statistically related processes, while systems are simply devices that transform the processes. The stochastic models are very similar to deterministic models except that a random process is the input to the system and the effects are analyzed statistically.

Deterministic models have finite sets of input–output vectors. Each signal is simulated by an explicit formula expressed as a function of time. In contrast, stochastic signals do not have explicit formulas. Instead, the stochastic signals are characterized by defining statistical time series descriptions such as the auto correlation or the spectral density. Another major difference between deterministic and stochastic systems lies in their long-term behaviour. Deterministic systems tend to produce output signals with regular steady state qualities such as constant, periodic, or chaotic states. Stochastic systems are usually random, even in the long run. Although the randomness still has no explicit definition, the output can still be characterized by the auto correlation and spectral density functions.

Table 1.3 *Comparisons of deterministic and stochastic signals (Severance, 2005)*

Signal	Deterministic	Stochastic
Input	Single input vector	Ensemble of input vectors
Output	Single output vector	Ensemble of output vectors
Analysis	Transient Phase	Initial non-stationery phase
	Steady state phase	Stationary phase
Defining input	Impulse	White noise
Signal descriptor	Explicit formula	Autocorrelation
		Spectral density

Table 1.3 shows several of the characteristic difference between deterministic and stochastic systems. In the deterministic case, the output can be a constant steady state or periodic. One of these two cases will always occur in a stable linear system. In a nonlinear system, its behaviour may be more exotic and perhaps even chaotic. A deterministic system is described using the formulas that are explicit functions of time. On the other hand, stochastic systems seem to have underlying deterministic behaviour with the randomness superimposed. In the case of linear systems, the output signal will have steady states analogous to those of the deterministic systems. If the steady

state appears essentially constant with a fixed amount of randomness superimposed, the signal has achieved the stationary condition, since all statistics are the same for each time slice. However, if there is no stationary, differing time slices have different averages.

1.6 BLACK BOX MODEL AND GREY BOX MODEL

The modelling of the system by the first principles model (physical, mechanistic) is known as a white box modelling. The requirement for a good understanding of the physical back ground of the problem at hand proves to be a severe limiting factor in practice when complex and poorly understood systems are considered. Difficulties encountered white box modelling can arise, for instance, from the poor underlying phenomena, inaccurate values of various parameters, or from the complexity of the resulting model.

In such cases, the process is described by a general ‘black box’ structure used as a function approximation. In black box modelling, the structure of the model is hardly related to the structure of the real system. The identification problem consists of estimating the parameters in the model. If representative process data is available, the black box model can be developed quite easily, without requiring process specific knowledge. Time series models, polynomial models, neural network models fall under the category. A severe drawback of this approach is that the structure and parameters of these models usually do not have any physical significance. Such models (i) cannot be used for analyzing the system behaviour otherwise than by the numerical simulation, (ii) cannot be scaled up or scaled down moving from one process scale to another. Therefore, the black box model is less useful for industrial practice. The black box model is valid only in a limited range.

Neural network (NN) model is an example of black box modelling of a system. The neural network models have gained much attention because of their capability of nonlinear function approximation. Theoretically, neural networks with three layers can approximate any nonlinear function with arbitrary accuracy. This feature makes the neural networks a promising nonlinear modelling tool. The development of NN model involves three basic steps. These include the generation of (or compilation of available) data required for training of NN, and the evaluation and validation of the optimal configuration of the NN model. Training the NN models with such a large number of parameters can lead to a poor prediction.

There is a range of modelling methods that attempt to combine the advantages of white box and black box approaches, such that known parts of the system are modelled using the physical knowledge and the unknown or less certain parts are approximated in a black box manner, using process data and black box modelling structures with suitable approximation properties. These methods are often denoted by hybrid, semi-mechanistic or grey box modelling. Attention can be given on the semi-parametric approach, which combines a neural network with a fixed form of a parametric model, either in series or in parallel. For example, a first principle model can be used to describe a particulate solid drying process, whereas, the unknown parameters in the first principle model can be approximated by a black box model. Figure 1.3 shows the architecture of a serial grey box model structure. The serial grey box modelling technique with black box network offers substantial advantages over a black-box (such as neural networks) modelling approach. The training of the model is easier and the model can be updated and it is more reliable for prediction purposes.

Sometimes, we have a situation, where a complete description of the entire process is not available. For example, in an exothermic reactor, the heating/cooling system is well studied but the kinetics of the reaction system, may not be easily modelled. The serial approach cannot be applied here, but an alternate (parallel) approach can be used (refer to Fig. 1.4)

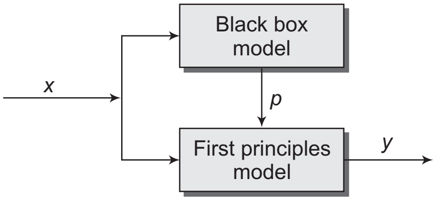


Fig. 1.3 Serial structure of a grey-box model with black box model (Xiong and Jutan, 2002)

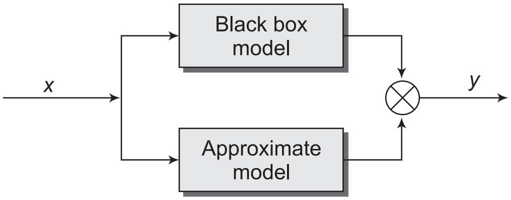


Fig. 1.4 Parallel structure of a grey-box model with black box model (Xiong and Jutan, 2002)

Review Problems

1. What is meant by mathematical modelling of systems?
2. Discuss briefly analysis, synthesis and compensation of a system.
3. Describe briefly the development of mathematical models.
4. With relevant equations, explain what is meant by nonlinear differential equations.
5. What are the classifications of mathematical models?
6. Explain briefly black box modelling and grey box modelling.
7. Discuss briefly random processes.

2

Model Development for Simple Systems

In the present chapter, examples are given for the development of mathematical models for simple systems. Understanding of the physical systems and identifying the control volume are required. Suitable assumptions are made so that the resulting equations can be solved. Applications of the mass balance or/and energy balance or/and momentum balance(s) are required**.** The mathematical model equations, for some case studies, are solved by the analytical methods or for several cases by the numerical methods. An example is presented for the development of model equations, the solution and the analysis of the system.

2.1 SETTLING VELOCITY OF A PARTICLE

A small spherical ball is dropped in a viscous fluid in a tall column of water in a marked jar. After a brief transient time, the sphere falls with a constant terminal (or settling) velocity. It is required to calculate the settling velocity of the ball. Three forces acting (Fig. 2.1) on the ball are: gravity, F_G; buoyancy, F_B; and the drag, F_D. These forces are described by the following equations:

$$F_G = -\left(\frac{\pi D^3 g}{6}\right)\rho_p \tag{2.1}$$

$$F_B = +\left(\frac{\pi D^3 g}{6}\right)\rho \tag{2.2}$$

$$F_D = \left(\frac{\pi}{8}\right)\rho\,(V^2{}_p\, D^2{}_p C_D) \tag{2.3}$$

Here ρ is the density of the fluid, ρ_p is the density of the solid sphere and g is the gravitational acceleration (9.8 m/s^2). The gravity force is given by the weight of the sphere. The buoyancy is equal to the weight of the displaced fluid (the buoyant force exerted on a submerged particle by the surrounding fluid is equal to the weight of fluid displaced by the solid. This theorem is known as Archimedes' theorem).

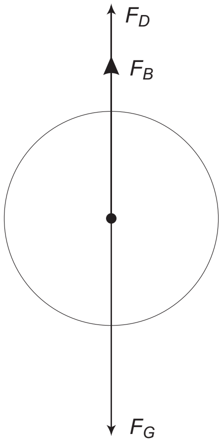


Fig. 2.1 Force balance on a spherical particle in a liquid (Denn, 1980)

When a particle is in relative motion to an enveloping fluid, a drag force is exerted on the particle. This force is due to the shear stress exerted in the boundary layer of the fluid next to the surface of the particle. As is the case of the flow through a conduit, this shear stress is due to the viscosity of the fluid and the velocity gradient between the fluid and particle. Experimental work has shown that this drag force is a function of particle size, the relative velocity between fluid and particle and the kinematic viscosity of the fluid.

The drag force is expressed as

$$F_D = C_D A\left(\frac{\rho V_P^2}{2}\right) \tag{2.4}$$

where, C_D is the dimensionless drag coefficient. A is the cross section area of particle projected on a plane perpendicular to the direction of flow, ρ is the fluid density, u_p is the relative velocity between particle and bulk velocity of the fluid. The sphere is assumed to move in a straight line with no change in velocity. The sum of the forces (on the sphere algebraically) is zero.

$$F_G + F_B + F_D = 0 \tag{2.5}$$

For Stokes' region [when Re < 1): $C_D = 24/\mathrm{Re}$, Eq. (2.5) gives:

$$V_P = \frac{[gD_P^2(\rho_P - \rho)]}{(18\mu)} \tag{2.6}$$

For the intermediate range $[1 \le \mathrm{Re} \le 10^3]$, $C_D = 18/\mathrm{Re}^{0.6}$, Eq. (2.5) gives

$$V_P = \left(\frac{2g}{27}\right)\left[\left(\frac{\rho_P}{\rho}\right) - 1\right]^{5/7} D_P{}^{8/7}\left(\frac{\rho}{\mu}\right)^{3/7} \tag{2.7}$$

For Newton's region, $[10^3 \leq \mathrm{Re} \leq 2 \times 10^5]$, $C_D = 0.44$, Eq. (2.5) gives

$$V_P = \left[3D_P g\left(\frac{\rho_P}{\rho}\right) - 1\right]^{1/2} \tag{2.8}$$

The falling sphere viscometry set-up requires the measurement of the terminal velocity of a sphere, usually by measuring the time (t_P) required to fall between two marks a distance apart. The terminal velocity is calculated from $V_P = \dfrac{L}{t_P}$. Usually the measurements are made in Stokes' region giving the expression for the viscosity as:

$$\mu = \frac{[gD^2{}_P\,(\rho_p - \rho)\,t_p]}{(18L)} \tag{2.9}$$

2.2 COOLING OF A SMALL SPHERE IN A STAGNANT FLUID

A hot solid sphere of diameter D_P at temperature T_S is kept in a stagnant cold fluid maintained at a temperature T_i. Consider a control of spherical shell at radius r and thickness Δr. From the energy input at r and energy output of the control volume at $r = r + \Delta r$, we get:

$$\left[4\pi r^2\left(\frac{\partial T}{\partial r}\right)\right]\Bigg|_r - \left[4\pi r^2\left(\frac{\partial T}{\partial r}\right)\right]\Bigg|_{(r+\Delta r)} = 0 \tag{2.10}$$

$$\left(\frac{1}{r^2}\right)\frac{\partial}{\partial r}\left(\frac{r^2 \partial T}{\partial r}\right) = 0 \tag{2.11}$$

The solution of Eq. (2.11) is given by: $T = \left[\dfrac{D_P(T_s - T_i)}{2r}\right] + C_2$ (2.12)

$$\text{B.C: } r = 0.5\,D_P\,,\ T = T_s \tag{2.13a}$$

$$r = \infty,\ T = T_i \tag{2.13b}$$

The solution becomes: $T = 0.5(T_S - T_r)\left(\dfrac{D_P}{R}\right) + T_i$ (2.14)

The heat transfer rate can be written as:

$$\mathrm{Q} = hA(T_S - T_i) = -k_f\ A\left(\frac{dT}{dr}\right)\Bigg|_R = \frac{0.5\,k_f A(T_s - T_i)D_P}{\left(\dfrac{D_P}{2}\right)^2} \tag{2.15}$$

Hence, $Nu = \dfrac{hD_P}{k_f} = 2$ (2.16)

2.3 VAPORIZATION FROM A SINGLE DROPLET IN QUIESCENT AIR

Consider a droplet of initial diameter D_o suddenly exposed to a higher temperature (T_o) quiescent air (Fig. 2.2). The assumptions made are: (i) the thermal layer around the droplet is spherical (negligible buoyancy effect); (ii) the temperature in the droplet is uniformly equal to the liquid saturation temperature (boiling point) T_b; and (iii) surrounding air is at constant pressure so that the liquid vapour density and the heat of vaporization remain constant.

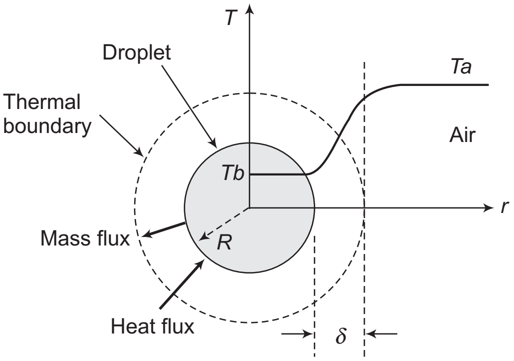


Fig. 2.2 Sketch of system involved in evaporation of a spherical droplet (McAllister et al. 2011)

The rate of change of mass of the droplet must be equal to surface area multiplied by heat flux per unit area. This leads to the equation:

$$-\left[\frac{d}{dt}\right]\left[\rho_l\left(\frac{4}{3}\right)\pi(0.5D)^3 h_{fs}\right]=\pi D^2\, q_s'' \tag{2.17}$$

where, q'' is the heat flux per unit area of droplet surface, and is given by

$$q''= k\frac{dT}{dt}=k\,\frac{(T_a-T_b)}{\delta} \tag{2.18}$$

ρ_l is the density of liquid droplet, D is the diameter of the sphere, h_{fg} is the heat of vaporization at T_b. Here k is the thermal conductive and δ is the thickness of the thermal layer surrounding the droplet. The value of δ depends on the physical properties of the problem but it is proportional to the characteristic length of the process, the droplet diameter. We assume that $\delta = C_1 D$. Hence the above differential equation can be rewritten as:

$$2D\,\frac{dD}{dt}=-\,\beta_0 \tag{2.19}$$

where,
$$\beta_0=\frac{4k(T_a-T_b)}{(\rho h_{fg}C_1)} \tag{2.20}$$

C_I is assumed here for simplicity as 0.5, i.e., the thermal layer is equal to the radius of the droplet. The term β_0 is called the 'vaporization constant' since it is fixed at a given air temperature.

The solution of Eq. (2.19) can be written as:

$$D^2 = D_0^{\,2}-\beta_0\, t \tag{2.21}$$

The above solution is referred as ‘*D* squared law’ (D^2 law). The instantaneous evaporation rate of the droplet can be obtained as:

$$\frac{dm_I}{dt} = \frac{d\left[\rho\left(\frac{\pi}{6}\right)D^3\right]}{dt} = \rho_1\left(\frac{\pi}{4}\right)D\,\frac{dD^2}{dt} \tag{2.22}$$

$$= -\left(\frac{\pi}{4}\right)\rho_1 D\beta_0 \tag{2.23}$$

$$= -\left(\frac{\pi}{4}\right)\rho_1\beta_0\,[D_0^2 - \beta_0 t]^{0.5} \tag{2.24}$$

2.3.1 Droplet vaporization by convection flow

In this situation, we have:

$$q'' = h(T_a - T_b) \tag{2.25}$$

where, h is the convective heat transfer coefficient.

$$Nu = \frac{hD}{k} = 2 + 0.4\,Re_p^{\;0.5}\,Pr^{0.333} \tag{2.26}$$

Similar to the steps carried out in the previous section, it can be shown that

$$D^2 = D_0^{\;2} - 2C_1\,\beta_0 t - \beta t \tag{2.27}$$

where,

$$\beta_0 = 1.6\text{k}\,(Re_P)^{0.5}\,Pr^{0.333}\,(T_a - T_b)/(\rho h_{fg}) \tag{2.28a}$$

$$Re_P = \rho(D_0/2)u_d/\mu \tag{2.28b}$$

2.4 PARALLEL COUETTE FLOW

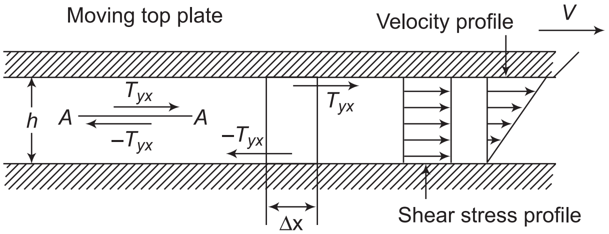


Fig. 2.3 Fluid in shear flow (Pneuli, 1992)

It is named after Couette who introduced it in 1880 to measure the viscosity, and it is a fully developed flow induced between two infinite parallel plate placed at a distance h apart, when one of them (say the upper one) is moving steadily with a speed V relative to the other (refer to Fig. 2.3). We assume the pressure does not depend on x. Hence, the shear stress on this fluid rectangle at the top, where it touches the upper plate, must be balanced by that at the bottom. The same considerations apply to a block which extends from the top plate to the A-A plane, is the same as on the top plate. The shear stress is the same on all planes parallel to the plates. It is known from experiments that the fluid adjacent to the upper plate, at $y = h$, moves with the velocity V. which that at the lowest plate, at $y = 0$, is at rest. The uniform stress, i.e., force per unit area, exerted on the viscous fluid by the upper plate T_{yx}, is expressed by the Newton’s law of viscosity:

$$\tau_{yx} = \mu\left(\frac{du}{dy}\right) \tag{2.29}$$

This equation can be integrated using $u = 0$ at $y = 0$ as

$$u = \tau_{yx}\,\frac{y}{\mu} \tag{2.30}$$

Using u (at $y = h$) $= V$, we get

$$V = \left(\frac{\tau_{yx}}{\mu}\right)h \tag{2.31}$$

Hence

$$u = \left(\frac{V}{h}\right)y \tag{2.32}$$

The flow obtained is known as the plane Couette flow or the plane shear flow.

We considered here the case of constant shear in a moving fluid. In the next section, we will consider a case where the shear in the moving fluid is not constant.

2.5 PLANE POISEUILLE FLOW

Plane Poiseuille flow, named after the channel experiments by Poiseuille in 1840, occurs when a fluid is forced between two stationary infinite flat plates under a constant pressure gradient $\frac{\partial p}{\partial x}$ and zero gravity. The flow is induced by a constant pressure drop, $-\frac{\Delta P}{\Delta x}$, along the axis.

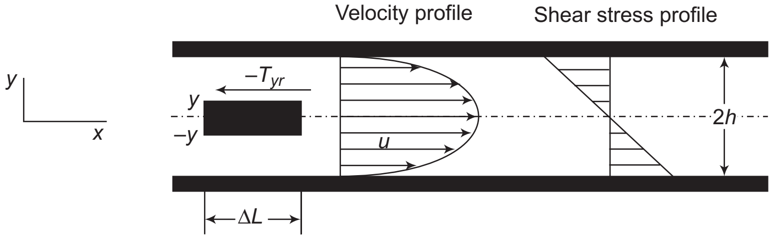


Fig. 2.4 Flow between two stationary plates, plane Poiseuille flow (Pnueli, 1992)

We consider a rectangular fluid block of length ΔL and height $2y$, extending from $-y$ to $+y$ as shown in Fig. 2.4. The pressure difference between its two vertical sides is:

$$\Delta P_L = -\left(\frac{\Delta P}{\Delta x}\right)\Delta L \tag{2.33}$$

And hence the force pushing it to the right is given by

$$2y\,\Delta P_L = 2y\left(-\frac{\Delta P}{\Delta x}\right)\Delta L \tag{2.34}$$

(note: $\frac{\Delta P}{\Delta x} < 0$). This force is balanced by the shear on the upper and lower sides: $-\tau_{yx}\,2\,\Delta L$.

Hence, $$\tau_{yx} = -\left(-\frac{\Delta P}{\Delta x}\right)y \tag{2.35}$$

And by Newton's law: $$\mu\left(\frac{du}{dy}\right) = -\left(-\frac{\Delta P}{\Delta x}\right)y \tag{2.36}$$

Integration yields: $$u = -\left(\frac{0.5}{\mu}\right)\left(-\frac{\Delta P}{\Delta x}\right)y^2 + C \tag{2.37}$$

which with the no slip boundary condition $u(h) = 0$ yields the velocity profile:

$$u = -\left(\frac{0.5h^2}{\mu}\right)\left(-\frac{\Delta P}{\Delta x}\right)\left[1-\left(\frac{y}{h}\right)^2\right] \tag{2.38}$$

This is known as a plane Poiseuille Flow. It can be checked from Eq. (2.38) that at $y = 0$, we get $u_{\max}$ as:

$$u_{\max} = \left(-\frac{\Delta P}{\Delta L}\right)\left(\frac{0.5h^2}{\mu}\right) \tag{2.39}$$

Hence Eq. (2.38) becomes:

$$u = u_{\max}\left[1-\left(\frac{y}{h}\right)^2\right] \tag{2.40}$$

2.5.1 Plane Poiseuille flow with slip

Consider again the fully developed plane Poiseuille flow of the previous example, and assume that slip occurs along the two plates according to the slip law (Papanastasiou, 2000):

$$\tau_w = \beta\, u_w \text{ at } y = H \tag{2.41}$$

where, β is the material slip parameters, τ_w is the shear stress exerted by the fluid on the plate:

$$\tau_w = -\tau_{\text{yx}} \text{ (at } y = H) \tag{2.42}$$

and u_w is the slip velocity. Our interest is to calculate the velocity distribution. The flow is still symmetric with respect to the centreline. In this case, the boundary conditions are:

$$\tau_{yx} = \mu\left(\frac{du_x}{dy}\right) = 0 \text{ at } y = 0 \tag{2.43a}$$

$$\tau_w = \tau\, u_w \text{ at } y = H \tag{2.43b}$$

We have $$u_x\,(y) = \left(\frac{0.5}{\mu}\right)y^2\left(\frac{\partial p}{\partial x}\right) + C_1 y + C_2 \tag{2.44a}$$

$$\tau_{yx} = \left(\frac{\partial p}{\partial x}\right)y + \mu C_1 \tag{2.44b}$$

The conditions at $y = 0$ yields $C_1 = 0$. (2.44c)

Therefore, $$u = \left(\frac{0.5}{\mu}\right)\left(\frac{\Delta P}{\Delta x}\right)y^2 + C_2 \tag{2.45}$$

$$\tau_{yx} = \left(\frac{\Delta P}{\Delta x}\right)y \text{ implies } \tau_{\text{w}} = -\left(\frac{\Delta P}{\Delta x}\right)H \tag{2.46}$$

Applying the condition at $y = H$, we get

$$u_w = \left(\frac{1}{\beta}\right)\tau_w \tag{2.47}$$

$$u_x(H) = -\left(\frac{1}{\beta}\right)\left(\frac{\Delta P}{\Delta x}\right)H \tag{2.48}$$

Using this relationship in Eq. (2.45), we get

$$C_2 = -\left(\frac{0.5}{\mu}\right)\left(\frac{\Delta P}{\Delta x}\right)\left[H^2 + \left(\frac{2\mu H}{\beta}\right)\right] \tag{2.49}$$

and

$$u_x = -\left(\frac{0.5}{\mu}\right)\left(\frac{\Delta P}{\Delta x}\right)\left[H^2 + \left(\frac{2\mu H}{\beta}\right) - y^2\right] \tag{2.50}$$

This equation reduces to the Poiseuille flow profile when $\beta \to \infty$. Since the slip velocity is inversely proportional to the slip coefficient, β, the standard no-slip condition is recovered. An alternate expression of the velocity distribution is:

$$u_x = u_w - \left(\frac{0.5}{\mu}\right)\left(\frac{\Delta P}{\Delta x}\right)[H^2 - y^2] \tag{2.51}$$

which indicates that u_x is just the superposition of the slip velocity u_w to the velocity distribution of the previous example.

2.6 MODELLING OF A SURGE TANK

Liquid is supplied by upstream which due to some reasons fluctuates. The fluctuations can be modelled as 'a sin(ωt)'. Hence, the overall flow is given by:

$$q = q_b + \text{a}\sin(\beta t) \qquad (2.52$$

In order to smooth out the fluctuations, we introduce the stream in to a tank (called a surge tank) having a free surface (refer to Fig. 2.5). Then the liquid flows out of the bottom of the tank through a valve and goes to the next stream. For the sake of simplicity, we assume the flow through the valve is kh, where, h is the fluid level (height) in the tank. The material balance across the tank gives:

$$\frac{Adh}{dt} = q_b + a\sin(\omega t) - q_{\text{out}} \tag{2.53}$$

$$\frac{Adh}{dt} = q_b + a\sin(\omega t) - \text{kh} \tag{2.54}$$

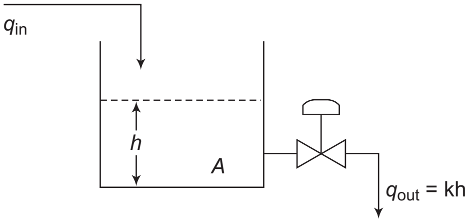


Fig. 2.5 Surge tank

We know that at steady state:

$$q_b = \text{kh} \tag{2.55}$$

Introducing the deviation variable: $y = h - h_s$; and defining $\tau = \dfrac{A}{K}$; $p = \dfrac{a}{K}$, Eq. (2.54) becomes

$$\frac{\tau dy}{dt} + y = p\sin(\omega t) \tag{2.56}$$

The Laplace transform of the system output can be obtained as:

$$y = \left[\frac{1}{(\tau s + 1}\right]\left[\frac{(p\omega)}{(s^2 + \omega^2)}\right] \tag{2.57}$$

The inverse of the Laplace transform gives $y(t)$.
After the initial dynamics die out, we get:

$$y = \frac{p\sin(\omega t + \phi)}{[(1 + \tau^2\omega^2)^{0.5}]} \tag{2.58}$$

If we want the output low deviation is 10% of the input deviation, then we get

$$\frac{1}{[(1 + \tau^2\omega^2)^{0.5}]} = 0.1 \tag{2.59}$$

Hence:
$$\tau = \frac{(99)^{0.5}}{\omega} \tag{2.60}$$

Hence:
$$A = K\frac{(99)^{0.5}}{\omega} \tag{2.61}$$

We can thus calculate the area of the tank. From the steady inlet flow, we can get the nominal height of the tank (h_b). The actual height should be about $\left(\dfrac{a}{A}\right)$ higher than this value in order to accommodate the fluctuation in the inlet flow. An additional safety factor should be added to ensure that the tank will not overflow.

2.7 RAPID THERMAL PROCESSING

Rapid thermal processing (RTP) is commonly used in the semiconductor manufacturing processes such as annealing, oxidation and chemical vapour deposition (CVD) (refer to Fig. 2.6 for a schematic diagram). The heating is provided by the incandescent lamps. The heat intensity

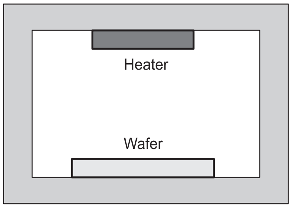


Fig. 2.6 Rapid thermal processing. Upper box – heater; Lower box – wafer

(control action), the furnace temperature, the wafer temperature (controlled variable) and the ambient temperature, are denoted by u, T_F, T_w and T_a, respectively. We shall develop a simplified model. Here, the heat is transferred by radiation and is governed by the Stefan–Boltzmann's law:

$$Q = \alpha\,[T^4_r - T^4] \tag{2.62}$$

where, Q, T_r and T represent the radiated heat (energy), the temperature of the radiator and the temperature of the receiver (the surroundings), respectively. We can write the energy balance as:

$$\beta_1 \frac{dT_F}{dt} = u(t) - \alpha_{FW}\,(T_F^{\;4} - T_W^{\;4}) - \alpha_{FA}\,(T_F - T_a) \tag{2.63}$$

$$\beta_2 \frac{dT_W}{dt} = \beta_2\,(T_F^{\;4} - T_W^{\;4}) \tag{2.64}$$

where $\alpha_{FW}\,(T_F^{\;4} - T_W^{\;4})$ represents the heat transmitted by radiation to the wafer, and,

$\alpha_{FA}\,(T_F - T_a)$ represents the heat transmitted by convection (losses) to the surroundings of the system.

2.8 MODELLING OF A PH PROCESS

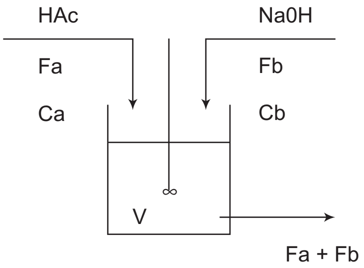


Fig. 2.7 Schematic diagram of the neutralization process

A process stream of weak acid (HAC of strength 0.1 N) enters a well-mixed vessel as the feed and is neutralized by a strong base (NaOH of strength 0.2 N). V is the volume of the contactor. F_a and F_b are the acid and base flow rates, respectively. The concentration of acid and base are C_a and C_b, respectively. x_a and x_b are the state variable concentration (total ion concentration) of the acid and base at the outlet, respectively. The sum of F_a and F_b is the flow rate of the outlet stream. Material balance for HAc and NaOH through the contactor is expressed as:

$$\frac{Vdx_a}{dt} = F_a C_a - (F_a + F_b)\,x_a \tag{2.65}$$

$$\frac{Vdx_b}{dt} = F_b C_b - (F_a + F_b)\,x_b \tag{2.66}$$

Definition of equilibrium constants and total ion concentration for acid and base:
For HAc:

$$\text{HAc} \rightleftharpoons H^+ + \text{Ac}^- \tag{2.67}$$

$$K_{\mathrm{HAc}} = \frac{[H^+][Ac]}{[HAc]} \tag{2.68}$$

Since HAc is a weak acid it will not dissociate completely in the solutions. So at any time, we can find some un-dissociated acid and the dissociated acid in the form of Ac$^-$. The dissociated constant for HAc, $K_a = 1.83 \times 10^{-5}$ at 25°C.
Hence the total ion concentration of acid is given by:

$$x_a = [\mathrm{HAc}\} + [\mathrm{Ac}^-] \tag{2.69}$$

Using Eq. (2.68), we get:

$$[\mathrm{Ac}^-] = \frac{x_a}{\left[1 + \left(\frac{H^+}{K_a}\right)\right]} \tag{2.70}$$

Similarly, for NAOH:

$$\mathrm{NaOH} \rightleftharpoons \mathrm{Na}^+ + \mathrm{OH}^- \tag{2.71}$$

$$K_{\mathrm{NaOH}} = \frac{[\mathrm{Na}^+][\mathrm{OH}^-]}{[\mathrm{NaOH}]} \tag{2.72}$$

Since NaOH is a strong base, it will dissociate completely. Hence [NaOH] = 0.

i.e.,

$$K_{\mathrm{NaOH}} = \infty \tag{2.73}$$

So, the total ion concentration of the base is given by

$$x_b = [\mathrm{Na}^+] + [\mathrm{NaOH}] = [\mathrm{Na}^+] \tag{2.74}$$

For the acid and base equilibrium, the electrical neutrality is to be satisfied, i.e., the total charge on positive ions equals to that of the total charge of negative ions.

$$[\mathrm{Na}^+] + [\mathrm{H}^+] \leftrightarrow [\mathrm{OH}^-] + [\mathrm{Ac}^-] \tag{2.75a}$$

By using Eqs. (2.74) and (2.70), Eq. (2.75a) can be written as:

$$x_b + [\mathrm{H}^+] \leftrightarrow [\mathrm{OH}^-] + \frac{x_a}{\left[1 + \left(\frac{[\mathrm{H}^+]}{K_a}\right)\right]} \tag{2.75b}$$

$$-\left[\frac{x_a}{\left[1 + \left(\frac{[\mathrm{H}^+]}{K_a}\right)\right]}\right] + x_b + [\mathrm{H}^+] - [\mathrm{OH}^-] = 0 \tag{2.75c}$$

We have

$$[\mathrm{H}^+]\,[\mathrm{OH}^-] = 10^{-14}. \tag{2.76a}$$

$$\mathrm{pH} + \mathrm{pOH} = \mathrm{pKw};\ \mathrm{pK_w} = 14 \tag{2.76b}$$

$$[\mathrm{H}^+] = 10^{-\mathrm{pH}};\ [\mathrm{OH}^-] = 10^{-\mathrm{pOH}} = 10^{\mathrm{pH}-14} \tag{2.76c}$$

Equation (2.75c) can be written as:

$$-\left\{\frac{x_a}{[1 + 10^{(\mathrm{pka}-\mathrm{pH})}}\right\} + x_b + 10^{-\mathrm{pH}} - 10^{\mathrm{pH}-\mathrm{pKw}} = 0 \tag{2.77}$$

The above nonlinear equation is to be solved to get the pH value from the state variable concentration x_a and x_b. The Eqs. (2.65), (2.66) and (2.77) constitute the model equations for the pH process.

2.9 MODELLING OF A LONG CHAIN POLYMERIZATION REACTION

The synthetic fabric industry relies on chemical reaction that produces long chain organic polymers. It is important to study such reactions. The reaction can be written symbolically:

$$\mathrm{A} + M_n \rightarrow M_{n+1} + \mathrm{CO}_2 \tag{2.78}$$

The compound M_n is called a polymer of length n. For fixed temperature and pressure, the rate of the above chemical reaction is given by $k_n\,[A]\,[M_n]$. It is assumed that the rate constant k_n is practically the same for all n since the mechanism is the same. A typical reaction starts with a concentration $a(0)$ of $\underline{\mathrm{A}}$ and $m_0(0)$ of M_0 . Since the concentration of the monomer does not change in the batch system, we have the conservation equation:

$$\sum m_n(t) = m_0(0) \tag{2.79}$$

The summation is carried out over n = 0 to ∞ and m_n (t) is $[M_n]$ at time t. Using Eq. (2.78) with n =0, we can write the following equations:

$$\frac{dm_0}{dt} = -k\,a(t)\,m_0(t) \tag{2.80}$$

$$\frac{dm_n}{dt} = k\,a(t)\,[m_{n-1}(t) - m_n(t)], \qquad n \geq 1 \tag{2.81}$$

$$\frac{da}{dt} = -k\,a(t)\sum m_n(t) \tag{2.82}$$

$$= -k\,a(t)\,m_0(0) \tag{2.83}$$

Equation (2.83) has the solution:

$$a(t) = a(0)\exp(-\lambda t), \text{ where } \lambda = k\,m_0(0) \tag{2.84}$$

We can define a variable y such that

$$dy = k\,a(t)\,dt \tag{2.85}$$

With $y = 0$ at $t = 0$, Eqs. (2.80) and (2.81) become:

$$\frac{dm_0(y)}{dy} = -\,m_0(y) \tag{2.86}$$

$$\frac{dm_n(y)}{dy} = m_{n-1}(y) - m_n(y) \tag{2.87}$$

These equations are solved by inductively to get:

$$\frac{m_n(y)}{m_0(0)} = \exp(-y)\,\frac{y^n}{n!} \tag{2.88}$$

which is a Poisson distribution with a parameter y. The mean chain length is y and the variance of the length is also *y*. From Eq. (2.84) and Eq. (2.85) we get:

$$y(t) = \int k\, a(0) \exp(-\lambda t)\, dt \text{ (the integral limit is from 0 to } t) \tag{2.89}$$

$$= a(0)\, \frac{[1 - \exp(-\lambda t)]}{m_0(0)} \tag{2.90}$$

Using the above equation, we can calculate the time required to produce polymers of desired length *l*.

2.10 DIFFUSION OF DOPANTS IN THE SEMICONDUCTOR SUBSTRATE

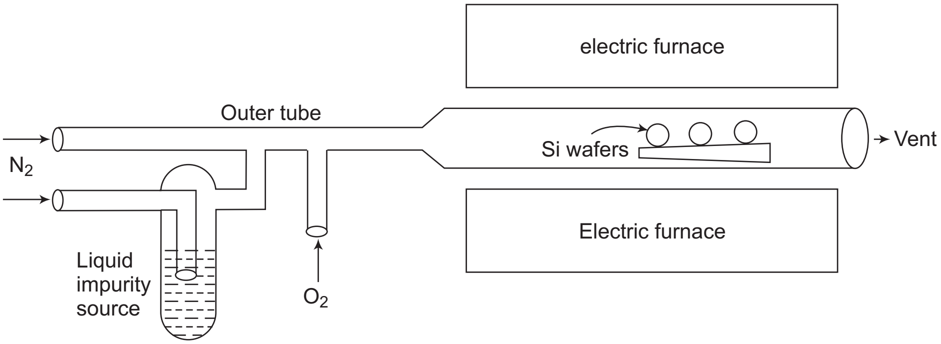


Fig. 2.8 Schematic diagram of a typical open-tube diffusion system (May and Sze, 2004)

Impurity doping is the introduction of controlled amounts of impurity dopants to the semiconductors in order to change the electrical properties of the semiconductors. Diffusion of impurities is typically carried out by placing the semiconductors wafers in a carefully controlled high temperature quartz tube furnace and passing a gas mixture that contains the desired dopant through it. The number of dopant atoms that diffuse in to the semiconductor is related to the partial pressure of the dopant impurity in the gas mixture. Figure 2.8 shows the schematic diagram of the furnace and gas flow arrangement for a liquid source of dopant ($POCl_3$). The reaction is given by:

$$4POCl_3 + 3O_2 \rightarrow 2P_2O_5 + 6Cl_2 \tag{2.91}$$

The P_2O_5 forms a glass-on-silica wafer and then reduced to phosphorous by silicon:

$$2P_2O_5 + 5Si \rightarrow 4P + 5SiO_2 \tag{2.92}$$

Diffusion in a semiconductor can be as the atomic movement of the diffusant (dopant atoms) in the crystal lattice by vacancies or interstitials. The basic diffusion of impurity atoms is similar to that of charge carriers (electrons or holes). Let F be the flux (number of dopant atoms passing through a unit area in a unit time) and C be the dopant concentration per unit volume. Then we have:

$$F = -\frac{D\partial c}{\partial x} \tag{2.93}$$

$$\frac{\partial c}{\partial t} = -\frac{\partial F}{\partial x} \tag{2.94}$$

$$= \frac{\partial F}{\partial x} = \frac{\partial\left(\frac{D\partial c}{\partial x}\right)}{\partial x} \tag{2.95}$$

When the concentration of the dopant is low, the diffusion coefficient D can be considered to be independent of C.

$$\frac{\partial c}{\partial t} = \frac{D\partial^2 c}{\partial x^2} \tag{2.96}$$

The above equation is known as the Fick's law. To solve the model equation, we need to give the boundary conditions:

2.10.1 Constant surface concentration

$$C(x, 0) = 0;\ C(0, t) = C_s\ ;\ C(\infty, t) = 0. \tag{2.97}$$

The solution is given by $C(x, t) = C_s \operatorname{erfc}\left[\frac{x}{2(Dt)^{0.5}}\right]$ (2.98)

where

$$\operatorname{erf}(x) = \left(\frac{2}{\pi^{0.5}}\right) \int \exp(-y^2)\, dy \text{ with the limit of integration from 0 to } x. \tag{2.99}$$

The various properties of erf are given by:

$$\operatorname{erfc}(x) = 1 - \operatorname{erf}(x) \tag{2.100}$$

$$\operatorname{erf}(0) = 0;\ \operatorname{erf}(\infty) = 1 \tag{2.101}$$

The total amount of dopant atoms per unit area of the semiconductor is given by:

$Q(t) = \int C(x, t)\, dx$ (with the limit from 0 to ∞) (2.102a)

$$= \left[\left(\frac{2}{\pi^{0.5}}\right) C_s\right] (Dt)^{0.5} = 1.13\ C_s\ (Dt)^{0.5} \tag{2.102b}$$

2.10.2 Constant total dopant

A fixed (or constant) amount of dopant is deposited on to the semiconductor surface in a thin layer, and the dopant subsequently diffuses in to the semiconductor. The initial condition is the same as before considered. The boundary conditions are:

$$\int c(x, t) = S;\ c(\infty, T) = 0 \text{ (limit from 0 to } \infty) \tag{2.103}$$

where, s is the total amount of dopant per unit area. The solution is given by

$$C(x, t) = \left[\frac{1}{(\pi Dt)^{0.5}}\right] S \exp\left[-\frac{x^2}{(4Dt)}\right] \tag{2.104}$$

The expression is the Gaussian distribution. In integrated circuit processing, a two-step diffusion process is commonly used, in which a pre-deposition diffusion layer first formed under the constant surface concentration condition. This step is followed by a drive-in diffusion (also called redistribution diffusion) under a constant total dopant condition. The penetration of the pre-deposition profile can be regarded to be negligible small compared with that of the final profile that results from the drive-in step.

2.11 MODELLING OF A TRANSPORT REACTOR

In a transport reactor, catalyst particles (of size 20 to 100 micron meter diameter) are physically carried out (transported) through a vertical pipe line by a concurrently upward flowing reactant gas stream. The transport reactors have been employed in situations of rapid catalyst deactivation, in which case the reactor offers the shorter residence time of the particles and of continuous addition of fresh catalyst at the feed and simultaneous with drawl of the deactivated catalyst at the reactor exit for subsequent regeneration of the catalyst. The reaction is assumed to take place at the surface of the catalyst. The gas and the solid particles are assumed to move by plug flow. The residence time of the reactor is shorter (few seconds) so that there is no catalyst deactivation. Consider a control volume of A ΔZ (Fig. 2.9) at a distance z from the inlet and thickness Δz.

The mass balance of the gaseous component through the control volume is given by:

$$[U_G A \varepsilon_G C_G]_z - [U_G A \varepsilon_G C_G]_{z+\Delta z} - k_m\, a\,(1-\varepsilon_G) A\, \Delta z\,(C_{G,\,av} - C_{S,\,av}) = 0 \tag{2.105}$$

Similarly consider the film around the particle also moves along with the particle with the same velocity

$$[U_P A(1-\varepsilon_G) C_S]_z - [U_P A(1-\varepsilon_G) C_S]_{z+\Delta z} + k_m\, a(1-\varepsilon_G) A\, \Delta z (C_{G,\,av} - C_{S,\,av}) - k_1 a\,(1-\varepsilon_G) A\, \Delta z\, C_{S\,av} = 0 \tag{2.106}$$

The subscript '*av*' indicates the average value in the control volume.

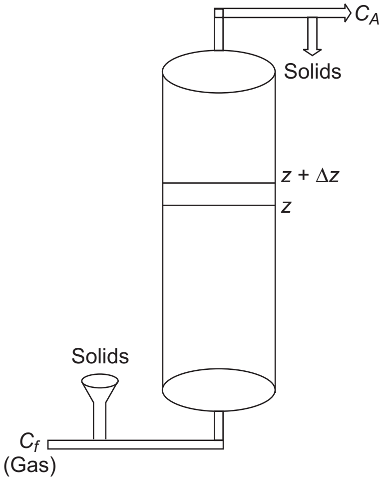


Fig. 2.9 Transport reactor for gas–solid catalyzed gas phase reaction

Divide throughout by Δz and then by making $\Delta z \to 0$, we get

$$\frac{dC_1}{dZ} = -N(C_1 - C_2) \tag{2.107}$$

$$\frac{dC_2}{dZ} = M(C_1 - C_2) - Q_1 C_2 \tag{2.108}$$

at
$$Z = 0;\ C_1 = 1;\ C_2 = 0 \tag{2.109}$$

$$C_1 = \frac{C_G}{C_f}, C_2 = \frac{C_S}{C_f}, C_f \text{ = feed concentration in the gas phase} \tag{2.110}$$

$$N = \frac{k_m a(1-\varepsilon_G)L}{V_G}, M = \frac{k_m aL}{U_P}, Q = \frac{k_1 aL}{U_P}, U_G = \frac{V_G}{\varepsilon_G} \tag{2.111}$$

$$a = \text{mass transfer area} = \frac{6}{dp}\ \frac{\text{cm}^2}{(\text{cm}^3 \text{ of solid volume})} \tag{2.112a}$$

V_G = superficial velocity of gas; U_G = actual velocity of gas in the reactor (2.112b)
$U_P = U_G$ (under the assumption of no-slip condition)

Otherwise $U_P = U_G - U_t$ (2.112c)

U_t = terminal velocity of a single particle (free or hindered velocity of particle)

$$= \frac{d_P^2(\rho_p - \rho_G)g}{(18\mu)} \text{ for Re}_\text{P} \geq 0.1;\ \text{Re}_\text{P} = \frac{d_P(U_G - U_P)\rho_G}{\mu} \tag{2.113a}$$

$$= 0.15\, d_P^{1.14}\ g^{0.71}\ \frac{(\rho_p - \rho_G)^{0.71}}{[\mu^{0.43}\ \rho_G^{0.29}]} \text{ for } 2 \leq \text{Re}_\text{P} \leq 1000 \tag{2.113b}$$

$$K_m \frac{d_P}{D_m} = 2 + 0.63\ (\text{Sc})^{0.33}\ (\text{Re}_\text{P})^{0.5} \tag{2.113c}$$

where, μ is the viscosity of gas; $\text{Sc} = \dfrac{\mu}{(\rho_G D_m)}$ (2.113d)

D_m = molecular diffusion coefficient in the gas phase,(cm^2 /s);
k_m = gas film mass transfer coefficient, cm/s
Mass balance of particle in the reactor:

$$(\rho_p - \rho_G)\left(\frac{\pi d_T^2}{4}\right) V_P = W_S \tag{2.114}$$

$$(1 - \varepsilon_G) = \frac{4W_s}{[(\rho_p - \rho_G)(\pi d_T^2)U_P]}, \tag{2.115}$$

Note: $U_G = \dfrac{V_G}{\varepsilon_G}, V_G =$ Superficial velocity (i.e., based on entire cross section of the reactor).

For improved correlation for u_t refer to Chidambaram (Chemicals and Petrochemicals J., 1992).

2.11.1 Numerical evaluation and discussion

Table 2.1 shows the values of the parameters used for the numerical evaluation. Figure 2.1 shows the fractional solid hold up (ε_S) in the reactor versus the particle diameter increase slightly with d_P. For higher values of d_P , the values of ε_S increases steeply with d_P. The value of ε_S increases as ρ_P increases and V_G decreases. This is due to decrease in particle velocity (U_P) with increase in d_P (refer to Eq. 2.113b).

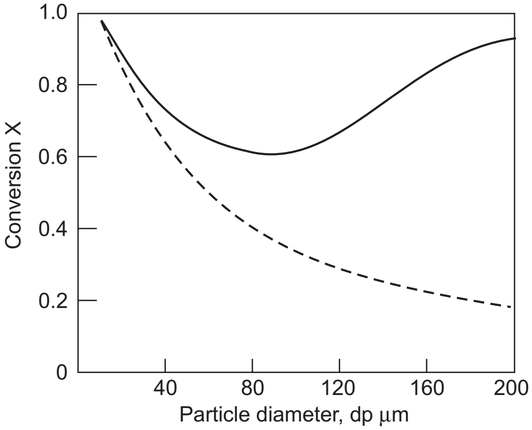


Fig. 2.10 Effect of particle diameter on the gas reactant conversion (Chidambaram, 1984) V_G = 100 cm/sec: ρ_P = 2.5 g/cm^3; Other conditions as in Table 2.1

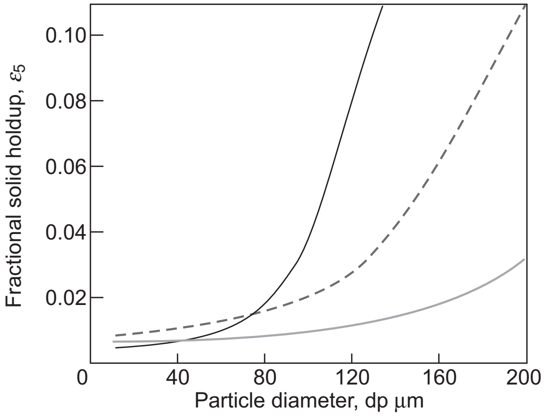


Fig. 2.11 Effect of particle diameter on the fractional solid hold up (Chidambaram, 1984)

Figure 2.10 shows gas reactants conversion (X) versus particle diameter (d_P) behaviour. This figure shows an interesting behaviour. It shows a minimum in the conversion with the particle size. As d_P increases the mass transfer area (a) and the mass transfer coefficient (k_m) decrease. These result in decrease in mass transfer rate. In the lower range of d_P, the increase in ε_S is small. In this range of d_P, the decrease in conversion due to decrease in k_m and a is more than the increase in conversion due to increase in ε_S. Hence, the conversion decreases with d_P. For higher values of d_P, the solid hold up (ε_S) increases steeply (Fig. 2.11). In this range, the increase in conversion due to increase in a_S offsets more than the decrease in conversion due to decreased k_m and a. Therefore, the conversion shows an increasing trend. Hence, there is a minimum in X versus d_P characteristics.

Table 2.1 *Values of parameters used for simulation*

Reactor diameter, d_T	6.72 cm
Particle diameter, d_P	10, 20,40,60,80,100,120,140,160,180,200 μm
Solid Flow rate, W_s	100 g/sec
Superficial gas velocity, V_G	100,150,200 cm/sec
Reactor Length	800 cm
Particle density, ρ_p	2.5, 5.0 g/cm^3
Gas Density , ρ_G	0.001 g/cm^3
Gas Viscosity, μ	1.8×10^{-4} g/(cm. sec)
Molecular diffusion coefficient in the gas film, D_m	0.01 cm^2/sec
Reaction rate constant, k_r	0.01 cm/sec

Other conditions as in Table 2.1

Figure 2.12 shows that the particle diameter at which the minimum conversion occurs, decreases as ρ_p increases V_G decreases. This is due to the steeper rise of ε_S with d_P. The value of the minimum conversion itself decreases as ρ_p increases and V_G increases. In the higher range of $d_{P,}$ conversion increases with ρ_p.

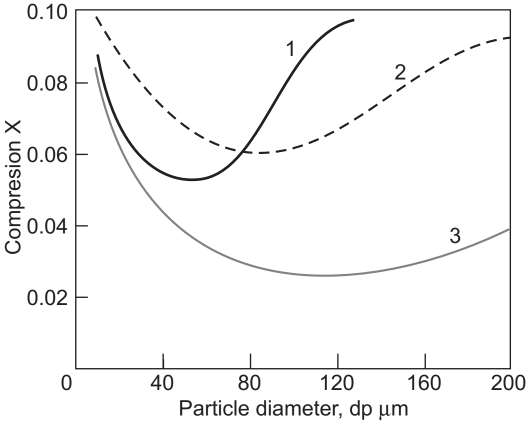


Fig. 2.12 Effect of ρ_p and V_G on X versus dp

Key	$V_{G,}$ cm/sec	$\rho_{p,}$ g/cm^3
1	100	5.0
2	100	2.5
3	150	2.5

The discussion clearly indicates that the transport reactors can be designed to give a desired conversion with a larger particle sizes as well. From economic point of view, operation with larger particle size is preferable since this results in enormous savings in the investment in the particles and more so in the separation of the particles from the outlet stream.

2.12 PDE MODEL FOR TUBULAR REACTOR WITH AXIAL DISPERSION MODEL

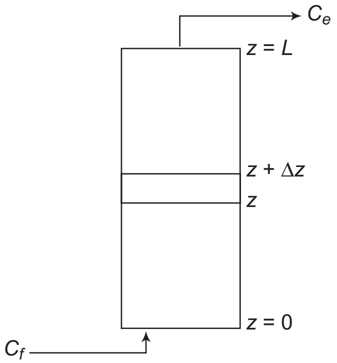


Fig. 2.13 Control volume in a tubular reactor

Consider a control volume (refer to Fig. 2.12) at a distance z of thickness Δz. The flow is both by the axial dispersion and by the convection flow. Let us write the mass balance across the control volume.

Accumulation in the control volume = input to the control volume at z - output from the control volume at ($z + \Delta z$) – consumption by a first order reaction which occurs in the control volume.

The input term at $z = \left[\mathrm{vAc} - \mathrm{AD}\dfrac{dc}{dz} \right]_z$ (2.116a)

The output at $z + \Delta z = \left[\mathrm{vAc} - \mathrm{AD}\dfrac{dc}{dz} \right]_{z+\Delta z}$ (2.116b)

Material consumed by reaction (first order kinetics) = $k_r\, \mathrm{c}_{\mathrm{ave}}\, A\Delta z$ (2.116c)

where, c_{ave} = average concentration in the control volume

Accumulation in the control volume = $\Delta z\ \dfrac{\partial (Ac_{\mathrm{ave}})}{\partial t}$ (2.116d)

The dynamics material balance is written now and after dividing throughout by A Δz and make the limit Δz tends to zero, to get:

$$\frac{\partial c}{\partial t} = -\frac{v\,\partial c}{dz} + D\frac{\partial^2 c}{\partial z^2} - k_r c \tag{2.117}$$

The boundary conditions are to be written at $z = 0$ and $z = L$.

At $z = 0$:

While writing the boundary condition, we make additional assumptions than what we assumed in developing the differential equation model at any z. Since the boundary condition is so small, we can assume negligible reaction and no accumulation. The material enters only by convection and on entering the reactor, the flow is by both convection and dispersion.

$$0 = v\, c_f - vc_Z + D\left[\frac{\partial c}{\partial z}\right]_Z \tag{2.118a}$$

Similarly at $z = L$;

$$0 = vc_{z+} - vc_L + D\left[\frac{\partial c}{\partial z}\right]_{Z^+} \tag{2.118b}$$

Analyzing the balance at $z = L$, we find that the gradient is from outside to inside the reactor at L which is not possible. Only way to overcome the problem is make the derivative $[\partial c/dz]_{Z=L} = 0$;

Hence the boundary condition at $z = L$ is given by $\dfrac{\partial c}{\partial z} = 0$

Now introducing the dimensionless variables: $x = \dfrac{z}{L}; C = \dfrac{c}{c_f}; Pe = \dfrac{uL}{D}, Q = \dfrac{k_r L}{u}$, the model equation becomes:

$$\frac{\partial C}{\partial \theta} = \frac{\partial^2 C}{\partial x^2} - \frac{1}{Pe}\frac{\partial C}{\partial Z} - QC \tag{2.119}$$

Boundary conditions are:

$$\frac{\partial C}{\partial x} = C_f - P\frac{\partial C}{\partial x} \quad \text{at } x = 0 \tag{2.120}$$

$$\frac{\partial C}{\partial x} = 0 \text{ at } x = 1 \tag{2.121}$$

Review Problems

1. Develop a model for the settling velocity of a spherical particle in a stagnant liquid.
2. Show that Nu =2 for cooling a small sphere in a stagnant fluid.
3. A naphthalene spherical particle is suspended in a quiescent air. Show that Sh = 2.
4. Derive a suitable expression for vaporization from a single liquid droplet in a quiescent air.
5. What is a Couette flow? For such a flow, derive $u = \left(\frac{V}{h}\right)y$, where V is the velocity of moving top plate.
6. What is a plane Poiseuille flow? For such a flow, derive $u = u_{\max}\left[1 - \left(\frac{y}{h}\right)^2\right]$.
7. Derive the corresponding equation for the velocity in a Poiseuille flow with a slip.
8. Find the area of a surge tank to smooth out flow variation of 10% amplitude of the inlet oscillation.
9. Develop a suitable model for a rapid thermal processing.
10. Develop set of model equations for a weak acid and strong base pH system.
11. Discuss the modelling of long chain polymerization reaction: $A + M_n \rightarrow M_{n+1} + CO_2$.
12. Derive the expression for total amount of dopant atoms per unit area of semiconductor.
13. Write down the model equation of a catalytic transport reactor. State all the assumptions made.
14. Derive the PDE model for a tubular reactor with the axial dispersion model.
15. Mott and Green [2015. *Chemical Engg Commun.* 202. 739–745.] have discussed on the Danckwerts' boundary conditions for the plug flow with dispersion /reaction model. Please read the paper and prepare a report on the work.

3

Model Development for Complex Systems

In this chapter, some examples of complex systems are given for the development of mathematical model equations. We define complex systems as simple models, which show a wide variety of interesting dynamics and hence are useful for understanding the complications of several real life phenomena. Usually, numerical methods are applied to get the solutions of the model equations. In some cases, analytical solution methods are possible.

3.1 ISOTHERMAL CONTINUOUSLY STIRRED TANK REACTOR (CSTR)

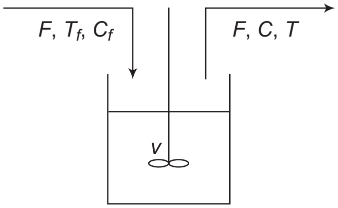


Fig. 3.1 Isothermal CSTR for single reaction

Consider an isothermal continuously stirred tank reactor (CSTR), (Fig. 3.1), wherein a single reaction to a product takes place (A→B). The reaction rate is given by $\dfrac{k_1 C}{(k_2 C + 1)^2}$ mol/(L.s). The model equation for the transient condition is given by the transient mass balance equation:

Accumulation = Input – output – consumption by reaction

$$V\frac{dC}{dt} = F\,(C_f - C) - \left[V\,\frac{k_1 C}{(k_2 C + 1)^2}\right] \tag{3.1}$$

where, F is the inlet flow rate and C_f is the feed concentration of the reactant A. The values of the operating conditions and the parameters are given as: F = 0.03333 L/s; V =1 L; k_1 =10 L/s; k_2 = 10 L/mol

For the nominal value of C_f = 3.288 mol/L, the steady state solution of the model equation gives the following three stable steady states at C = 1.3065, 1.7673 and 0.01424 mol/L On linearizing the transient equation around the operating point C = 1.3065, we get an unstable transfer function as $\frac{\Delta C(s)}{\Delta C_f(s)} = \frac{3.3226}{(99.70s-1)}$. Here Δ is the deviation variable from the steady state solution and s is the Laplace variable. The linearization of the dynamic equations around the other two equilibrium points (1.7673 and 0.01424 mol/L) give the characteristic root as negative, indicating they are stable steady states.

3.1.1 Linearization of a nonlinear system

Given the nonlinear systems: $\frac{dx}{dt} = f(x, u)$ (3.2)

$$\text{at } t = 0,\ x = x_s;\ u = u_s \tag{3.3}$$

Applying the Taylor's series around the operating condition (x_s, u_s):

$$f(x, u) = f(x_s, u_s) + \left(\frac{\partial f}{\partial x}\right)_{(x_s, u_s)} (x - x_s) + \left(\frac{\partial f}{\partial u}\right)_{(x_s, u_s)} (u - u_s) + \text{higher order terms.} \tag{3.4}$$

For smaller value of the deviation variables, we can neglect the higher order terms.

Let $$\Delta x = x - x_s \tag{3.5}$$

Equation (3.2) can be rewritten as:

$$\frac{d(\Delta x + x_s)}{dt} = f(x_s, u_s) + \left(\frac{\partial f}{\partial x}\right)_{(x_s, u_s)} (x - x_s) + \left(\frac{\partial f}{\partial u}\right)_{(x_s, u_s)} (u - u_s) \tag{3.6}$$

At steady state condition we have: $\frac{dx_s}{dt} = f(x_s, us)$. (3.7)

Hence, the above equation becomes:

$$\frac{d(y)}{dt} = \left(\frac{\partial f}{\partial x}\right)_{(x_s, u_s)} (y) + \left(\frac{\partial f}{\partial u}\right)_{(x_s, u_s)} (v) \tag{3.8}$$

where, $$y = \Delta x = x - x_s;\ v = u - u_s \tag{3.9}$$

The terms $\left(\frac{\partial f}{\partial x}\right)_{(x_s, u_s)}$ and $\left(\frac{\partial f}{\partial u}\right)_{(x_s, u_s)}$ are evaluated from the given $f(x, u)$ to get the constant values.

$$\frac{dy}{dt} = a_1 y + b_1 v \tag{3.10}$$

at $$t = 0;\ y = 0. \tag{3.11}$$

On taking the Laplace transformation, we get the transfer function model as

$$\frac{y(s)}{u(s)} = \frac{b_1}{(-a_1 s + 1)} \tag{3.12}$$

If a_1 is positive, then the system is called an unstable system.

3.1.2 Linearization of coupled ODEs

Similarly, one can linearize the coupled ODEs:

$$\frac{dx_1}{dt} = f_1\,(x_1, x_2, u) \tag{3.13}$$

$$\frac{dx_2}{dt} = f_2(x_1, x_2, u) \tag{3.14}$$

The steady state solution is denoted by x_{1s} and x_{2s}.

The Taylor's series is given by:

$$f_1(x_{1s}, u) = f_1(x_{1s}, u_s) + \left(\frac{\partial f_1}{\partial x_1}\right)_{(x_{1s}, x_{2s}, u_s)} (x_1 - x_{1s}) + \left(\frac{\partial f_1}{\partial x_2}\right)_{(x_{1s}, x_{2s}, u_s)} (x_2 - x_{2s})$$
$$+ \left(\frac{\partial f_1}{\partial u}\right)_{(x_{1s}, x_{2s}, u_s)} (u - u_s) + \text{higher order terms.} \tag{3.15}$$

$$f_2(x_2, u) = f_2(x_{2s}, u_s) + \left(\frac{\partial f_2}{\partial x_1}\right)_{(x_{1s}, x_{2s}, u_s)} (x_1 - x_{1s}) + \left(\frac{\partial f_2}{\partial x_2}\right)_{(x_{1s}, x_{2s}, u_s)} (x_2 - x_{2s})$$
$$+ \left(\frac{\partial f_2}{\partial u}\right)_{(x_{1s}, x_{2s}, u_s)} (u - u_s) + \text{higher order terms.} \tag{3.16}$$

The higher order terms can be neglected.

$$\frac{dy_1}{dt} = a_{11}\, y_1 + a_{12}\, y_2 + b_1 u \tag{3.18}$$

$$\frac{dy_2}{dt} = a_{21}\, y_1 + a_{22}\, y_2 + b_2 u \tag{3.19}$$

If the original nonlinear system has multiple steady state solutions, then the matrix A (= $[a_{ij}]$) can be calculated for each of the steady state solution. The eigenvalues (λ) of the corresponding matrix, can then be obtained. The nature of the system around these operating points will be classified (refer to Fig. 3.2) as stable node (if the each λ is negative and real), stable focus (if each λ is complex conjugate with the real part negative). The nature of the steady state can be given as unstable node (if the each λ is positive and real), unstable focus (if each λ is complex conjugate with the real part positive) and saddle (all λ are real but the sign of some of the λ differs). The stable node indicates that the system response monotonically changes and stable focus indicates the response is underdamped (oscillatory) to reach the final value.

A saddle point means that the system is unstable. With the given initial conditions, the solution of the above two linear ODEs gives the solution of x_1 versus t and x_2 versus t. These two graphs can, then be combined as a single curve by plotting x_2 versus x_1 with time as the parameter (Fig. 3.2). Such a plot is called the phase plane diagram. The behaviour of the system shown in Fig. 3.2 is valid only around a small operating point around each of the steady-state conditions [refer to Fig. 3.3a]. The numerical solution of the nonlinear ODEs will give the behaviour for large perturbations [refer to Fig. 3.3b].

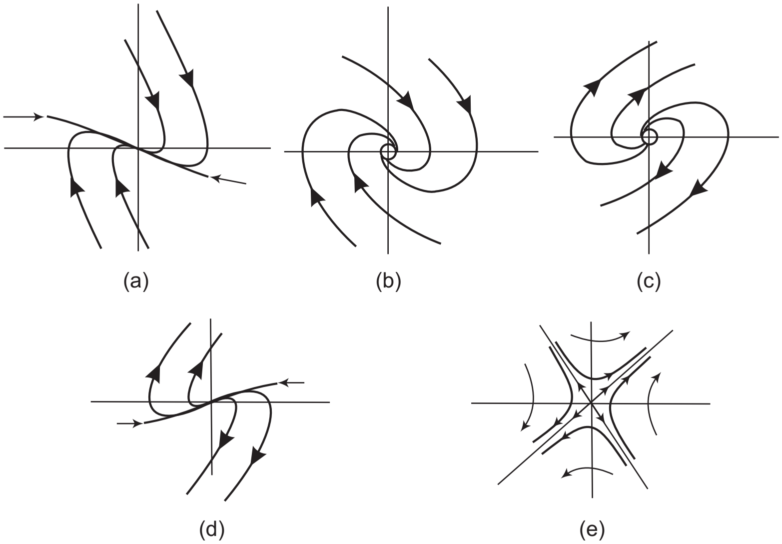


Fig. 3.2 x_2 versus x_1 local behaviour from a linear system (a) stable node, (b) stable focus, (c) unstable focus, (d) unstable node, (e) saddle point

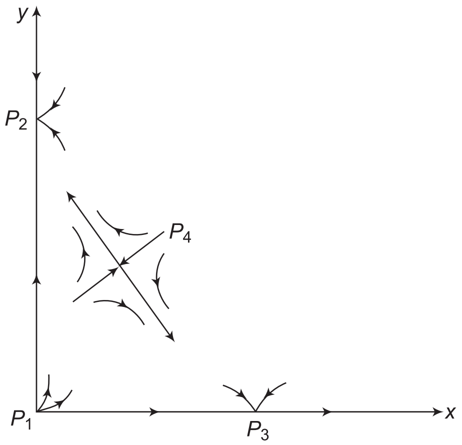


Fig. 3.3a Local information of system with 4 equilibrium states. y-axis: x_2 and x-axis: x_1; P_1: unstable Node; P_2 and P_3: stable nodes; P_4: saddle

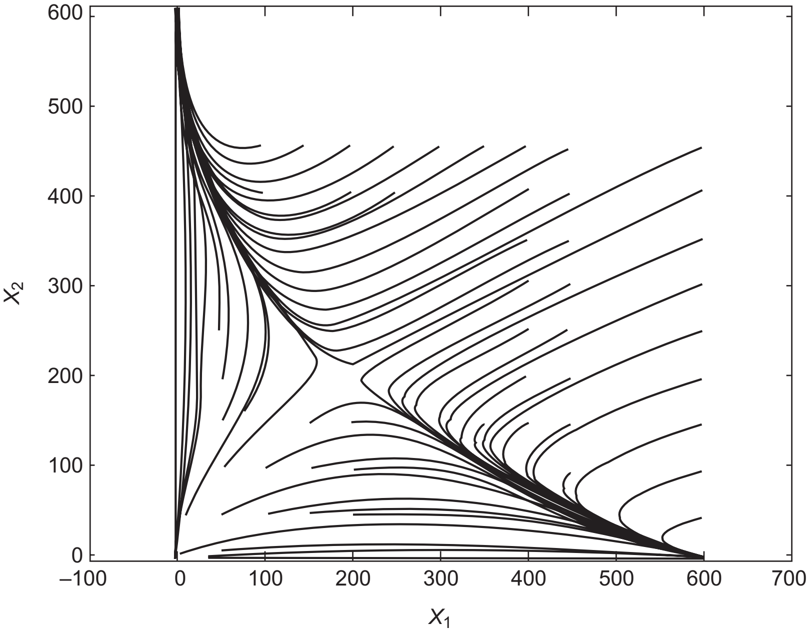


Fig. 3.3b The full phase portrait from the solution of a nonlinear dynamical system. Unstable node (0,0); stable node (600,0), (0,600); saddle (200,200). The direction of arrows as in Fig. 3.3a

3.2 BIOREACTOR MODELLING

The unsteady state model equations of a bioreactor (Fig. 3.4) for describing the cell concentration and the substrate concentration can be derived as:

$$\text{Accumulation} = \text{input} - \text{output} \tag{3.20}$$

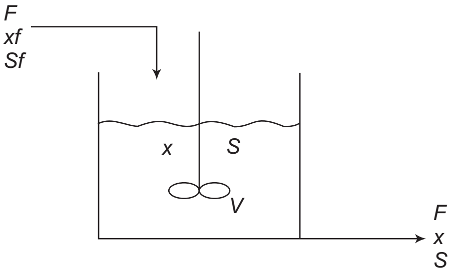


Fig. 3.4 Schematic representation of the example CSTB

There is no biomass in the feed. It is generated by the reaction (autocatalysis) with a rate $V\mu X$ where, μ is the specific growth rate of biomass. The rate of biomass produced is defined by $V\mu X$. The biomass leaves the reactor and the rate of output is given by FX where F is the flow rate of feed (equals to the exit flow).

$$\frac{Vdx}{dt} = V\mu X - FX \tag{3.21}$$

The above equation can be rewritten as:

$$\frac{dX}{dt} = (\mu - D)X \tag{3.22}$$

Similarly for the substrate, we can write the mass balance as:

$$\frac{dS}{dt} = (S_f - S)D - \left(\frac{\mu X}{\gamma}\right) \tag{3.23}$$

where the specific growth rate is given by (Agrawal and Lim, 1984):

$$\mu = \mu_{\max} \frac{S}{(K_m + S + K_1\, S^2)} \tag{3.24}$$

$D\left(= \frac{F}{V}\right)$ is called the dilution rate. In chemical reaction engineering subject, we call $\frac{F}{V}$ as a space–time. The reactant concentration is termed in biochemical engineering as substrate concentration. The stoichiometric coefficient is called the yield factor, γ.

The model parameters are given by:

$$\gamma = 0.4 g/g;\ \mu_m = 0.53\,\text{h}^{-1};\ D = 0.3\,\text{h}^{-1};\ K_m = 0.12 g/L;\ K_I - 0.4545 L/g;\ S_f = 4 g/L \tag{3.25}$$

Here X and S are the concentrations of the cell and substrate respectively. By making the terms $\frac{dX}{dt}$ and $\frac{dS}{dt}$ each zero, we get two non-linear algebraic equations. Analytical solutions of the equations give three steady state solutions (Agrawal and Lim, 1984): ($X = 0$, $S = 4$), (0.9951, 1.5122) and (1.5301, 0.1746). It is desired to operate the system at unsteady steady state ($X = 0.9951$, $S = 1.5122$). On local linearization of the unsteady state nonlinear equations around the steady state (0.9951, 1.5122) gives the transfer function as:

$$\frac{\Delta X(s)}{\Delta D(s)} = -\frac{5.89}{(5.86s - 1)} \tag{3.26}$$

Under a suitable feedback control scheme, the reactor can be stabilized.

3.3 MAGNETIC LEVITATION SYSTEM

The ‘maglev’ experiment is a magnetic ball suspension system which is used to levitate steel ball in the air by the electromagnetic force generated by an electromagnet (Fig. 3.5). The maglev system consists of an electromagnet, a ball rest, a ball position sensor, and a steel ball. The maglev system is completely encased in a rectangular enclosure. The focus is how to levitate the ball against gravity by applying an electromagnetic field. The applied control is the voltage applied (which is converted in to current by a driver embedded within the unit). The current passes through an electromagnet, which creates the corresponding electromagnetic field in the vicinity. The sphere is kept along the vertical axis of the electromagnet. The measured position is determined from an array of infrared transmitters and detectors, positioned such a way that the infrared beam is intersecting by the sphere. The infrared photo sensor is assumed to be linear in the required range of operation. Let us consider the system without any feedback control action. The force, experienced by the ball under the influence of electromagnet, is given by the nonlinear electro-mechanical equation:

$$F = \text{mg} + f(x, i) \tag{3.27}$$

where, $f(x, i)$ is the magnetic control force given by

$$f(x, i) = -\frac{ki^2}{x^2} \tag{3.28}$$

Here m is the mass of the steel ball, g is the acceleration due to gravity, x is the distance of the ball from the electromagnet and i is the current through the coil and k is a constant depending on the coil (electromagnet) parameters.

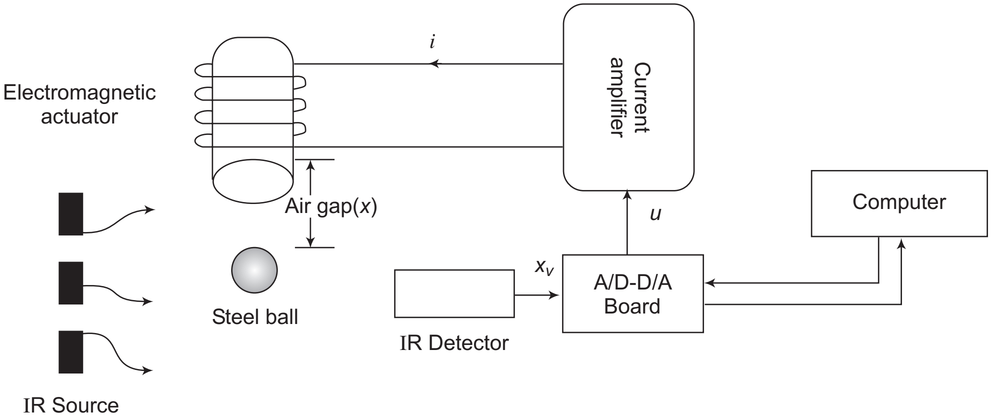


Fig. 3.5 Schematic of the MAGLEV system

Using Newton's second law, a differential equation is obtained:

$$m\frac{d^2x}{dt^2} = \text{mg}-\frac{ki^2}{x^2} \tag{3.29a}$$

The parameters and the nominal operating conditions are given by:

$$m = 0.02 \text{ kg}, k = 0.0001477 \text{ Newton-(m/A)}^2; i = 0.8 \text{ A}; x = -1.5 \text{ V}; g = 9.81 \text{ m/s}^2 \tag{3.29b}$$

The above equation is linearized around the operating point to get

$$\frac{\Delta X(s)}{\Delta I(s)} = -\frac{K_i}{(s^2 - K_x)} \tag{3.30a}$$

where,

$$K_i = \left(\frac{2K_{i0}}{x_0^2}\right), K_x = \left(\frac{2k_{i0}^2}{x_0^3}\right) \tag{3.30b}$$

where, $K_x = -0.2613$ and $K_i = 0.49$, and hence the poles are 0.511 and –0.511. Under the feedback control system, the magnetic levitation can be stabilized.

3.4 BALANCING A STICK ON A FINGER

Consider balancing a stick on the finger as shown in Fig. 3.6. The input variable is acceleration of the finger in one direction and the output is the angle of the stick (θ) with respect to a vertical line. The length of the stick is l and its mass is m. Let us consider the horizontal motion by the finger along a line. The position is given by the coordinate x. The input is then $u = \dfrac{d^2x}{dt^2}$. The centre of mass has the horizontal coordinate $x + 0.5l\sin(\theta)$ and the vertical coordinate $0.5\,l\cos(\theta)$

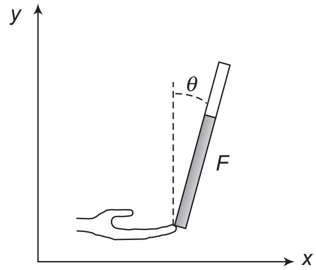


Fig. 3.6 Stick balancing; the lower end point of the stick has the coordinates x and y = 0 (Glad and Ljung, 2000)

Let us look at the point of contact between the finger and the stick. For the y-component, the force equation gives:

$$F\cos\theta - \mathrm{mg} = md^2[0.5\,l\cos(\theta)]\,/dt^2 = (0.5\,l\,\mathrm{m})\,[-\theta''\sin\theta - \theta'^2\cos\theta] \tag{3.31}$$

For the x-component, we have

$$F\sin\theta = mx'' + md^2\,[(0.5\,l\sin\theta)]/\mathrm{dt}^2 = mu + [\mathrm{m}\,0.5l\,]\,[\theta''\cos\theta - \theta'^2\sin\theta] \tag{3.32}$$

where, $$\theta' = \frac{d\theta}{dt},\ \theta'' = \frac{d^2\theta}{dt^2}$$

On multiplying Eq. (3.31) by $\cos\theta$ and Eq. (3.32) by $\sin\theta$ and adding the resulting two equations we get:

$$0.5\,l\,\theta'' - g\sin\theta = -u\cos\theta \tag{3.33}$$

For small angles, we get the transfer function [relating $\Delta\theta(s)$ to $\Delta u(s)$] as:

$$G(s) = -\frac{\left(\dfrac{2}{l}\right)}{\left[s^2 - \left(\dfrac{2g}{l}\right)\right]} \tag{3.34}$$

The roots of the denominator are $+\sqrt{\dfrac{2g}{l}}$ and $-\sqrt{\dfrac{2g}{l}}$ and the system is unstable. Feedback action (movement of the finger) is continuously required to make the system stable, i.e., to keep the stick vertical).

3.5 CHOLETTE'S MODEL WITH INPUT MULTIPLICITIES

We consider an isothermal CSTR with the reaction rate given by $\frac{-k_1 c}{(1+k_2 c)^2}$. The non-ideal mixing is described by the Cholette's model (Liou and Chien, 1991). In Fig. 3.7, n is the fraction of the reactant feed that enters the zone of the perfect mixing and m is the fraction of the total volume of the reactor where the reaction occurs [i.e., $(1 - m)$ fraction of the volume is a dead zone]. The $(n - 1)$ q fraction of the inlet flow by the mixing & dead zone and leave the reactor such like that. This is shown in Fig. 3.7 for clarity as if this fraction is bypassing the reactor. The transient equation of the reactor is given by:

$$\frac{dC}{dt} = \left[\left(\frac{nq}{mV}\right)(C_f - C)\right] - \frac{k_1 C}{(k_2 C + 1)^2} \tag{3.35}$$

$$\text{at } t = 0,\ C = C_0 \tag{3.36}$$

C and C_e are related by

$$nC + (1 - n)\,C_f = C_e \tag{3.37}$$

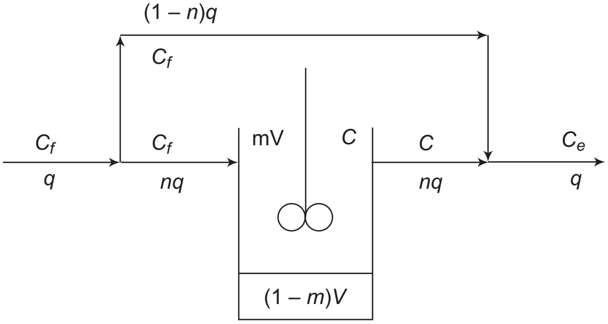


Fig. 3.7 Schematic representation of the Cholette's model of a CSTR (Liou and Chien, 1991)

At the steady state condition, the corresponding equations from Eqs. (3.35) and (3.36) give the relation to calculate C_f in terms of C_e as:

$$g^3 + p_1 g^2 + p_2 g + p_3 = 0 \tag{3.38}$$

where,

$$g = k_2 C_e - k_2 (1 - n) C_f \tag{3.39}$$

where p_1, p_2 and p_3 are functions of C_e

$$p_1 = (2n - nk_2 C_e) \tag{3.40}$$

$$p_2 = [n_2 - 2n^2 k_2 C_e + \text{Dmn}(1 - n)] \tag{3.41}$$

$$p_3 = -n^3 k_2 C_e \tag{3.42}$$

For the given values of the parameters:

$$n = 0.75,\ m = 0.75 \text{ and } D = 300;\ k_1 = 10 \text{ L/s},\ k_2 = 10\ L\text{/mol and } V = 1\ L. \tag{3.43}$$

To get $C_e = 1.8$ mol/L, the numerical solution of Eq. (3.36) gives

$$C_f = 7.024,\ 6.848 \text{ and } 3.288 \text{ mol/}L \tag{3.44}$$

To get a specified value of C_e, we get three values of C_f. This behaviour is called the input multiplicity behaviour. Similarly, the steady state equation for C_e in terms of C_f is obtained from Eqs. (3.35) and (3.37) as

$$C_e^{\ 2} + p_4\, C_e^{\ 2} + p_5\, C_e + p_6 = 0 \tag{3.45}$$

where

$$p_4 = (2n-3)C_f + \frac{2n}{k_2} \tag{3.46}$$

$$p_5 = \frac{\{[k_2(1-n)(3-n)\,C_f - 2n(2-n)]k_2C_f + n^2 + \text{Dmn}\}}{k_2^2} \tag{3.47}$$

$$p_6 = -\frac{\{[k_2(1-n)C_f - n]^2 + \text{D mn}(1-n)\}C_f}{k_2^2} \tag{3.48}$$

For $C_f = 7.024$ mol/L, we get the following values for C_e:

$$C_e = 6.692,\ 1.8 \text{ and } 1.894 \text{ mol/}L \tag{3.49}$$

For a give input value of C_f, we get three values of output C_e. This behaviour is called the output multiplicity behaviour.

Similarly for C_f =6.484, we get

$$C_e = 6.1212,\ 1.655 \text{ and } 1.8 \text{ mol/}L \tag{3.50}$$

Similarly for $C_f = 3.288$ mol/L, we get

$$C_e = 2.148,\ 0.8327 \text{ and } 1.8 \text{ mol/}L \tag{3.51}$$

The corresponding values of C can be obtained from Eq. (3.37).

3.6 ISOTHERMAL CSTR WITH INPUT MULTIPLICITIES

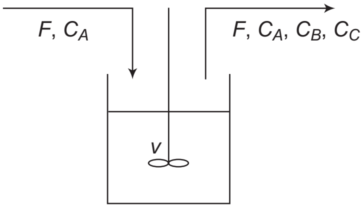


Fig. 3.8 Isothermal CSTR for consecutive reaction

We consider (Fig. 3.8) here a continuous stirred tank reactor (CSTR) with the following isothermal series/parallel reactions (Van de Vase, 1966):

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$$2A \xrightarrow{k_3} D \tag{3.52}$$

The product B is the desired one. The transient mass balance equations for A and B are given by

$$\frac{dx_1}{dt} = -k_1 x_1 - k_3 x_1{}^2 + (C_{A,0} - x_1)u \tag{3.53}$$

$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 - x_2 u \tag{3.54}$$

where

$$x_1 = C_A,\ x_2 = C_B,\ u = \frac{F}{V} \tag{3.55}$$

and F is the flow rate (L/min), V is the volume of the reactor (L), C_A and C_B are the concentrations of A and B in the reactor (mol/L) and $C_{A,0}$ is the feed concentration of A (mol/L). The analytical solution for the steady state concentration of A and B are given by:

$$x_{1,s} = \frac{[-b + \{b^2 + 4k_1 C_{A,0}\, u_s\}^{0.5}}{(2k_1)} \tag{3.56}$$

$$u_s = \frac{[f_2 \pm \{f_2^2 - 4f_1 f_2\}^{0.5}]}{(2f_1)} \tag{3.57}$$

where,

$$b = k_1 + u_s; f_1 = d_2{}^2 - 1; f_2 = -2\,d_1\,d_2 + 2k_1 + d_3; f_3 = d_1{}^2 - k_1{}^2 \tag{3.58}$$

$$d_1 = \frac{(2k_3 k_2 x_{2,s} + k_1^2)}{k_1}; d_2 = \frac{[2k_3 x_{2,s} + k_1]}{k_1}; d_3 = 4k_3 C_{A,0} \tag{3.59}$$

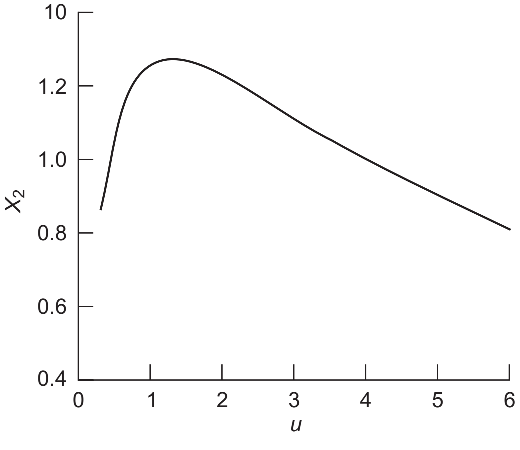


Fig. 3.9 Steady state x_2 versus u (Reddy and Chidambaram, 1996)

The parameters considered for the present work are given by k_1 = 0.8333 (L/min); k_2 = 1.6667 (*L*/min), k_3 = 0.16667 (*L*/mol. min), $C_{A,\,0}$ = 10 mol/*L*. The steady state behaviour of x_2 versus u_s is shown in Fig. 3.9. This figure shows that the steady state input multiplicities in u_s on the product concentration ($x_{2,\,s}$). Two values of u_s give the same value of $x_{2,\,s}$. For example, $x_{2,\,s} = 1.117$ can be obtained at $u_s = 0.5714$ and also at u_s =2.8746. The gain (the slope) is + 0.5848 at $u = 0.5714$ whereas the gain is –0.1208 at $u = 2.8746$.

3.7 MODEL FOR PREDATORS AND PREY POPULATIONS

Let x denote the number of prey per unit area and $y(t)$ the number of predators per unit area.

Rate of change of prey = rate of natural prey births – rate of natural prey death – rate of prey killed by predators (3.60)

Rate of change of predators = rate of predator births – rate of natural predator deaths (3.61)

Since the overall rates are the per capita rates multiplied by the respective population densities:

Rate of prey births = $b_1\,X(t)$, (3.62)

Rate of prey natural deaths = $a_1\,X(t)$ (3.63)

Rate of predator birth = $b_2\,Y(t)$ (3.64)

Rate of predators death = $a_2\,Y(t)$ (3.65)

For the prey deaths, we denote the per capita death rate as $C_1\,Y(t)$, since it is proportional to the predator density, with C_1 as the positive constant of proportionality. Thus the rate at which the prey are eaten is given by $C_1\,X(t)\,Y(t)$. The predator birth rate has a component, which is proportional to this rate of prey eaten:

Rate of prey killed by predators = $C_1\,X(t)\,Y(t)$ (3.66)

Corrected rate of predators birth = $b_2Y(t) + f\,C_1Y(t)\,X(t)$ (3.67)

where *f* is also a positive constant of proportionality. Substituting the above derived equations in Eqs. (3.60) and (3.61), we get the model equations as:

$$\frac{dX}{dt} = b_1X - a_1X - c_1\,XY \tag{3.68}$$

$$\frac{dY}{dt} = b_2Y + fc_1\,XY - a_2Y \tag{3.69}$$

the above equations can be rewritten as:

$$\frac{dX}{dt} = \beta x - c_1XY \tag{3.70}$$

$$\frac{dY}{dt} = c_2XY - a_2Y \tag{3.71}$$

where, β_1, α_1, c_1 and c_2 are all positive constants given by:

$\beta_1 = b_1 - a_1$; $-\alpha_2 = b_2 - a_2$ and $c_2 = fc_1$ (3.72)

The system of equations is called the Lotka–Volterra predator–prey system after two mathematicians who first studied these systems. The parameters c_1 and c_2 are known as interaction parameters as they describe the manner in which the populations interact. To get a feel for the behaviour of the system, let us assume the parameters as: $\beta_1 = 1$, $\alpha_2 = 0.5$, $c_1 = 0.01$, $c_2 = 0.005$ with the initial conditions as: $X_0 = 200$ and $Y_0 = 80$. The time behaviour of the system is given in Fig. 3.10. A sustained oscillatory behaviour is obtained in both X and Y.

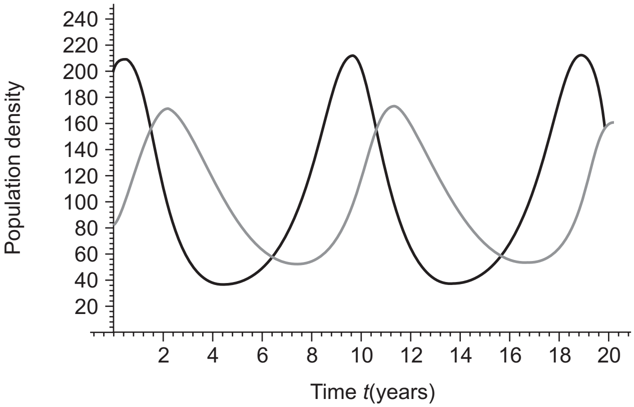


Fig. 3.10 Sustained oscillatory behaviour of prey and predator population densities; solid: prey; dot: predator (Barnes and Fulford, 2009)

Certain systems exhibit steady-state behaviour, while others oscillate in a regular periodic fashion. Still others vary in an irregular, seemingly haphazard manner, and, even when observed for a long period of time, do not appear their previous history. It is sometimes possible to get particular solutions of the system equations analytically, especially when the solutions are periodic or invariant with time. Ordinarily, however, the non-periodic solutions can not readily be determined except by the numerical procedures.

3.8 WEATHER FORECASTING

Weather forecasting has to be performed by the numerical solution of complicated equations (systems of coupled nonlinear partial differential equations) that involve several variables (as the three velocity components in space and temperature). To see the basic features of such systems of partial differential equations (like the weather prediction), it is helpful to consider highly simplified approximations to the system – as given by the Lorenz (1953) model. E. Lorenz, a professor of Meteorology at MIT, was simulating a reduced order model of the atmosphere, which consists of 12 ODEs. He discovered a very important aspect of certain types of the nonlinear systems that of extreme sensitivity to initial condition. A very small difference in the initial conditions leads to different output behaviour for a long run. He pointed out that the long term prediction of certain systems (such as the weather) will never be possible. He reduced the model of the atmosphere to three that could describe the essentials of the original higher order model equations.

Consider a fluid between two parallel plates (Fig. 3.11). When the top plate temperature (T_2) is equal to the bottom plate temperature (T_1), there is no heat flow and the system is in equilibrium. Let us increase the bottom temperature. At low temperature differences, there is still no flow because the viscous forces are greater than the buoyancy forces. Finally at some critical temperature differences, the buoyancy forces overcome the viscous forces and the fluid begins to move and form convection rolls. As the temperature difference is increased, the fluid movement becomes more and more vigorous. The speed of the convection rolls can be considered as the wind speed in a 'weather model' and the direction of the convection rolls as wind direction. The simplified model is given by the following equations:

$$\frac{dy_1}{dt} = P_R\,(y_2 - y_1) \tag{3.72}$$

$$\frac{dy_2}{dt} = y_1(R - y_3) - y_2 \tag{3.73}$$

$$\frac{dy_3}{dt} = y_1 y_2 - b y_3 \tag{3.74}$$

Here y_1 measures the strength and direction of atmospheric circulation, and y_2 and y_3 measure the horizontal and vertical temperature variation, respectively. The variable that essentially controls the dynamics of this equation system is $R\left[=\frac{g\alpha H^3 \Delta T}{(\gamma k)}\right]$, which is proportional to the vertical temperature difference.. Here α = coefficient of expansion; H = distance between plates; g = gravitational acceleration; ΔT = temperature difference between the plates ($T_1 - T_2$); γ= kinematic viscosity; k = thermal conductivity.

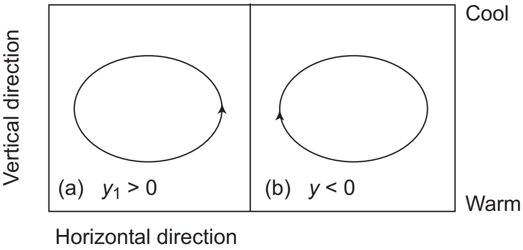


Fig. 3.11 An illustration of convection according to Lorenz's equation

The model parameters Pr is the Prandtl number (the ratio of diffusivities of momentum and heat), and b is defined by $b = \frac{4}{(1 + a^2)}$. The parameter 'a' is a horizontal wave number for the convection cells, and b measures the width to height ratio of the convection layer. The important model parameter is R, which is proportional to the vertical temperature difference (the driving force of the system). R is defined by $R = \frac{R_a}{R_c}$, where R_a refers to Rayleigh number, and R_c refers to the critical value of Rayleigh number (R_c is required for the onset of convection).

Let us consider $a^2 = 0.5$ and hence $b = \frac{8}{3}$. Let Pr = 10 (for water). $R = 28$. Two solutions to these equations, which differ by a minor difference of the initial value for y_1 (one at 5 and the other at 5.005) are shown in Fig. 3.12. A small variation of the initial condition may result in a completely different solution, which indicates that a long-range weather forecasting may be impossible. Several chemical reactors exhibit similar behaviour. It is necessary to have three nonlinear autonomous differential equations for chaos to occur. Chaos can also occur in a system of two nonlinear, non-autonomous differential equations (i.e., if some type of periodic input forcing function is used). The chaos can also occur in a single discrete nonlinear equation.

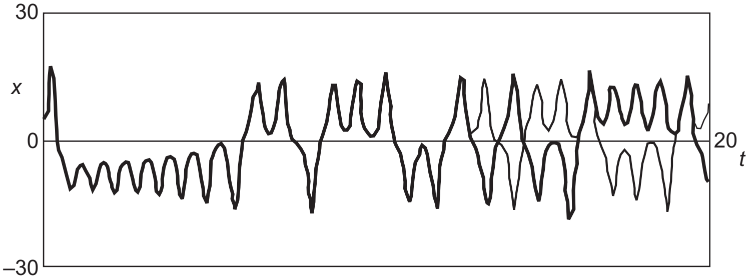


Fig. 3.12 Chaotic behaviour of Lorenz equation for r = 28, $(x, y, z)=(x_0, 5, 5)$ at t = 0; bold curve: $x_0 = 5.000$, the lighter curve: $x_0 = 5.005$ (Acheson, 1997)

3.9 POPULATION MODEL

Let $x(t)$ represents the number of individuals in a population at time t. Two factors influence its growth: the birth rate [$b(t)$] and the death rate [$d(t)$]. The model equation for x is given by

$$\frac{dx}{dt} = b(t) - d(t) \tag{3.75}$$

In this model (known as Malthusian growth model), the birth and death rates are assumed to be proportional to the number in the population. Thus

$$\frac{dx}{dt} = \beta x - \delta x \tag{3.76a}$$

$$= \frac{x(t)}{\tau} \tag{3.76b}$$

$$x(t) = x(0)\ \exp\left(\frac{t}{\tau}\right) \tag{3.76c}$$

where $x(0)$ is the initial population. $\frac{1}{\tau}$ is called Malthusian parameter. The above model may be reasonable one for a shorter time. It does not take in to account the growth factors such as disease, overcrowding and competition for food that come into play for large populations which are not seen in the small populations. It is reasonable to assume that as population grows, the birth rate decreases and death rate increases. The capita birth rate in the Malthusian model, $\frac{b(t)}{x(t)} = \beta$ is constant. This will be assumed to decrease with the population: $\frac{b(t)}{x(t)} = [\beta - k_1\, x(t)]$, for some positive constant k_1.

Similarly $\dfrac{d(t)}{x(t)} = [\delta + k_2\, x(t)]$ for some positive constant of k_2. Hence we get:

$$\frac{dx(t)}{dt} = b(t) - d(t) \tag{3.77}$$

$$= \left[1 - \left(\frac{x}{N}\right)\right]\left(\frac{x}{\tau}\right) \tag{3.78}$$

where $\tau = \dfrac{1}{(\beta - \delta)}$ and $N = \dfrac{(\beta - \delta)}{(k_1 + k_2)}$. This equation is called *Logistic* differential equation or the *Verhulst* population differential equation. N is called carrying capacity of the population, which represents the maximum population possible under the given model. The name 'logistic' was first coined by the French army under Napolean. This equation is used for the planning of 'logement' of troops in the camps. Now, this model is used to simulate a population growth model.

3.9.1 Two competing species

In this section, we consider a specific model, which describes the population changes of two species competing for the same food. When x_1 is large, there is less than the required food for each member of the species, This has the effect of decreasing the death–rate because of the increased probability of disease and starvation, and of decreasing the birth rate because the offspring are less healthy and hence have less chance of survival. If only one species were present, its population changes can be described in most circumstances by the logistic equation:

$$\frac{dx_1}{dt} = \left(\frac{x_1}{\tau_1}\right)\left(1 - \frac{x_1}{N_1}\right) \tag{3.79}$$

N_1 is called equilibrium (saturation) value for species 1.

The effect of species 2 is to decrease the food supply to species 1 by an amount proportional to x_2. Thus the equations

$$\frac{dx_1}{dt} = \left(\frac{x_1}{\tau_1}\right)\left(1 - \frac{x_1}{N_1} - \frac{\sigma_1 x_2}{N_2}\right) \tag{3.80}$$

$$\frac{dx_2}{dt} = \left(\frac{x_2}{\tau_2}\right)\left(1 - \frac{x_2}{N_2} - \frac{\sigma_2 x_1}{N_1}\right) \tag{3.81}$$

are a reasonable model for the two competing species. Consider the equilibrium condition (make the derivative terms zero in the above equations). From the first equation, we get:

$$x_1 = 0 \text{ (or) } \left(1 - \frac{x_1}{N_1} - \frac{\sigma_1 x_2}{N_2}\right) = 0 \tag{3.82}$$

From the second equation, we get:

$$x_2 = 0 \text{ (or) } \left(1 - \frac{x_2}{N_2} - \frac{\sigma_2 x_1}{N_1}\right) = 0 \tag{3.83}$$

To get the solution for the model, we must get one condition from each equation as:

$$(x_1 = 0, x_2 = 0) \tag{3.84}$$

Substituting $x_1 = 0$ from the first condition in Eq. (3.82) in the second condition of Eq. (3.83) we get

$$x_1 = 0 \text{ and } x_2 = N_2 \tag{3.85}$$

Similarly, by substituting $x_2 = 0$ from the second set of condition in Eq. (3.83) in the first set we get:

$$x_1 = N_1, x_2 = 0$$

Similarly, we get: $$1 - \frac{X_{1i}}{N_1} - \frac{\sigma_1 x_{2j}}{N_2} = 0 \text{ and } 1 - \frac{x_{2i}}{N_2} - \frac{\sigma_2 x_1}{N_1} = 0 \tag{3.86}$$

As a specific example, let us consider; $N_1 = 300$; $N_2 = 300$; $\sigma_1 = 2$ and $\sigma_2 = 2$, $\tau_1 = 0.2$; $\tau_2 = 1$ year. The four equilibrium solutions are given by (0, 0), (0, 300), (300, 0) and (100, 100). The linearization of the dynamic equations around the equilibrium point (0, 0) give the eigenvalues as (both positive real) indicating it is a unstable node. Similarly the equilibrium points at (300, 0) gives the eigenvalues as each negative real indicating it is a stable node. Similarly, the third equilibrium point (100, 100) gives one positive real eigenvalue and the other negative real eigenvalue, indicating the equilibrium points corresponds to a saddle condition. Similarly, the fourth equilibrium point (0, 300) gives both the eigenvalues as negative real indicating it is a stable node.

The phase plane diagram for the nonlinear system is shown in Fig. 3.13. The space of points with coordinates $(x_1, x_2,\ldots, x_n)$ is known as *phase space*, or when $n = 2$, it is called the *phase plane*. The numerical solution of Eq. (3.80) and Eq. (3.81) gives the solution of x_1 versus t and x_2 versus t. These two graphs can be merged to a single curve by plotting x_2 versus x_1 with time as the parameter. By changing the initial conditions, we can generate such curves. Such a plot is called a phase plane diagram. For a given initial condition, Fig. (3.13) will show what the steady state solution will be. Ball (1985) gives additional details of the model equations.

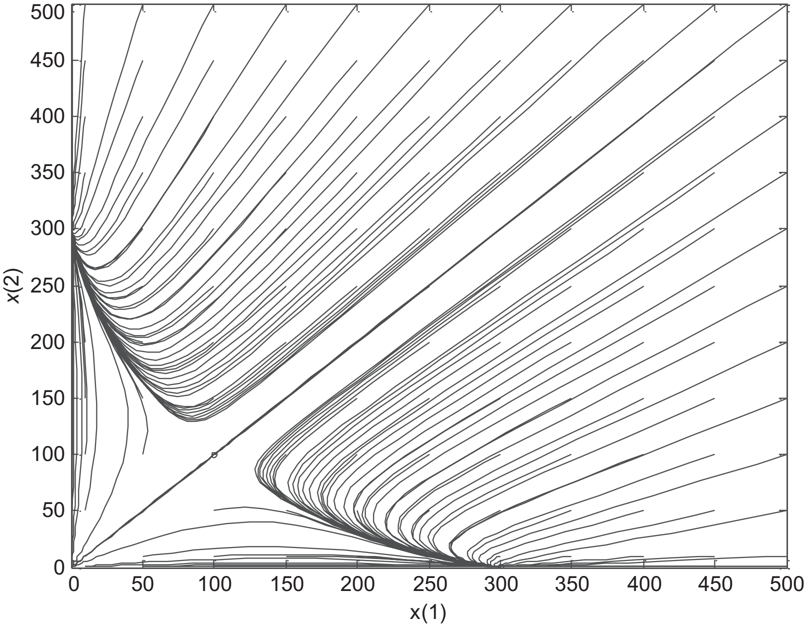


Fig. 3.13 Phase plane diagram for the system
Profile at (0, 0) is outward. The profile at (300, 0) & (0, 300) inward

3.10 EPIDEMIOLOGICAL MODEL

The problem of epidemics is to assess how a group of individuals with a communicable infection spreads to a population that will be able to catch it (Ghezzi and Picard, 1993). Consider a population of constant size, where individuals are susceptible, i.e., they can contact the disease, or infective, i.e., they can spread the disease, or recovered, i.e., they have become permanently immune. If the population has unitary size and consists of S susceptible individuals, I infective individuals and R recovered individuals, then we have:

$$S(t) + I(t) + R(t) = 1 \text{ for all } t \geq 0 \tag{3.87}$$

Suppose that newborns are all susceptible, and that birth and death rates are the same and equal to η with $\eta > 0$. Assume that the vaccination program turns susceptible into recovered, i.e., permanently immune individuals, at a rate $u(t)$.

The infective disease is transmitted by contact between the individuals. If the population is homogeneous and uniformly mixed, contacts between susceptible, contacts between susceptible and the infective are proportional to SI. It is assumed that the infective in the unit of times are $\beta\,(t)$ SI, where β is the contact rate. Since traditional childhood diseases (e.g., measles, mumps, rubella and chicken pox) strike mainly when schools are open, the contact rate β is seasonally dependent, i.e., it is periodic with a period equal to one year. Finally, assume that the infectives recover at a rate γ, with $\gamma > 0$.

The governing differential equations are:

$$\frac{dS}{dt} = \eta - [\eta + u]S - \beta SI \tag{3.88}$$

$$\frac{dI}{dt} = \beta SI - (\eta + \gamma)I \tag{3.89}$$

where
$$\beta = \beta_0\,[1 + \varepsilon \sin(2\pi t)] \tag{3.90}$$

at
$$t = 0,\ S = S_0,\ I = I_0 \tag{3.91}$$

with $\beta_0 > 0$ and $0 < \varepsilon < 1$. If vaccination is ruled out ($u = 0$ for all $t \geq 0$), the previous model reduces to SIR model (Dietz, 1976) notably the periodic SIR models can display chaotic behaviours in accordance with real data (Olsen et al., 1988). The recurrence of large outbreaks is peculiar to such behaviours. The disease is transmitted by contact between susceptible and infective individuals. For the epidemic to unfold, a certain (very small) amount of infective must always be present. For $\varepsilon = 0$ (no seasonality) and consider a constant vaccination rate $u = u_0$.

The model equations have two states of equilibrium:

$$S = \frac{(\eta + \gamma)}{\beta_0},\ I = \left[\frac{\eta}{(\eta + \gamma)}\right] - \left[\frac{(\eta + u_0}{\beta_0}\right] \tag{3.92}$$

$$S = \frac{\eta}{(\eta + u_0)},\ I = 0 \tag{3.93}$$

For $u_0 < u_{cr} = \eta\left\{\left[\frac{\beta_0}{(n+\gamma}\right]-1\right\}$ both the equilibrium are nonnegative, with the first one being stable and the later unstable, as can be ascertained by linearization. A bifurcation can take place $u_0 = u_{cr}$, the two equilibrium collide, giving rise to exchange of stability. For $u_0 > u_{cr}$, only the later equilibrium, now a stable one, is nonnegative. All trajectories do converge to it. The epidemiological meaning is apparent; the epidemic can be eradicated by using a sufficiently large vaccination rate. Such a results carries over to the seasonal case $\varepsilon > 0$, we get:

$$S = \frac{\eta}{(\eta + u_0)}\ ;\ I = 0 \tag{3.94}$$

is still equilibrium. Based on the local linearized model, it can be shown that such an equilibrium is stable for $u > u_{cr}$, and unstable for $u < u_{cr}$. The various control techniques now available generally aim to replace a chaotic solution with a stationary or a periodic one. Ghezzi and Picard (1993) give details of the problem.

3.11 NON-ISOTHERMAL CONTINUOUS STIRRED TANK REACTOR

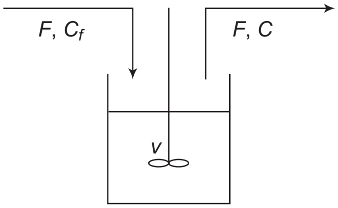


Fig. 3.14 Non-isothermal CSTR

The model equations for a non-isothermal CSTR (Fig. 3.14) can be written as:

$$\frac{VdC}{dt} = Q(C - C_f) - Vk_0C\ \exp\left[-\frac{E}{(RT)}\right] \tag{3.95}$$

$$V\left[(1-\phi)\rho c_p + \phi\rho c_p\right]\frac{dT'}{dt'} = -(\rho c_p Q)\ (T' - T_f) + (-\Delta H)Vk_rC\ \exp\left[-\frac{E}{(RT')}\right] \tag{3.96}$$

where, V is the volume of reactor, Q volumetric flow rate; C concentration in the reactor, T' Temperature in the reactor; k_r reaction rate constant; C_p specific heat capacity and $(-\Delta H)$ heat of reaction,

The non-dimensional form of these equations is given by (Finlayson, 2012):

$$\frac{dc}{dt} = (1-c) - c\ D_a\ \exp\left\{y\left[1-\left(\frac{1}{T}\right)\right]\right\} \tag{3.97}$$

$$L_e\frac{dT}{dt} = (1-T) + \beta D_a c\ \exp\left\{y\left[1-\left(\frac{1}{T}\right)\right]\right\} \tag{3.98}$$

where,
$$c = \frac{C}{C_f},\ T = \frac{T'}{T_f},\ t = \frac{Qt'}{V} \tag{3.99}$$

The dimensionless numbers are defined by:

$$D_a = \left(\frac{Vk_0}{Q}\right)\exp\left(-\frac{E}{RT'_f}\right) \tag{3.100}$$

$$Le = \frac{[\phi(\rho C_p)_f + (1-\phi)(\rho C_p)_f]}{(\rho C_p)_f} \text{ and } \gamma = \frac{E}{(RT'_f)},\ \beta = \frac{(\Delta H)c'_f}{[(\rho C_p)_f T_f]} \tag{3.101}$$

At steady state conditions, we have:

$$\left(\frac{Q}{V}\right)(1-c) = c\ D_a\ \exp\left\{\gamma\left[1-\left(\frac{1}{T}\right)\right]\right\} \tag{3.102}$$

$$\left(\frac{Q}{V}\right)(1-T) = -\beta\ D_a\ c\exp\left\{\gamma\left[1-\left(\frac{1}{T}\right)\right]\right\} \tag{3.103}$$

Multiplying the first equation by β and adding to it to the second equation we get:

$$\beta(1-c) + (1-T) = 0 \tag{3.104}$$

The equation is solved for T:

$$T = 1 + \beta(1-c) \tag{3.105}$$

Then, Eq. (3.102) can be simplified as:

$$\left(\frac{Q}{V}\right)(1-c) = c\ D_a\ \exp\left\{\gamma\left[1-\frac{1}{(1+\beta-\beta c)}\right]\right\} \tag{3.106}$$

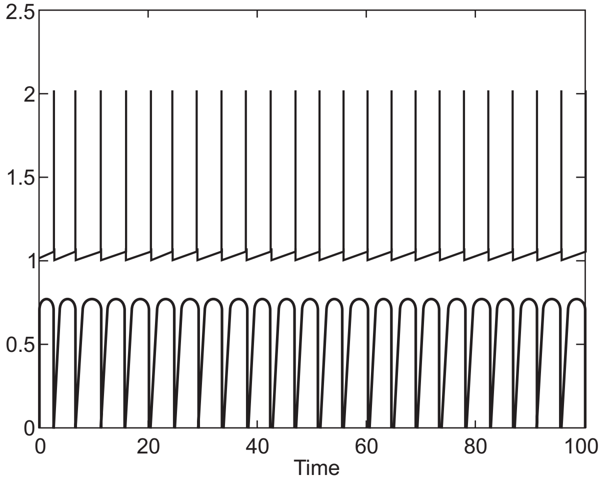


Fig. 3.15 Sustained oscillatory response of CSTR (c versus θ) (Finlayson, 2006)

For the values of $\left(\frac{Q}{V}\right) = 25$; $\beta = 0.25$ and $\gamma = 30$; the above equation is solved numerically (with different initial guess values of c varying from 0 to 1) or graphically for c. For these set of parameters, the numerical solution gives the following multiple solutions for c: 0.0863, 0.5577 and 0.9422. On substituting the values of c in Eq. (3.105), we get the corresponding values of T. To get the phase plot, we can solve the transient model equations with the different start up conditions. For the parameters values of $\beta = 0.15$, $\gamma = 30$, $L_e = 0.1$, $D_a = 0.115$, and $T_f = 1$, the numerical solution of the transient equations gives a sustained oscillation in c and θ as shown in Fig. 3.15.

3.12 THE BELOUSOV–ZHABOTINSKI (OSCILLATING) REACTION

Periodic chemical reaction such as the Belousov–Zhabotinski reaction provides a wonderful example of relaxation oscillations. The first experiment was conducted by the Russian biochemist Boris Belousov in the 1960s and the results were not confirmed until as late as 1968 by Zhabotinski. Consider the following recipe for a Belousov periodic chemical reaction:

Solution A: Malonic acid, 15.6 g/*L*

Solution B: Potassium bromate, 41.75 g/*L*, and potassium bromide, 0.006 g/*L*

Solution C: Cerium IV sulphate, 3.23 g/*L* in 6M sulfuric acid

Solution D: Ferroin indicator

Add 20 mL solution of A and 10 mL of solution B to a mixture of 10 mL of solution C and 1 mL of solution D. Stir continuously at room temperature. The mixture remains blue for about 10 minutes and then begins to oscillate blue-green-pink and back again with a periodic of approximately two minutes. The reactions are given by:

$BrO_3^- + Br^- \rightarrow HBrO_2 + HOBr$ rate = $k_1\,[BrO_3^-]\,[Br^-]$

$HBrO_2 + Br^- \rightarrow 2HOBr$ rate = $k_2\,[HBrO_2][Br^-]$

$BrO_3^- + HBrO_2 \rightarrow 2HBrO_2 + 2\,M_{OX}$ rate = $k_3[BrO_3^-]\,[HBrO_2]$

$2HBrO_2 \rightarrow BrO_3^- + HOBr$ rate = $k_4\,[HBrO_2]^2$

$OS + M_{OX} \rightarrow (1/2)\,CBr^-$ rate = $k_5\,[OS][M_{OX}]$ (3.107)

where OS represents all oxidizable organic species and *C* is kept constant. Note that in the third equation, species $HBrO_2$ is an auto catalyst (Product also one of the reactants). The model equations, for the well mixed reactor, are given by (Lynch, 2004):

$$\frac{dx}{dt} = k_1ay - k_2xy + k_3ax - 2k_4x^2 \tag{3.108}$$

$$\frac{dy}{dt} = -k_1ay - k_2xy + \left(\frac{1}{2}\right) \text{C}\, k_5bz \tag{3.109}$$

$$\frac{dz}{dt} = 2k_3ax - k_5bz \tag{3.110}$$

where $x = [HBrO_2]$; $y = [Br^-]$, and $z = [M_{OX}]$ (3.111) and a = [BrO_3^-], b= [OS] are assumed to be constant. By introducing the following variables X, Y, Z and τ,

$$X = \frac{(2k_4x)}{(k_5a)}; Y = \frac{(k_2y)}{(k_3a)}; Z = \frac{(k_5k_4bz)}{(k_3a)^2} \text{ and } t = k_5bt, \tag{3.112}$$

the above equations become:

$$\frac{dX}{dt} = \frac{[qY - XY + x(1-X)}{\varepsilon_1} \tag{3.113}$$

$$\frac{dY}{dt} = \frac{(-qY - XY + CZ)}{\varepsilon_2} \tag{3.114}$$

$$\frac{dZ}{dt} = X - Z \tag{3.115}$$

where
$$\varepsilon_1 = \frac{k_5b}{(k_3a)}; \varepsilon_2 = \frac{2k_5k_4b}{(k_2k_3a)}; q = \frac{2k_1k_4}{(k_2k_3)} \tag{3.116}$$

If we assume that $\varepsilon << 1$ so that $\frac{dY}{dX}$ is large unless the numerator ($-qX - XY + CZ$) is also small. Further at all times $Y = \frac{CZ}{(q+X)}$, so that bromide concentration Y = [Br^-] is in a steady state compared to X. In this way, three dimensional system of differential equations is reduced to a two-dimensional system of autonomous ODEs:

$$\varepsilon_1\frac{dX}{dt} = X(1-X) - \left[\frac{(X-q}{(X+q)}\right]CZ \tag{3.117}$$

$$\frac{dZ}{dt} = X - Z \tag{3.118}$$

For certain parameters values (for example, $\varepsilon_1 = 0.05$; $q = 0.01$ and $C = 1$) the above two equations show a limit cycle behaviour (sustained oscillation). Additional details can be found from Lynch (2004).

3.13 BREATHING MODEL

The arterial carbon dioxide level controls our rate of breathing. To develop a suitable model, the following assumptions are made: (i) production of carbon dioxide is at a constant arte (λ) due to metabolic activity and (ii) the removal of carbon dioxide from the blood stream is proportional to both the current carbon dioxide concentration and to the ventilation. Ventilation is defined as the volume of the gas exchanged by the lungs per unit time, is controlled by the carbon dioxide level in the blood. The carbon dioxide concentration is detected by receptors in the brain stem. There is a time lag due to the blood transport from the lungs to the heart and then back to the brain requires time. The modal equation is given by Mackey and Glass (1988) as:

$$\frac{dc}{dt} = \lambda - \alpha R_{\max}\, c\, R'_{(t-\theta)} \tag{3.119}$$

where R' is the rate of ventilation and it is given by the Hill function $[R'(t) = \frac{c^n}{(b^n + c^n)}$. $R_{\max}$, b, n and α are constants. Here $R_{(t-\theta)}$ means the value of R at $(t - \theta)$. Hence

$$R'_{(t-\theta)} = \frac{[c_{(t-\theta)}]^n}{[b + \{c_{(t-\theta)}\}^n]} \tag{3.120}$$

For the parameters values given by Keener and Sneyd (2009): $\lambda = 6$, $\alpha = 0.3$, $R_m = 0.1$, $b = 1$. $n = 3$ with the initial history of 1.2 and $\theta = 0.25$, the concentration of carbon dioxide versus time behaviour shows a sustained oscillation (Fig. 3.16).

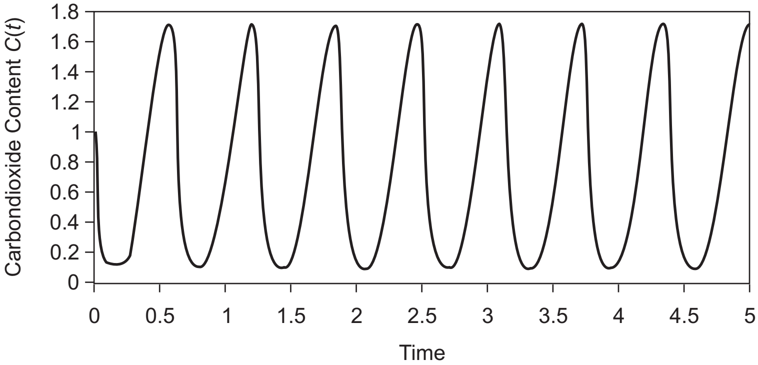


Fig. 3.16 The oscillatory behaviour of carbon dioxide content (Keener and Sneyd, 2009)

3.14 NONLINEAR PHENOMENA

There are 'essential nonlinear phenomena' that can take place only in the presence of nonlinearity; hence, they cannot be predicted by linear models. The following are the examples of essentially nonlinear phenomena (Khalil, 2015):

- Finite escape time: The state of an unstable linear system goes to a larger value (infinity) as time approaches larger values; a nonlinear system's state however can go to a larger value (infinity) in a finite time (Of course the model equations under these conditions may not continue to be valid).
- Multiple isolated equilibria: A linear system can have only one isolated equilibrium point; thus it can have only one steady-state operating point that attracts the state of the system irrespective of the initial state. A nonlinear system can have more than one isolated equilibrium point. The state may converge to one of the several steady-state operating points, depending on the initial state of the system.
- Limit cycles: For a linear time invariant system to oscillate, it must have a pair of eigenvalues on the imaginary axis, which is a non-robust condition that is almost impossible to maintain in the presence of perturbations. Even if we do, the amplitude of oscillation will be dependent on the initial state. In real life, a stable oscillation must be produced by nonlinear systems. There are nonlinear systems that can go into an oscillation of fixed amplitude and frequency, irrespective of the initial state. This type of oscillation is known as a limit cycle.

- Sub-harmonic, harmonic and almost-periodic oscillations: A stable linear system under a periodic input produces an output of the same frequency. A nonlinear system under periodic excitation can oscillate with frequencies that are submultiples or multiples of the input frequency. It may even generate an almost-periodic oscillation, an example is the sum of periodic oscillations with frequencies that are not multiples of each other.
- Chaos: A nonlinear system can have a more complicated steady-state behaviour that is not equilibrium, periodic oscillation, or almost–periodic oscillation. Such a behaviour is usually referred to as a chaos. Some of these chaotic motions exhibit randomness, despite the deterministic nature of the system.
- Multiple modes of behaviour: It is not unusual for the two or more modes of behaviour to be exhibited by the same nonlinear system. An unforced system may have more than one limit cycle. A forced system with periodic excitation may exhibit harmonic, sub-harmonic, or more complicated steady state behaviour, depending upon the amplitude and frequency of the input. It may even exhibit a discontinuous jump in the mode of behaviour as the amplitude or frequency of the excitation is smoothly changed.

The chaos indicates that (i) the underlying dynamics is deterministic (ii) no external noise has been introduced (iii) seemingly erratic behaviour of individual trajectories depends sensitivity on small changes of initial conditions (iv) in contrast to a single trajectory some global characteristics are obtained by averaging over many trajectories or over long time that do not depend on initial conditions and (v) when a parameter is tuned, the erratic state is reached via a sequence of events, including the appearance of one or more sub harmonics.

3.15 ONE ROUTE TO CHAOS: PERIOD DOUBLING

Systems which exhibit chaotic oscillations typically do so for some ranges of the relevant parameters but not for others, so one matter of obvious interest is how the chaos appears (or disappear) as one of the parameters is gradually varied. The Rossler equations are:

$$\frac{dx}{dt} = -y - z \tag{3.121}$$

$$\frac{dy}{dt} = x + 0.2y \tag{3.122}$$

$$\frac{dz}{dt} = 0.2 + (x - c)z \tag{3.123}$$

where c is a constant parameter. In contrast to the Lorenz equation, they have just one nonlinear term, namely xz in Eq. (3.123). The set of first order equations, Eqs. (3.121) – (3.123), are proposed by Otto Rossler in 1976. The equations provide a good example of a common route to chaos called period doubling. Let us start the system with $c = 2.5$. For a wide range of initial conditions, we end up eventually with the simple limit cycle oscillation shown in Fig. 3.17(a). If we then gradually increase c there are slow and unremarkable changes in the amplitude and period of oscillation until c increase beyond about 2.83. At this point, the path in the phase plane just fails to close up on itself after one circuit, and does so instead after two circles (Fig. 3.17b). By $c = 3.5$, this has become rather more pronounced (Fig. 3.17c), and at $c = 3.84$ the same happens again, leading to an oscillation pattern which only repeats itself after four cycles (Fig. 3.17d). After c is increased still further, the period doublings occur ever more frequently until $c = 4.2$, the oscillation pattern is chaotic, never exactly repeating itself.

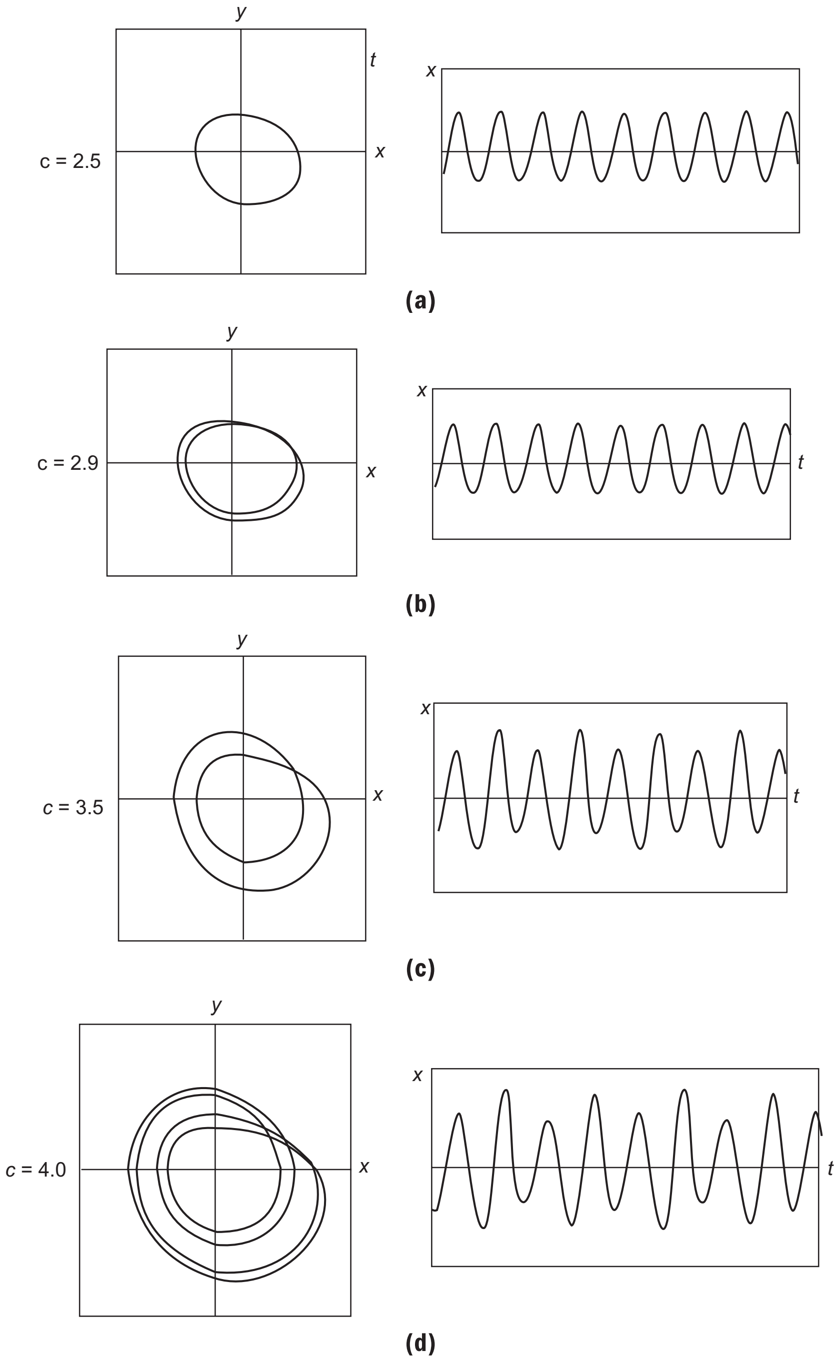


Fig. 3.17 A period doubling sequence for the Rossler equations (Acheson, 1997)

Review Problems

1. Find the stationary points and the local nature of the stationary points of:

$$\frac{dx_1}{dt} = 2x_1\left\{1 - \left[\frac{(x_1 + 3x_2)}{400}\right]\right\};\ \frac{dx_2}{dt} = x_2\left\{1 - \left[\frac{(3x_1 + x_2)}{400}\right]\right\}$$

2. Write down the model equations for transient conditions of a continuously well mixed bioreactor with substrate inhibition kinetics and show the system can have three multiple steady-states. Derive the transfer function model relating ΔX to ΔS_f in Laplace domain.
3. Write down the model equations for transient conditions of an adiabatic continuously stirred tank reactor (CSTR) with a first order kinetics and exothermic reaction and show for particular operating conditions the system can have three multiple steady-states.
4. What is Cholette's model for a non-ideal CSTR. Write down the relevant differential equations. Show that the system can have both the input and output multiplicity behaviour.
5. Write down the model equations for transient conditions of an adiabatic continuously stirred tank reactor (CSTR) with a first order kinetics and exothermic reaction and show for particular operating conditions the system can have three multiple steady-states.
6. Derive the model equation of a magnetic levitation system and show the system is unstable.
7. Develop a suitable model for weather forecasting.
8. Write down for the transient condition the mass balance equations of a CSTR for carrying out the Van de Vusse reaction.
9. Derive model equations for two competing species population model equation.
10. Derive the model equation for an epidemiological situation.
11. Write down the model equations of a non-isothermal CSTR for transient conditions.
12. Explain briefly the Belousov–Zhabotinski oscillating reaction. Write down the relevant ODEs.
13. Write down the relevant ODE for the breathing situation.
14. What are the characteristics of a chaos. With the example of Rossler equations, explain the development of chaos through double period up.
15. Chien [2000. *Biochemical Engg Journal.* 6. 51–17] has given a study on multiple steady states biochemical reactions under substrate and product inhibition. Prepare a report on the work .
16. Li and Li have reported the occurrence of isolas, mushrooms and other forms of multi-stability in isothermal bimolecular reacting systems (1989. *Chemical Engg Sci.* 44. 2995–3000). Read the paper and give a summary of the work reported on the complex behaviour of such an isothermal system.

4

Analytical Solutions of Model Equations

In this chapter, methods of solving analytically the linear, initial value problems in Ordinary Differential Equations (IVP ODEs), linear, boundary value ODEs (BVP ODEs) and linear Partial Differential equations (PDEs) are given.

4.1 HOMOGENEOUS ODES WITH CONSTANT COEFFICIENTS

In an ordinary differential equation (ODE), all the derivatives are with respect to a single independent variable. The order of the differential equation is the order of the highest derivative that appears in the equation. An nth order linear homogeneous constant coefficient ODE has the form:

$$a_0 \frac{d^n y}{dt^n} + a_1 \frac{d^{n-1} y}{dt^{n-1}} + \cdots + a_{n-1} \frac{dy}{dt} + a_n y = 0 \tag{4.1}$$

where, $a_0, \ldots, a_n$ are real constant coefficients. Note that the right side term is zero. In a physical system, a homogeneous ODE may represent the situation in which the dynamic system does not have any input or force applied to it and its response is due to some nonzero initial conditions.

The solution may be anticipated in the form $y = \exp(\gamma t)$ with appropriate values of γ. On substituting this solution in the differential equation we get:

$$(a_0\gamma^n + a_1\gamma^{n-1} + \ldots. + a_{n-1}\,\gamma + a_n)\exp(\gamma t) = 0 \tag{4.2}$$

i.e.,

$$(a_0\,\gamma^n + a_1\,\gamma^{n-1} + \ldots + a_{n-1}\,\gamma + a_n) = 0 \tag{4.3}$$

is called the characteristic equation of the above ODE (obtained by replacing $\frac{d^i y}{dt^i}$ by γ^i where $i = 1, 2, \ldots n$, in Eq. 4.1). A polynomial degree of n has n roots, say, $\gamma_1, \gamma_2, \ldots, \gamma_n$. The characteristic equation is represented in the form:

$$(\gamma - \gamma_1)(\gamma - \gamma_2)\ldots(\gamma - \gamma_n) = 0 \tag{4.4}$$

Solving the roots of characteristic equation (Eq. 4.3 can be solved analytically or numerically) gives $\gamma_1, \gamma_2, \ldots, \gamma_n$. If the roots area real and distinct, then the general solution can be written as:

$$y = c_1 \exp(\gamma_1 t) + c_2 \exp(\gamma_2 t) + \cdots + c_n \exp(\gamma_n t) \tag{4.5}$$

the constants $c_1, c_{2,}\ldots, c_n$ will be determined by using the n initial conditions of the ODE. The initial conditions are specified values of: $y(t = 0)$, $\frac{dy}{dt}$ $(t = 0)$, $\frac{d^2y}{dt_2}(t=0)$, … $\frac{d^{n-1}y}{dt^{n-1}}(t=0)$. Satisfying n initial conditions gives n linear algebraic equations with n unknown integration constants c_1, $c_2, \ldots, c_n$.

If the roots are complex conjugate ($\alpha \pm j\omega$) and non-repeating, and $(n - 2)$ real roots, then the general solution is given by:

$$y = c_1 \exp(\alpha t) \cos(\omega t) + c_2 \exp(\alpha t) \sin(\omega t) + c_3 \exp(\gamma_3 t) + \ldots + c_n \exp(\gamma_n t) \tag{4.6}$$

Repeated Real Roots

If a real root γ is repeated q times, then the corresponding solutions are written as

$$\exp(\gamma t),\ t \exp(\gamma t),\ t^2 \exp(\gamma t), \ldots.\ t^{q-1}\exp(\gamma t) \tag{4.7}$$

It can be verified by substituting the above solution in the ODE (Eq. 4.1).

Repeated Complex Roots

If the complex root ($\alpha \pm j\omega$) is repeated p times, then we have $2p$ solutions because the complex roots always appear as conjugate pairs (for characteristic equations with real coefficients). The solution can be written as

$$\exp(\alpha t) \cos(\omega t),\ t \exp(\alpha t) \cos(\omega t),\ t^2 \exp(\alpha t) \cos(\omega t), \ldots,\ t^p \exp(\alpha t) \cos(\omega t), \tag{4.8}$$

$$\exp(\alpha t) \sin(\omega t),\ t \exp(\alpha t) \sin(\omega t),\ t^2 \exp(\alpha t) \sin(\omega t), \ldots\ldots,\ t^p \exp(\alpha t) \sin(\omega t) \tag{4.9}$$

It can be shown that the above solutions satisfy the given ODE.

Example 1.1

Find the general solution of ODE:

$$\frac{d^2y}{dt^2} + 4\frac{dy}{dt} + 3y = 0 \tag{4.10}$$

The characteristic equation is given by

$$\gamma^2 + 4\gamma + 3 = 0 \tag{4.11}$$

The roots are: –1, –3.
The general solution is given by:

$$y = c_1 \exp(-t) + c_2 \exp(-3t) \tag{4.12}$$

If the initial conditions are given, then the integration constants can be obtained.

Example 1.2

$$\frac{d^2y}{dt^2} + 4\frac{dy}{dt} + 5y = 0 \tag{4.13}$$

The characteristic equation is given by

$$\gamma^2 + 4\gamma + 5 = 0 \tag{4.14}$$

the roots are: $-2 \pm j$.
The general solution is given by:

$$y(t) = c_1 \exp(2t) \cos(\omega t) + c_2 \exp(2t) \sin(\omega t) \tag{4.15}$$

Example 1.3

$$\frac{d^2 y}{dt^2} + 4\frac{dy}{dt} + 4y = 0 \tag{4.16}$$

The characteristic equation is given by

$$\gamma^2 + 4\gamma + 4 = 0$$

The roots are: $-2, -2$.
The general solution is given by:

$$y = c_1 \exp(-2t) + c_2\, t \exp(-2t) \tag{4.17}$$

Example 1.4

$$\frac{d^4 y}{dt^4} + 4\frac{d^2 y}{dt^2} + 4y = 0 \tag{4.18}$$

The characteristic equation is given by

$$\gamma^4 + 4\gamma^2 + 4 = 0 \tag{4.19}$$

i.e.,

$$(\gamma + i)^2 (\gamma - i)^2 = 0$$

The roots are: $i, i, -i, -i$
The general solution is given by

$$y(t) = c_1 \cos(t) + c_2\, t \cos(t) + c_3 \sin(t) + c_4\, t \sin(t) \tag{4.20}$$

4.2 NON-HOMOGENEOUS ODE WITH CONSTANT COEFFICIENTS

If the system is subjected to some input or forcing function $f(t)$, the system is given by:

$$a_0 \frac{d^n y}{dt^n} + a_1 \frac{d^{n-1}}{dt^{n-1}} + \cdots + a_{n-1}\frac{dy}{dt} + a_n y = f(t) \tag{4.21}$$

If the right side of the ODE, $f(t)$, is zero (0), then the resulting ODE is called the homogeneous equation. The general solution of the above equation is the sum of the solution of the homogeneous part of the ODE and a particular solution of the non-homogeneous ODE. Let the solution of the homogeneous part of the ODE be denoted by $y_h(t)$ and the particular solution by $y_p(t)$.

$$a_0 \frac{d^n y_h}{dt^n} + a_1 \frac{d^{n-1} y_h}{dt^{n-1}} + \cdots + a_{n-1}\frac{dy_h}{dt} + a_n y_h = 0 \tag{4.22}$$

$$a_0 \frac{d^n y_p}{dt^n} + a_1 \frac{d^{n-1} y_p}{dt^{n-1}} + \cdots + a_{n-1}\frac{dy_p}{dt} + a_n y_p = f(t) \tag{4.23}$$

Adding the two equations we get:

$$a_0 \frac{d^n (y_h + y_p)}{dt^n} + a_1 \frac{d^{n-1}(y_h + y_p)}{dt^{n-1}} + \cdots + a_{n-1} \frac{d(y_h + y_p)}{dt} + a_n (y_h + y_p) = f(t) \tag{4.24}$$

which proves that $$y(t) = y_h + y_p. \tag{4.25}$$

For a simple forcing function $f(t)$, it is sometimes possible to guess the form of the particular solution with a certain number of underdetermined coefficients that will make this candidate solution satisfy the non-homogeneous ODE. This method is called the method of under determined coefficients. Table 4.1 gives simple cases those are commonly encountered in practice.

Table 4.1 *Particular solution for simple forcing functions*

Se. No.	Forcing function	Particular solution $y_p(t)$ to try
1	constant	a
2	t	$at + b$
3	t^2	$at^2 + bt + c$
4	sin(wt)	a sin (wt) + b cos(wt)
5	exp(pt)	a exp(pt)

The total solution (general solution) is the sum of homogeneous solution and the particular solution. Then the integration constants are to be obtained by using the initial conditions.

4.2.1 Particular integrals: method of variation of parameters

Consider the general linear second-order equation (Jenson and Jeffreys,1997) :

$$\frac{d^2 y}{dx^2} + a_1(x)\left(\frac{dy}{dx}\right) + a_2(x)\, y = Q(x) \tag{4.26}$$

The coefficients a_1 and a_2 may be functions of x. It is assumed that the two functions, which form the complementary solution, are known:

$$Z = c_1 y_1 + c_2 y_2 \tag{4.27}$$

It is assumed that a particular integral of (4.26) is of the form

$$I = u\, y_1 + V\, y_2 \tag{4.28}$$

Here u and V are functions of x. Two equations are required to determine u and V. One equation results from the condition that Eq. (4.28) must satisfy Eq. (4.26). The second equation is arbitrary in the sense that it can be set by the analyst. However, the success of the method rests upon the procedure used to obtain the second equation. Differentiate Eq. (4.28) to obtain the condition to satisfy Eq. (4.26):

$$\frac{dI}{dt} = (uy_1' + vy_2') + \left(u' y_1 + V'\, y_2\right) \tag{4.29}$$

If we take the derivative of Eq. (4.29) and substitute it in Eq. (4.26), we introduce the second derivative of the unknown functions u and V. To avoids this requirement, we set

$$u_1' y_1 + V' y_2 = 0 \tag{4.30}$$

Equation (4.30) is the second conditions imposed on u and V. Equation (4.29) becomes:

$$\frac{dI}{dt} = (uy_1' + Vy_1') \tag{4.31}$$

The derivative of the above equation gives:

$$\frac{d^2I}{dx^2} = (uy_1'' + Vy_2'') + (u'\,y_1' + V'\,y_2') \tag{4.32}$$

When Eqs. (4.28), (4.30) and (4.31) are substituted in Eq. (4.26), we get:

$$u_1'y_1' + V'\,y_2' = Q(x) \tag{4.33}$$

Equation (4.30) and Eq. (4.33) are solved for u' and V', to get:

$$u' = \frac{du}{dx} = -\frac{y_2\,Q(x)}{(y_1y_2' - y_2y_1')} \tag{4.34}$$

$$V' = \frac{dV}{dx} = \frac{y_1Q(x)}{(y_1y_2' - y_2y_1')} \tag{4.35}$$

The functions y_1 and y_2 and $Q(x)$ are known. Hence, u and V are found by direct integration, and the particular integral can be obtained as:

$$I = uy_1 + V\,y_2 \tag{4.36}$$

4.3 APPLICATION OF LAPLACE TRANSFORM TO SOLVE A LINEAR PDE

The Laplace transform of $u(x, t)$, with respect to time, is defined as

$$L\,[u(x,t)] = \int \exp(-st)\,u(x,t)\,dt \tag{4.37}$$

$$= U(s, t)$$

The limit for the integration is from 0 to ∞. The transform U is a function not only of s but also of the untransformed variable, x.

$$L\left(\frac{\partial u}{\partial x}\right) = \frac{dU}{dx}$$

$$L\left(\frac{du}{dt}\right) = sU - u(x, 0)$$

$$L\left(\frac{\partial^2 u}{\partial t^2}\right) = s^2U - su(x, 0) - \left(\frac{\partial u}{\partial t}\right)_{t=0}$$

$$L\left(\frac{\partial^n u}{\partial t^n}\right) = s^nU - s^{n-1}u(x,0) - s^{n-2}\left(\frac{\partial u}{\partial t}\right)_{t=0} - s^{n-3}\left(\frac{\partial^2 u}{\partial t^2}\right)_{t=0} - \cdots - \left(\frac{\partial^{n-1} y}{\partial^{n-1}}\right)_{t=0} \tag{4.38}$$

The steps in applying the Laplace transformation to solve the PDE are given in Fig. 4.1 The PDE in $u(x, t)$ is transformed to ordinary differential equation in $u(x, s)$. Refer to Table 4.2 for Laplace transform of few functions.

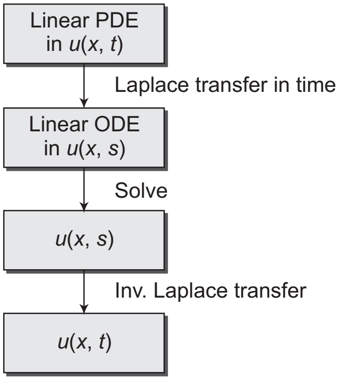


Fig. 4.1 Steps in solving a linear PDE by Laplace transform (Powers, 2005)

4.3.1 Important theorems

For a given U, Laplace transform of $u(t)$, the following theorems will be useful (without carrying out the Laplace inverse):

$$
\begin{aligned}
&u(t=0) = (sU)_{s\to\infty} && \text{(initial value theorem)} \\
&u(t=\infty) = (sU)_{s=0} && \text{(final value theorem)} \\
&L[u(t-L)] = \exp(-Ls)\,U && \text{(Laplace transform of delayed function)}
\end{aligned}
\tag{4.39}
$$

Table 4.2 *Laplace transform of some functions*

f(t)	F(s)
$\delta(t)$	1
t	$\frac{1}{s^2}$
t^n	$\frac{n!}{s^{n+1}}$
$\exp(-at)$	$1/(s+a)$
$t\exp(-at)$	$1/(s+a)^2$
$\sin(at)$	$\frac{a}{(s^2+a^2)}$
$\cos(at)$	$\frac{s}{(s^2+a^2)}$

4.3.2 Solution of linear ODE

Before we apply the Laplace transform method to solve a linear PDE, we apply the method for the solution of a constant coefficient linear ODE (Powers, 2005).

Example 1.5

Solve the following ODE by Laplace transform method.

$$y'' + y' - 12\,y = \exp(2t)$$

$$y(t = 0) = 3 \text{ and } y'\,(t = 0\,) = 0$$

By taking Laplace transformation of the above ODE, we get:

$$s^2Y - sy(t = 0) - y'\,(t = 0) + [sY - y(t = 0)] - 12Y = \left[\frac{1}{(s-2)}\right]$$

We get the solution for Y (in Laplace domain) as:

$$Y = \frac{(3s^2 - 3s - 5)}{[(s^2 + s - 12)(s - 2)]}$$

Now, we have to take the Laplace inverse to get the solution for $y(t)$. The Laplace inverse can be carried out by the partial fraction method. The roots of the denominator are $s = -4$, $s = 3$ and $s = 2$. Hence, we can write Y as:

$$Y = \frac{A_1}{(s+4)} + \frac{A_2}{(s-3)} + \frac{A_3}{(s-2)}$$

The values of A_1, A_2, A_3 can be obtained by multiplying both sides of the equations by the term $[(s^2 + s - 12)(s - 2)]$, and get the limiting values by substituting $s = -4$, $s = 3$ and $s = 2$, respectively, to get the values for A_1 , A_2 and A_3 as 1.309, 1.857 and (1/6).

Hence, the Laplace inverse for each term by term gives the solution as:

$$y(t) = 1.309 \exp(-4t) + 1.857 \exp(3t) + (1/6) \exp(2t)$$

Let us now apply the Laplace transformation method to a PDE (Powers, 2005):

Example 1.6

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} \tag{4.40}$$

$$u(0, t) = 1 \tag{4.41}$$

$$u(1, t) = 1 \tag{4.42}$$

$$u(x, 0) = 1 + \sin(\pi x) \tag{4.43}$$

The partial differential equation and the boundary conditions (that is, everything that is valid for $t > 0$) are converted in to Laplace domain as:

$$\frac{D^2U}{dx^2} = sU - [1 + \sin(\pi x)] \tag{4.44}$$

$$U(0, s) = 1/s; \tag{4.45a}$$

$$U(1, s) = 1/s \tag{4.45b}$$

The boundary value problem is solved to obtain

$$U(x, s) = \left(\frac{1}{s}\right) + \left[\frac{(\sin(\pi x))}{(s + \pi^2)}\right] \tag{4.46}$$

The Laplace inverse of Eq. (4.46) gives the solution as:

$$U(x, t) = 1 + [\sin(\pi x)] \exp(-\pi^2 t) \tag{4.47}$$

Example 1.7

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t} \tag{4.48}$$

$$u(0, t) = 1 \tag{4.49a}$$

$$u(1, t) = 1 \tag{4.49b}$$

$$u(x, 0) = 0 \tag{4.50}$$

The transformed problem is given by

$$\frac{d^2 U}{dx^2} = sU \tag{4.51}$$

$$U(0, s) = 1/s \tag{4.52}$$

$$U(1, s) = 1/s \tag{4.53}$$

The general solution of the differential equation is well known to be combination of $\sinh(\sqrt{s} \cdot x)$ and $\cosh(\sqrt{s} \cdot x)$. Application of the boundary conditions yields:

$$U(x, s) = (1/s)\ \cosh(\sqrt{s} \cdot x)\ + \left\{ \frac{\left[\{1 - \cosh(\sqrt{s})\} \{\sinh(\sqrt{s} \cdot x)\} \right]}{s \cdot \sinh(\sqrt{s})} \right\} \tag{4.54}$$

$$= \frac{\sinh(x\sqrt{s}) + \sinh[(1 - x)\sqrt{s}]}{s \cdot \sinh(\sqrt{s})} \tag{4.55}$$

This function rarely appears in a table of Laplace transforms. However, by extending the Heaviside formula, we can compute the inverse transform (Powers, 2005).

When U is the ratio of two transcendental functions (not polynomial) of s, we wish to write

$$U(x, s) = \sum A_k(x) \left[\frac{1}{(s - r_k)} \right] \tag{4.56}$$

In this formula, the numbers r_k are the values of s for which the denominator of U is zero or rather, for which mod $[U(x, s)]$ becomes infinite; and the A_k are functions of x but not s. From this form we expect to determine

$$U(x, t) = \sum A_k \exp(r_k t) \tag{4.57}$$

The convergence of the series solution should be checked.

The hyperbolic sine (also the cosh, cos, sin, and exponential functions) is not infinite for any finite value of its argument. Thus $U(x, s)$ becomes infinite only where s or $\sinh\sqrt{s}$ is zero. Since $\sinh\sqrt{s} = 0$ has no real root besides zero, we seek complex roots by setting $\sqrt{s} = \zeta + i\eta$ (where ζ and η are real).

The addition rules for hyperbolic and trigonometric functions remain valid for complex arguments. Furthermore, we know that

$$\cosh(iA) = \cos(A) \text{ and } \sinh(iA) = i\sin(A) \tag{4.58}$$

By combining the addition rule and the above identities we get:

$$\sinh(\zeta + i\eta) = \sinh\zeta\cos\eta + i\cosh\zeta\sin\eta \tag{4.59}$$

This function is zero only if both the real and imaginary parts are zero. Thus ζ and η must be chosen to satisfy simultaneously

$$\sinh(\zeta)\cos(\eta) = 0 \tag{4.60}$$

$$\cosh(\zeta)\sin(\eta) = 0 \tag{4.61}$$

Of the four possible combinations, only

$$\sinh(\zeta) = 0 \text{ and } \sin(\eta) = 0 \tag{4.62}$$

produce solutions.

Therefore $$\zeta = 0 \text{ and } \eta = \pm n\pi \; (n = 0, 1, 2, \ldots) \tag{4.63}$$

whence $$\sqrt{s} = \pm \text{ in } \pi \text{ and } s = -n^2\pi^2 \tag{4.64}$$

Recall that only the value of s, not the value of $\sqrt{s}$, is significant.

Finally then, we have located

$$r_0 = 0, \text{ and } r_k = -n^2\pi^2 \; (n = 1, 2, 3). \tag{4.65}$$

We proceed to find the $A_k(x)$ by the partial fraction method. The computations are carried out by piece meal and then the solution is assembled.

Part a ($r_0 = 0$). In order to find A_0, we multiply both sides of our proposal partial fractions development

$$U(x, s) = \sum\left[\frac{A_k(x)}{(s - r_k)}\right] \tag{4.66}$$

by $s - r_0 = s$, and take the limit as s approaches r_0. The index is from $k = 0$ to ∞. The right hand side goes to A_0. On the left we have,

$$\lim_{s\to 0} \frac{s\left[\{\sinh(\sqrt{s}\cdot x) + \sinh[\sqrt{s}\cdot(1-x)\}\right]}{[s\cdot\sinh\sqrt{s})} = 1 \tag{4.67}$$

Thus the part of $u(x, t)$ corresponding to $s = 0$ is 1 exp(0t) = 1, easily recognized as the steady state solution:

Part *b* ($r_0 = -n^2\pi^2$, $n = 1, 2, 3, \ldots$). For these cases, we find

$$A_n = \frac{q(r_0)}{p'(r_0)} \tag{4.68}$$

where q and p are the obvious choices. We take

$$\sqrt{r} = +\text{in}\pi \tag{4.69}$$

in all the calculations:

$$P'(s) = \sinh\sqrt{s}\ = s\ (0.5\sqrt{s})\cosh\sqrt{s} \qquad 4.70)$$

$$P'\,(r_0) = (0.5\ \text{in}\pi)\cosh(\text{in}\ \pi) \qquad (4.71)$$

$$= 0.5\ \text{in}\pi\cos(n\pi) \qquad (4.72)$$

$$Q(r_0) = \sinh(\text{in}\pi x) + \sinh[\text{in}\pi(1-x)] \qquad (4.73)$$

$$= i\ [\sin(n\pi x) + \sin[n\pi(1-x)] \qquad (4.74)$$

Hence the portion of $u(x, t)$ which arises from each r_0 is

$$A_n(x)\exp(r_0 t) = 2\ [\{\sin(n\pi x) + \sin[n\pi(1-x)\}]\ \exp(-n^2\pi^2 t)/[n\pi\cos(n\pi)] \qquad (4.75)$$

Part *c* On assembling the various pieces of the solution, we get:

$$U(x,t) = 1+\left(\frac{2}{\pi}\right)\sum\frac{[\{\sin(n\pi x)+\sin[n\pi(1-x)\}]\exp(-n^2\pi^2 t)}{[n\pi\cos(n\pi)]} \qquad (4.76)$$

The index for the summation index is from 1 to ∞.

The same solution can be derived by the method of separation of variables to be discussed in a later section.

4.4 SERIES SOLUTION OF VARIABLE COEFFICIENT LINEAR ODE

Example 1.8

We consider the variable coefficient ODE (Kaplan, 1962):

$$\left[2t^2D^2+(t^2-5t)D+(3+t)\right]x=0 \qquad (4.77)$$

Let $x = t^\alpha$ in the above differential equation. Then we get:

$$L[t^\alpha]=2t^2\alpha(\alpha-1)t^{\alpha-2}+(t^2-5t)\alpha t^{\alpha-1}+(3+t)t^\alpha \qquad (4.78)$$

$$=2(\alpha^2-7\alpha+3)t^\alpha+(\alpha+1)t^{\alpha+1} \qquad (4.79)$$

The identical equation is given by

$$2\alpha^2 - 7\alpha + 3 = 0 \qquad (4.80)$$

The roots are $$\alpha_1=\frac{1}{2},\alpha_2=3 \qquad (4.81)$$

We set $$x_1=t^{\frac{1}{2}}\sum_{\beta=0}^{\infty}c_\beta t^\beta \qquad (4.82)$$

in Eq. (4.77) and combine terms into one series, finding

$$\sum_{\beta=0}^{\infty}\left[c_\beta(2\beta^2-5\beta)+c_{\beta-1}\left(\beta+\frac{1}{2}\right)\right]t^\beta=0 \qquad (4.83)$$

Accordingly, $$c_\beta=\frac{2\beta+1}{2\beta(5-2\beta)}c_{\beta-1};(\beta=1,2,3,...). \qquad (4.84)$$

The coefficient c_0 is arbitrary. We choose $c_0 = 1$ and obtain the solution

$$x_1(t) = t^{\frac{1}{2}}\left[1 + \sum_{\beta=1}^{\infty} \frac{3.5...(2\beta+1)}{2^{\beta}\beta!3.1.(-1)(-3)...(5-2\beta)} t^{\beta}\right] \tag{4.85}$$

valid in particular for $t > 0$. Similarly, with $\alpha = 3$,

$$x_2(t) = t^3\left[1 + \sum_{\beta=1}^{\infty} \frac{(-1)^{\beta}(\beta+1)(\beta+2)(\beta+3)}{6[7.9...(2\beta+5)]} t^{\beta}\right] \tag{4.86}$$

for all t. The solutions are linearly independent and, for proper interpretation of $t^{\frac{1}{2}}$, are also valid for complex t ($t \neq 0$ for $x_1(t)$). Kaplan (1962) gives the details of the method.

4.4.1 Equations with coefficients asymptotic to constants

The systems problems leading to time-variant equations with regular singular points are rather rare. But other equations are reducible to such equations by appropriate substitutions.

Example 1.9

$$\left[2D^2 + (7 - e^{-t})D + (3 + e^{-t})\right]x = 0 \tag{4.87}$$

Here there is no singular point, and we can obtain power series solutions $\sum c_{\beta} t^{\beta}$ converging for all t. However, computing the solutions numerically from the series is effective only for small $|t|$ increases. Instead of using power series in the given equation, let $z = e^{-t}$.

Since

$$\frac{dx}{dt} = \frac{dx}{dz}\frac{dz}{dt} = -e^{-t}\frac{dx}{dz} = -z\frac{dx}{dz} \tag{4.88}$$

$$\frac{d^2x}{dt^2} = -z\frac{d}{dz}\left(-z\frac{dx}{dz}\right) = z^2\frac{d^2x}{dz^2} + z\frac{dx}{dz} \tag{4.89}$$

We obtain the equation

$$2\left(z^2\frac{d^2x}{dz^2} + z\frac{dx}{dz}\right) + (7 - z)\left(-z\frac{dx}{dz}\right) + (3 + z)x = 0 \tag{4.90}$$

that is,

$$2z^2\frac{d^2x}{dz^2} + (z^2 - 5z)\frac{dx}{dz} + (3 + z)x = 0 \tag{4.91}$$

This is the same as Eq. (4.77), except that t is replaced by z. Hence the functions $x_1(z)$, $x_2(z)$ obtained from Eq. (4.85) and Eq. (4.86) are linearly independent solutions for all z except zero. Finally, $x_1(e^{-t})$, $x_2(e^{-t})$ are solutions of the given equation in t, valid for *all* t (Since $e^{-t} \neq 0$):

$$x_1(t) = e^{-\frac{1}{2}t}\left[1 + \sum_{\beta=1}^{\infty} \frac{3.5...(2\beta+1)}{2^{\beta}\beta!3.1.(-1)(-3)...(5-2\beta)} t^{\beta}\right] \tag{4.92}$$

$$x_2(t) = e^{-3t}\left[1 + \sum_{\beta=1}^{\infty} \frac{(-1)^{\beta}(\beta+1)(\beta+2)(\beta+3)}{6[7.9...(2\beta+5)]} e^{-\beta t}\right] \tag{4.93}$$

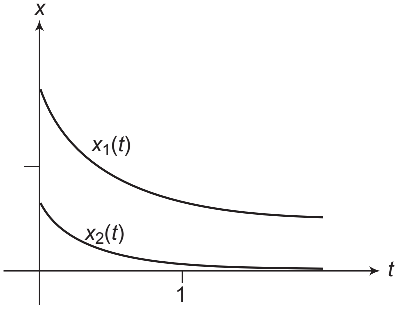


Fig. 4.2 Solution of the Eq. (4.87)

4.4.2 Summary of the series solution method

The differential equation

$$\frac{x^2 d^2 y}{dx^2} + x F(x)\frac{dy}{dx} + G(x)y = 0 \tag{4.94}$$

can be solved by substituting

$$y = \sum a_n x^{n+c} \ (a_0 \neq 0) \tag{4.95}$$

The summation is from 0 to ∞. If $F(x)$ and $G(x)$ can be expanded in a convergent series of non-negative powers of x for all mod(x) < R, the solution got will also be convergent for all mod(x) < R. Substitute Eq. (4.95) in Eq. (4.94). The indicial equation is found by equating the coefficient of the lowest power of x occurring in Eq. (4.94). The recurrence relation is found by equating coefficients of x^{c+r} in the same equation. If the two roots of the indicial equation are $c = c_1$ and $c_2 = c_1 + k$ and $k \geq 0$, then the following four cases arise.

Case (i) (k not an integer or not a zero): Two separate series of the form Eq. (4.95) are obtained, one for $c = c_1$ and the other for $c = c_2$. These two series added together with arbitrary constants give the complete solution.

Case (ii) (k is zero): Define the function $u(x, c)$ which satisfies the recurrence relation but not necessary the indicial equation. The solution then takes the form

$$y = Au(x, c_1) + B\,(\partial u/\partial c)_{c=c1}$$

Case (iiia) (k is an integer): Find the first recurrence relation in which a_j appears. When $c = c_1$, the coefficient of a_j will be zero, and if the rest of the equation is not zero. The solution takes the form

$$y = Au(x, c_2) + B\,\partial/\partial c\,[(c - c_1)\,u(x, c)\}]_{c=c1}$$

where, $u(x, c)$ satisfies the recurrence relation but not necessarily the indicial equation.

Case (iiib) (k is an integer): When $c = c_1$, the first recurrence relation in which a_k appears is identically zero leaving a_k indeterminate. The complete solution can be found in the form of equation (4.95) by substituting $c = c_1$ when a_0 and a_k will be the two arbitrary constants.

4.5 THE STURM–LIOUVILLE EQUATION

It describes any second order linear ordinary differential equation which can be written in the form (Jenson and Jeffreys, 1997):

$$d\,[p(x)\;dy/dx]\;/dx + [q(x) + \lambda\, r(x)]y = 0 \tag{4.96}$$

where λ is a constant, and p, q, and r are functions of x. It should be noted that the first and second order equation can always be combined into the form given in Eq. (4.96) by using an integrating factor as described earlier. For any particular set of functions p, q, and r, the solution of Eq. (4.96) for y will depend upon λ. Hence, if λ can take a set of discrete values λ_n, a corresponding set of solutions $y = \varphi_n(x)$ and $y = \varphi_m(x)$, then

$$(d/dx)\;[p(x)\;d\varphi_n/dx] + [q(x)+\lambda_n\; r(x)]\varphi_n = 0 \tag{4.97}$$

$$(d/dx)\;[p(x)\;d\varphi_m/dx] + [q(x)+\lambda_m\; r(x)]\;\varphi_m = 0 \tag{4.98}$$

Multiplying the first of these equation by φ_m, the second by φ_n, and subtracting the second equation from the first equation gives

$$\varphi_m\; d/dx[p(x)d\varphi_n/dx] - \varphi_n\; d/dx[p(x)d\varphi_m/dx]+(\lambda_n - \lambda_m]r(x)\;\varphi_n\;\varphi_m = 0 \tag{4.99}$$

Integrating the above equation with respect to x from a to b gives:

$$(\lambda_n - \lambda_m)\int r(x)\;\varphi_n\;\varphi_m\;dx = \int \varphi_n\,(d/dx)[p(x)d\varphi_m/dx]\;dx - \int \varphi_m\left(\frac{d}{dx}\right)\left[\frac{p(x)d\varphi_n}{dx}\right]dx \tag{4.100}$$

Evaluating the integrals on the right side of the above equation by parts and simplifying and combining to give:

$$(\lambda_n - \lambda_m)\int r(x)\;\varphi_n\;\varphi_m\;dx = \left[p(x)\left(\frac{\varphi_n d\varphi_m}{dx} - \frac{\varphi_m d\varphi_n}{dx}\right)\right]_a^b \tag{4.101}$$

Hence the functions φ_n and φ_m, which correspond to two different values (λ_n and λ_m) of the constant, will be orthogonal if the right side of the above equation is zero. There are three types of boundary conditions which are suitable for the orthogonality conditions:

1. At $x = a$, $y = 0$ (4.102a)

   Therefore, $\varphi_n = \varphi_m = 0$ (4.102b)

2. At $x = a$, $\dfrac{dy}{dx} = 0$ (4.103a)

   Therefore, $\dfrac{d\varphi_n}{dx} = \dfrac{d\varphi_m}{dx} = 0$ (4.103b)

3. At $x = a$, $\dfrac{dy}{dx} = \beta y$ (4.104a)

   Therefore, $\dfrac{d\varphi_n}{dx} = \beta\varphi_n$; $\dfrac{d\varphi_m}{dx} = \beta\varphi_m$ (4.104b)

Therefore, if both the boundary conditions are of the above three types (with duplication allowed), then the set of the function $\varphi(x)$ will be orthogonal with respect to the weighting function $r(x)$ which occurs in Eq. (4.96) in conjunction with λ.

4.6 METHOD OF SEPARATION OF VARIABLES

1. If the partial differential equation or a boundary condition or both are not homogeneous, first find a function $v(x)$, independent of t, which satisfy the partial differential equation and the boundary conditions. Since $v(x)$ does not depend on t, the partial differential equation applied to $v(x)$ to become an ordinary differential equation. Finding $v(x)$ is just a matter of solving the two point boundary value problem (Powers, 2005).
2. Determine the initial value boundary value problem satisfied by the' transient solution' $w(x, t) = u(x, t) - v(x)$. This must be a homogeneous problem. That is, the partial differential equation and the boundary conditions (but not usually the initial conditions) are satisfied by the constant function.
3. Assuming that $w(x, t) = \varphi(x)\, T(t)$, separate the partial differential equation into two ordinary differential equations, one for $\varphi(x)$ and one for $T(t)$, linked by the separate constant, $-\lambda^2$. Also reduce the boundary conditions to conditions on φ alone.
4. Solve the eigenvalue problem for φ. That is, find the values of λ^2 for which the eigenvalue problem has non-zero solutions. Label the eigen functions and the eigenvalues as $\varphi_n(x)$ and $\lambda_n^{\ 2}$.
5. Solve the ordinary differential equation for the time factors, $T_n(t)$.
6. Form the general solution of the homogeneous problem as a sum of constant multiples of the product solutions:
$$w(x, t) = \sum c_n \varphi_n(\mathrm{x}) T_n(x) \tag{4.105}$$
7. Choose the c_n so that the initial condition is satisfied. This may or may not be a routine Fourier series problem.
8. Form the solution of the original problem
$$w(x, t) = v(x) + w(x, t) \tag{4.106}$$
And check that all conditions are satisfied.

Example 1.10

The boundary conditions are usually specified either by u or by $\partial u/\partial x$. Now, we shall study a case where a condition of the third kind is involved. The physical model is conduction of heat in a rod with insulated lateral surface whose left end is held at constant temperature and whose right end is exposed to convective heat transfer. The boundary value-initial value problem satisfied by the temperature in the rod is given by Powers (2005).

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{k}\frac{\partial u}{\partial t},\ 0 < x < a,\ 0 < t \tag{4.107}$$

$$u(0,t) = T_0,\ 0 < t \tag{4.108}$$

$$-\kappa \frac{\partial u}{\partial x}(a,t) = h(u(a,t) - T_1),\ 0 < t \tag{4.109}$$

$$u(x,0) = f(x),\ 0 < x < a \tag{4.110}$$

The steady-state solution of this problem is found to be:

$$v(x) = T_0 + \frac{xh(T_1 - T_o)}{\kappa + ha}. \tag{4.111}$$

Now, since the original boundary conditions, Eq. (4.109), were non-homogeneous, we form the problem for the transient solution $w(x, t) = u(x, t) - v(x)$ By direct substitution in Eq. (4.107), we get

$$\frac{\partial^2 w}{\partial x^2} = \frac{1}{k}\frac{\partial w}{\partial t}, \qquad 0 < x < a, 0 < t \tag{4.112}$$

$$w(0,t) = 0,\ hw(a,t) + \kappa\frac{\partial w}{\partial x}(a,t) = 0,\ 0 < t \tag{4.113}$$

$$W(x, 0) = f(x) - v(x) = g(x) \quad 0 < x < a \tag{4.114}$$

The solution for $w(x, t)$ can now be found by the product method. On the assumption that w has the form of a product $\varphi(x)T(t)$ the variables can be separated exactly, giving two ordinary differential equation linked by a common parameter, λ^2:

$$\varphi'' + \lambda^2\varphi = 0 \quad 0 < x < a \tag{4.115}$$

$$T' + \lambda^2 kT = 0 \quad 0 < t. \tag{4.116}$$

Also, since the boundary conditions are linear and homogenous, they can be translated directly into conditions on φ:

$$W(0, t) = \varphi(0)T(t) = 0. \tag{4.117}$$

$$\kappa\frac{\partial w}{\partial x}(a,t) + hw(a,t) = [\kappa\varphi'(a) + h\varphi(a)]T(t) = 0 \tag{4.118}$$

Either $T(t)$ is identically zero (which would make $w(x, t)$ identically zero), or

$$\varphi(0) = 0 \qquad \kappa\varphi'(a) + h\varphi(a) = 0 \tag{4.119}$$

Combining the differential equation and boundary conditions on φ, we get the eigenvalue problem

$$\varphi'' + \lambda^2\varphi = 0 \quad 0 < x < a \tag{4.120}$$

$$\varphi(0) = 0 \quad \kappa\varphi'(a) + h\varphi(a) = 0. \tag{4.121}$$

The general solution of the differential equation is

$$\varphi(x) = a' \cos \lambda x + b' \sin \lambda x \tag{4.122}$$

The boundary condition at zero requires that $\varphi(0) = a' = 0$, (4.123)

leaving $\varphi(x) = b' \sin \lambda x$ Now, at the other boundary,

$$\kappa\varphi'(a) + h\varphi(a) = b'(\kappa\lambda\cos\lambda a + h\sin\lambda a) = 0. \tag{4.124}$$

Discarding the possibilities $b' = 0$ and $\lambda = 0$, which both lead to the trivial solution, we are left with the equation:

$$\kappa\lambda\cos\lambda a + h\sin\lambda a = 0,$$

or

$$\tan\lambda a = -\frac{\kappa}{h}\lambda \tag{4.125}$$

From sketches of the graphs of tan λa and $-\kappa\lambda/h$ (Fig.4.3), we see that there are an infinite number of solutions, $\lambda_1, \lambda_2, \lambda_3\ldots$ and that, for very large n, λ_n is given *approximately* by

$$\lambda_n \cong \frac{2n-1}{2}\frac{\pi}{a}. \tag{4.126}$$

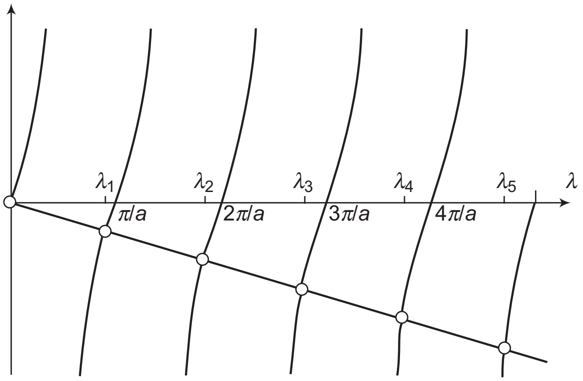


Fig. 4.3 Graphs of tan λa and $-\kappa\lambda/h$

(*Note:* Solutions are tabulated in *Handbook of Mathematical Functions* by Abramowitz and Stegun, 1965)

Thus we have for each $n = 1, 2, \ldots,$ an eigenvalue $\lambda^2{}_n$ and an eigenfunction $\varphi_n(x)$ which satisfies the eigenvalue problem Eqs. (4.115) and (4.116). Accompanying $\varphi_n(x)$ is the function

$$T_n(t) = \exp(-\lambda_n^2 kt) \tag{4.127}$$

that makes $w_n(x, t) = \varphi_n(x)T_n(t)$ a solution of the partial differential Eq. (4.112) and the boundary conditions Eq. (4.113). Since Eq. (4.112) and the conditions Eq. (4.113) are linear and homogeneous, any linear combination of solutions is a solution also. Therefore, the transient solution will have the form

$$w(x,t) = \sum_{1}^{\infty} b_n \sin(\lambda_n x)\exp(-\lambda_n^2 kt) \tag{4.128}$$

4.7 TYPES OF BOUNDARY CONDITIONS

The initial condition is described mathematically as:

$$u(x, 0) = f(x) \quad 0 < x < a \tag{4.129}$$

where, $f(x)$ is given function of x alone. In this way, the initial condition at every point of the system can be calculated.

The boundary conditions may take a variety of forms. First, the temperature at either end may be held constant, for instance, by exposing the end to an ice-water bath or to condensing them. We can describe such conditions by the equations

$$u(0, t) = T_0,\ u(a, t) = T_1,\ t > 0 \tag{4.130}$$

where T_0 and T_1 may be the same or different. More generally, the temperature at the boundary may be controlled in some way, without being held constant. If x_0 symbolizes an end point, the condition is:

$$u(x_0, t) = \alpha(t) \tag{4.131}$$

where α is a function of time. Of course, the case of a constant function is included here. This type of boundary condition is called **Dirichlet condition** or boundary condition of the first kind.

Another possibility is that the heat flow rate is controlled. Since the Fourier's law associates the heat flow rate and the gradient of the temperature, we can write

$$\left(\frac{\partial u}{\partial x}\right) \text{at } (x_0, t) \;= \beta(t) \tag{4.132}$$

where β is a function of time. This is called a **Neumann condition** or boundary condition of the second kind. Most frequently $\beta(t)$ to be identically zero:

$$\left(\frac{\partial u}{\partial x}\right) \text{at } (x_0, t) = 0 \tag{4.133}$$

corresponds to an insulated surface, for this equation, the heat flow is zero,
Another possible boundary condition is given by:

$$C_1\, u(x_0, t) + C_2\left(\frac{\partial u}{\partial x}\right) \text{at } (x_0, t) = g(t) \tag{4.134}$$

It is called the third kind or a **Robin condition.** This condition can also be realized physically. If the surface at $x = a$ is exposed to air or other fluid, then the heat conducted up to that surface from inside the rod is carried away by convection. Newton's law of cooling says that the rate at which heat is transferred from the body to the fluid is proportional to the difference in temperature between the body and the fluid. We have:

$$q(a, t) = h[u(a, t) - T(t)] \tag{4.135}$$

where $T(t)$ is the air temperature. After application of Fourier's law, this becomes

$$-k\left(\frac{\partial u}{\partial x}\right) \text{at } (a, t) = ku(a, t) - hT(t) \tag{4.136}$$

This equation is can be put in to the form of Eq. (4.134).

All of the boundary conditions given above involve the function u and / or its derivative at one point. If more than one point is involved, the boundary condition is called mixed. For example, if a uniform rod is bent into a ring and the ends $x = 0$ and $x = a$ are joined, appropriate boundary conditions would be:

$$u(0, t) = u(a, t) \text{ for } t > 0 \tag{4.137}$$

$$\left(\frac{\partial u}{\partial x}\right) \text{at } (0, t) = \left(\frac{\partial u}{\partial x}\right) \text{at } (a,\; t) \tag{4.138}$$

both of mixed type. An important feature common to all four types is that they involve a linear operation on the function u.

Review Problems

1. Find the homogeneous and particular integral $y_h(t)$ and $y_P(t)$ and hence y_{total} for a step change in u(t) of the system: $9(d^2y/dt^2) + 10\,(dy/dt) + y(t) = 2\,u(t)$ at $t = 0$, $y = 0$ and $y' = 0$.
2. By the Laplace transform method, find the solution y(t) for the problem given in P(1).

3. Solve the PDE by Laplace transform method:

$$\left(\frac{\partial^2 u}{\partial x^2}\right) = \left(\frac{\partial^2 u}{\partial t^2}\right) \quad 0 < x < 1, 0 < t$$

$u(0, t) = 0, u(1, t) = 0$

$u(x, 0) = \sin(\pi x)$; $\dfrac{\partial u}{\partial t}$ at $(x, 0) = -\sin(\pi x)$

4. Get the analytical solution for the semi-infinite domain problem: $\partial c/\partial t = \alpha\, \partial^2 c/\partial x^2$ with the IC and BCs as: $c(x,0) = 0$; $c(0, t) = c_s$; $c(\infty, t) = 0$.
5. Get the analytical solution of the linear PDE by the variable separable method

   $\partial c/\partial t = \alpha\, \partial^2 c/\partial x^2$ with the IC and BCs as: $c(x, 0) = 0$; $c(0, t) = 1$; $c(1, t) = 1$
6. Get the analytical solution of the linear PDE by Laplace transformation method followed by inversion by method of residues: $\partial c/\partial t = \alpha\, \partial^2 c/\partial x^2$ with the IC and BCs as: $c(x, 0) = 0$; $c(0, t) = 1$; $c(1, t) = 1$.
7. Solve the following variable coefficient equation by converting in to a standard form where the coefficient will be a polynomial in the independent variable: $[3D^2 + (3 - e^{-t})D + 2te^{-2t}]x = 0$.

5

Numerical Solutions of Model Equations

In this chapter, some of the numerical methods of solving nonlinear algebraic equations, nonlinear IVP ODEs, Nonlinear BVP ODEs and Nonlinear PDEs are reviewed.

5.1 NEWTON–RAPHSON (NR) METHOD

5.1.1 Scalar equation

The method is required for the numerical solution of a nonlinear algebraic equation

$$f(x) = 0 \tag{5.1}$$

Taylor's series of $f(x_{\mathrm{i}+1})$ around a value of x_i gives:

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \text{higher order derivatives terms} \tag{5.2}$$

By neglecting the second and higher order derivatives and letting $f(x_{i+1}) = 0$, we get the iteration equation as:

$$x_{i+1} = x_i - \left[\frac{f(x_i)}{f'(x_i)}\right] \tag{5.3}$$

Substituting the value of x_{i+1} in the left side of Eq. (5.3), we get the value of x_{i+2} The iterative process is to be continued till convergence is achieved.

The steps involved are:

Assume an initial guess of x_i;

Calculate x_{i+1} by Eq. (5.3).

We need to check the following stopping conditions:

1. Abs[$f(x_{i+1})$] ≤ given value, (say 10^{-2})
2. check abs($x_{i+1} - x_i$) ≤ abs(x_i 10^{-3})
3. or check the iteration not to exceed the maximum iteration ($N_{\max}$, say 100)

If stopping conditions (1) or (2) not met, iterate again. If the stopping condition (1) is to be given importance, then make the second condition stringent (small value, use x_i 10^{-5} than x_i 10^{-3}).

5.1.2 Multivariable equations

Consider the N simultaneous nonlinear algebraic equations:

$$f_1(x_1, x_2, \ldots x_{\mathrm{n}}) = 0$$

$$f_2(x_1, x_2, \ldots x_n) = 0$$

$$\ldots\ldots\ldots\ldots\ldots\ldots$$

$$f_N(x_1, x_2, \ldots x_n) = 0 \tag{5.4}$$

We can write the iteration equations, by the Newton–Raphson method, in vector form as:

$$X_{i+1} = X_i - J^{-1}(X_i)\, F(X_i) \tag{5.5}$$

where,
$$J = \left[\frac{\partial^2 f_i}{\partial x_i \partial x_j}\right]_{ij} \tag{5.6a}$$

$$F(X_i) = [f_1(X_i)\, f_2\, f_3 \ldots f_N]^T \tag{5.6b}$$

stopping conditions

1. for each f_{i}, check abs[$f(x_{i+1})$] ≤ given value, (say 10^{-3})
2. (or) check for each x: abs($x_{i+1} - x_i$) ≤ abs(x_i 10^{-3})
3. or check the iteration not to exceed the given maximum iteration (say, $N_{\max} = N * 100$)

If stopping condition (1) or (2) is not met with, the let X_i is replaced by X_{i+1} from Eq. (5.5) and then get the next improved value from

$$X_{i+1} = X_i - J^{-1}(X_i)\, F(X_i) \tag{5.7}$$

Repeat the above step till the stopping condition (1) or (2) is met. If the stopping condition is met, then X is the solution vector.

Example 5.1

Find x by the NR numerical method for the equation:

$$x = e^{-x} \tag{5.8}$$

Let
$$f(x) \Rightarrow xe^x - 1 = 0 \tag{5.9}$$

$$F'(x) = e^x + xe^x \tag{5.10a}$$

$$= (1 + x)\, e^x \tag{5.10b}$$

The NR iteration:

$$x_{i+1} = x_i - \left[\frac{f(x_i)}{f'(x_i)}\right] \tag{5.11}$$

$$= x_i - \frac{[x_i \exp(x_i)]}{[(1+x)\exp(x_i)]} \tag{5.12}$$

Every time update x_i by the latest value of x_i and use the above iterative equation to get the next improved x_{i+1}.

Let $$x_0 = 1.0 \tag{5.13}$$

Using Eq. (5.12), we get for various iterations:

$i = 1$: $$x_1 = 0.6839397 \tag{5.14a}$$

$i = 2$: $$x_2 = 0.5674545 \tag{5.14b}$$

$i = 3$: $$x_3 = 0.56714 \tag{5.14c}$$

Within 3 iterations, a good convergence is achieved

Example 5.2

By NR method, obtain the solution for the following simultaneous nonlinear algebraic equations.

$$f_1(x_1, x_2, x_3) = 0 \Rightarrow -0.5\, x_1 + \left(\frac{1}{3}\right)(x_2^{\,3} + x_3^{\,3}) + 0.3 = 0 \tag{5.15a}$$

$$f_2(x_1, x_2, x_3) = 0 \Rightarrow 0.5\, x_1 x_2 - 0.5\, x_2 + 0.2 x_3^{\,5} = 0 \tag{5.15b}$$

$$f_3(x_1, x_2, x_3) = 0 \Rightarrow \left(\frac{1}{3}\right)x_2^3 - \left(\frac{1}{4}\right)x_3 + 0.04 = 0 \tag{5.15c}$$

The Jacobian matrix Eq. (5.5) is obtained as:

$$J(X) = \begin{bmatrix} -0.5 & x_2^2 & x_3^2 \\ 0.5x_2 & 0.5(x_1 - 1) & x_3^4 \\ 0 & x_2^2 & -0.25 \end{bmatrix} \tag{5.16}$$

The iteration equations are

$$X_{i+1} = X_i - J^{-1}(X_i)\, F(X_i) \tag{5.17}$$

With the initial guess $$X_0 = [0\ 0\ 0]^T \tag{5.18}$$

The NR iteration steps are now executed. The results for 4 iterations are given below:

$i = 1$, $X = [0.60\ 0\ 0.16]^T$

$i = 2$, $X = [0.6027307\ 0.0001049\ 0.16]^T$

$i = 3$, $X = [0.6027307\ 0.0001056\ 0.16]^T$

$i = 4$, $$\text{X} = [0.6027307\ 0.0001056\ 0.16]^T \tag{5.19}$$

5.2 RUNGE–KUTTA (RK) METHODS FOR IVP ODES

Consider the scalar initial value nonlinear ODE.

$$\frac{dy}{dt} = f(y, t)$$

At $t = 0,\ y = y_0$

The numerical solution for y at various time intervals is required.

The Taylor series representation forms the basis of several methods for solving differential equations, including the Runge–Kutta methods (Palm, 1985). The Taylor series may be used to represent the solution $y(t + \Delta t)$ in terms of $y(t)$ and its derivatives as follows.

$$y(t+\Delta t) = y(t) + \Delta t y'(t) + \frac{1}{2}(\Delta t)^2 y''(t) + \frac{1}{6}(\Delta t)^3\, y'''(t) + \ldots \tag{5.20}$$

The required derivatives are calculated from the differential equation.

5.2.1 Development of second-order algorithm

We now demonstrate the development of the Runge–Kutta algorithms for the second-order case. For notational compactness, we replace the step size Δt with h. Thus, $t_{k+1} = t_k + h$. Also, let the subscript k denotes evaluation at time t_k. Truncating Eq. (5.20) beyond the second-order term gives

$$\begin{aligned} y_{k+1} &= y_k + hy_k' + \frac{1}{2}h^2 y_k'' \\ &= y_k + hf_k + \frac{1}{2}h^2\left(\frac{df}{dt}\right)_k \end{aligned} \tag{5.21}$$

But,

$$\begin{aligned} \frac{df}{dt} &= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y}\frac{dy}{dt} \\ &= \frac{\partial f}{\partial t} + \frac{\partial f}{\partial y} f \end{aligned} \tag{5.22}$$

In simpler notation, f_y denotes $\frac{\partial f}{\partial y}$, and f_t denotes $\frac{\partial f}{\partial t}$. Thus,

$$\frac{df}{dt} = f_t + f_y f \tag{5.23}$$

and

$$y_{k+1} = y_k + hf_k + \frac{1}{2}h^2 (f_t + f_y f)_k \qquad 5.24)$$

The second-order Runge–Kutta methods express y_{k+1} as

$$y_{k+1} = y_k + w_1 g_1 + w_2 g_2 \tag{5.25}$$

where, w_1 and w_2 are constant weighting factors, and

$$\begin{aligned} g_1 &= hf(t_k, y_k) \\ g_2 &= hf(t_k + \alpha h, y_k + \beta h f_k) \end{aligned} \tag{5.26}$$

for constant α and β. We now compare Eq. (5.25) with Eq. (5.26). First, expand f in g_2 in a two-variable Tayler series.

$$g_2 = h[f_k + (f_t)_k \alpha h + (f_y)_k \beta h f_k + \ldots] \tag{5.27}$$

where the omitted terms are of the order of h^2. Substituting this and g_1 into Eq. (5.25) and collecting terms give

$$y_{k+1} = y_k + h\left[w_1 f + w_2 f\right]_k + h^2\left[w_1 \alpha f_t + w_2 \beta f f_y\right]_k \tag{5.28}$$

Comparison with Eq. (5.24) for like powers of h shows that

$$\begin{aligned} w_1 + w_2 &= 1 \\ w_1 \alpha &= \frac{1}{2} \\ w_2 \beta &= \frac{1}{2} \end{aligned} \tag{5.29}$$

Thus, the family of second-order Runge–Kutta algorithms is characterized by the parameters (α, β, w_1, w_2), one of which can be chosen independently. The choice $\alpha = 2/3$ minimizes the truncation error term (Ralston, 1965). For $\alpha = 1$, the Runge–Kutta algorithm (Eq. 5.25 and Eq. 5.26) corresponds to the trapezoidal integration rule if f is a function of only t, and is the same as the predictor–corrector algorithm for a general $f(y, t)$.

5.2.2 Fourth-order algorithms

Second- and third-order Runge–Kutta algorithms have found extensive applications in the past. However, the fourth-order algorithm is now the most commonly used. Its derivation follows the same pattern as earlier, with all terms up to h^4 retained. The algebra required is extensive and is given by Hornbeck (1975). Here, we present the results. The algorithm is

$$y_{k+1} = y_k + w_1 g_1 + w_2 g_2 + w_3 g_3 + w_4 g_4 \tag{5.30}$$

$$\begin{aligned} g_1 &= hf[t_k, y_k] \\ g_2 &= hf[t_k + \alpha_1 h, y_k + \alpha_1 g_1] \\ g_3 &= hf[t_k + \alpha_2 h, y_k + \beta_2 g_2 + (\alpha_2 - \beta_2) g_1] \\ g_4 &= hf[t_k + \alpha_3 h, y_k + \beta_3 g_2 + \gamma_3 g_3 + (\alpha_3 - \beta_3 - \gamma_3) g_1] \end{aligned} \tag{5.31}$$

Comparison with the Taylor series yields eight equations for the ten parameters. Thus, two parameters can be chosen in light of other considerations. Three common choices are as follows (Palm, 1985).

1. Gill's Method

This choice minimizes the number of memory locations required to implement the algorithm and thus is well suited for programmable calculators.

$$\begin{aligned} &w_1 = w_4 = 1/6 && \alpha_1 = \alpha_2 = 1/2 && \alpha_3 = 1 \\ &w_2 = \left(1 - \frac{1}{\sqrt{2}}\right)\Big/3 && \beta_2 = 1 - \frac{1}{\sqrt{2}} && \beta_3 = -\frac{1}{\sqrt{2}} \\ &w_3 = \left(1 + \frac{1}{\sqrt{2}}\right)\Big/3 && \gamma_3 = 1 + \frac{1}{\sqrt{2}} && \end{aligned} \tag{5.32a}$$

2. Ralston's Method

This choice minimizes a bound on the truncation error.

$$w_1 = 0.17476028 \qquad w_2 = -0.55148066 \qquad w_3 = 1.20553560$$

$$w_4 = 0.17118478 \qquad \alpha_1 = 0.4 \qquad \alpha_2 = 0.45573725 \qquad \alpha_3 = 1$$

$$\beta_2 = 0.15875964 \qquad \beta_3 = -3.05096516 \qquad \gamma_3 = 3.83286476 \tag{5.32b}$$

3. Classical Method

$$w_1 = w_4 = 1/6 \qquad w_2 = w_3 = 1/3 \qquad \alpha_1 = \alpha_2 = 1/2 \qquad \alpha_3 = \gamma_3 = 1$$

$$\beta_2 = 1/2 \qquad \beta_3 = 0 \tag{5.32c}$$

For multivariable ODEs:

$$\frac{dy}{dt} = F(y, t) \text{ at } t = 0;\ y = y_0 \tag{5.33}$$

where y and F are vectors. By the classic RK method, we have:

$$y_{K+1} = y_k + (1/6)\,[g_1 + 2g_2 + 2g_3 + g_4] \tag{5.34}$$

where

$$g_1 = h\,F(y_k, t_k)$$

$$g_2 = h\,F(y_k + 0.5\,h, t_k + 0.5\,g_1)$$

$$g_3 = h\,F(y_k + 0.5\,h, t_k + 0.5\,g_2)$$

$$g_4 = h\,F(y_k + h, t_k + g_3)$$

where, g_1, g_2, g_3 and g_4 are vectors.

The numerical method should satisfy the convergence criterion and the stability criterion. The convergence criterion deals with the approach of the approximate numerical solution as the number of increments employed become infinite in number. The stability criterion deals with the growth of errors introduced in the calculation. A finite number of increments must be used and only finite number of significant figures can be carried out in the computations.

5.2.3 The Runge–Kutta method

From the preceding discussion, it should be clear that numerical methods developed, for first-order models, can be easily applied to higher models if they are in the state variable form. This is because the state variable form consists of a series of coupled first-order equations. The Runge–Kutta method given by Eq. (5.30) and Eq. (5.31) can be extended in this manner. First, all the g_1, terms for every state equation are evaluated with Eq. (5.30) using the same numerical values for h, α_i, β_i, and γ_i. After this is done, then all the updated values of the $y_i(t_{k+1})$ are calculated from Eq. (5.30). Care must be taken to observe the proper time indexing and update the state variables for time t_{k+1} only after *all* of the intermediate calculations have been made.

5.2.4 Conversion to state variable form

There are several ways of converting an ODE model to a state variable form. If the variables representing the energy storage in the system are chosen as the state variable, the model must then be manipulated algebraically to produce the standard state variable form. The required algebra is not always obvious. However, we note here that the model

$$\frac{d^n y}{dt^n} = f\left[t, y, \frac{dy}{dt}, \ldots, \frac{d^{n-1}y}{dt^{n-1}}, v(t)\right] \tag{5.35}$$

The initial conditions are:

At $t = 0,\ y = a_1;\ \frac{dy}{dt} = a_2;\ \ldots\ldots,\ \frac{dy^{n-1}}{dt^{n-1}} = a_n$

The input $v(t)$ can always be put into state variable form by the following choice of state variables:

$$\begin{aligned} x_1 &= y \\ x_2 &= \frac{dy}{dt} \\ &. \\ &. \\ &. \\ x_n &= \frac{d^{n-1}y}{dt^{n-1}} \end{aligned} \tag{5.36}$$

By differentiating Eq. (5.36), the resulting state model is obtained as:

$$\begin{aligned} x_1' &= x_2 \\ x_2' &= x_3 \\ &. \\ &. \\ &. \\ {x_{n-1}}' &= x_n \\ x_n' &= f\left[t, x_1, x_2, \ldots, x_n, v(t)\right] \end{aligned} \tag{5.37}$$

a$t = 0;\ x_1 = a_1;\ x_2 = a_2;\ x_3 = ..;\ x_n = a_n$

5.2.5 Coupled higher order models

Equation (5.37) is somewhat general in that it can be nonlinear, but it does not cover all cases. For example, consider the coupled higher order model.

$$\begin{aligned} y'' &= f_1(t, y, y', z, z') \\ z'' &= f_2(t, y, y', z, z') \end{aligned} \tag{5.38}$$

They have the appropriate initial conditions. Choose the state variables as

$$\begin{aligned} x_1 &= y \\ x_2 &= y' \\ x_3 &= z \\ x_4 &= z' \end{aligned} \tag{5.39}$$

By differentiating Eq. (5.39) we get state variable model as:

$$\begin{aligned} x_1' &= x_2 \\ x_2' &= f_1(t, x_1, x_2, x_3, x_4) \\ x_3' &= x_4 \\ x_4' &= f_2(t, x_1, x_2, x_3, x_4) \end{aligned} \tag{5.40}$$

5.2.6 Runge–Kutta implicit method

We have $$y_{i+1} = y_i + \sum w_j k_j \tag{5.41}$$

where $$k_i = hf[t_i + b_j h, y_i + \sum a_{jl} k_l] \tag{5.42}$$

The summation is from $j = 1$ to v. Here i is the step counter and h is step size. When $a_{jl} = 0$ for $l \geq j$, j are calculated in sequences, $j = 1, \ldots, m$, and the method is termed explicit. When $a_{jl} = 0$ for $l > j$, but $a_{jj} \neq 0$, k_j appear on both the sides of the above equation, the method is termed semi-implicit. Finally, when $a_{jl} \neq 0$ for some $l > j$, k_j are determined by solution of nonlinear equations and the method is termed implicit.

Hence, computation time per step, for the same v, is the least for explicit methods and the most for implicit methods. However, implicit methods give the highest accuracy, with local truncation errors equivalent to those of a $r = 2v$ degree Taylor series approximation. Explicit methods give lowest accuracy, with errors equivalent to a $r = v$ degree approximation.

A system of ODEs is stiff if the local Jacobian contains at least one eigenvalue that does not contribute significantly over the most of the domain of interest. This occurs when $[\mathrm{Re}(\lambda_{\max})]/\mathrm{Re}[\mathrm{abs}(\lambda_{\min})]$ is large. This ratio is called stiffness ratio and when this value is ≥ 100, the system is stiff. For solving stiff ODEs, we need to use predictor–corrector methods proposed by Gear (1971).

5.2.7 Predictor–corrector method

The single step numerical method needs only the information from one previous point for computing the successive point. For example to generate (t_{k+1}, x_{k+1}), the initial point (t_0, x_0) should be known. Let us discuss the multistep methods. At the starting, the four step approach requires total four initial points, namely (t_0, x_0), (t_1, x_1), (t_2, x_2) and (t_3, x_3) to compute the next points $[(t_{k1}. X_{k+1})$ for $k \geq 3$. The multi-step algorithm is developed based on the fundamental theorem of calculus:

$$x_{k+1} = x_k + \int f[t, x(t)]\, dt, \text{ the integration is from } t_k \text{ to } t_{k+1}.$$

One needs to integrate over a finite step using a simple interpolating polynomial approximation for $f(t, x)$ over the interval.

Adams–Bashforth method (prediction step)

Under this step, we need to fit a cubic polynomial to the function $f(t, x)$ through the points $(t_{k-3,} f_{k-3})$, $(t_{k-2,} f_{k-2})$, (t_{k-1}, f_{k-1}), (t_k, f_k). The function is then integrated over the interval t_k to t_{k+1} and the Adams–Bashforth predictor is obtained as:

$$P_{k+1} = x_k + \left(\frac{\Delta t}{24}\right) [55f_k - 59\,f_{k-1} + 37\,f_{k-2} - 9\,f_{k-3}] \tag{5.43}$$

Adams–Moulton method (corrector method)

By the same way, the corrector is developed. A second order polynomial for $f(t, k)$ is constructed based on the points (t_{k-2}, f_{k-2}), (t_{k-1}, f_{k-1}), (t_k, f_k) are the new point (t_{k+1}, f_{k+1}), where $f_{k+1} = f(t_{k+1}, P_{k+1})$. Integrating over t_k to t_{K+1}, the Adams–Moulton corrector is obtained as:

$$x_{k+1} = x_k = \left(\frac{\Delta t}{24}\right) (9f_{k+1} + 19f_k - 5f_{k-1} + f_{k-2}) \tag{5.44}$$

As mentioned, the Adams–Moulton method requires four initial points in advance. Typically, for an initial value problem, x_0 is only given and t_0 is obviously zero. In this multistep method, three additional starting values, $x_{1,}$ x_2, and x_3 are usually computed using the Runge–Kutta approach. The Adams-Bashforth-Moulton algorithm is of fourth order. This method is faster than the fourth-order Runge–Kutta approach since only two new functional evaluations are involved in each step. However, this algorithm is not self-starting and, therefore, the RK method is needed to initiate this multi-step approach. (i) We use RK method to determine x_1, x_2, x_3 (x_0 is known), (ii) calculate P_{k+1} using the above equation and estimate $f_{k+1} = f(t_{k+1}, P_{k+1})$, and (iii) to compute x_{k+1} using the above equation. Next, increment the t interval and repeat the above steps.

5.3 SOLUTION OF SECOND-ORDER NONLINEAR BVP ODES

We now consider a second-order nonlinear equation of the form

$$y'' = f(x, y, y'), a < x < b \tag{5.45}$$

Subject to the general two-point boundary conditions

$$\begin{aligned} &a_0 y(a) - a_1 y'(a) = \alpha, a_i \ge 0 \\ &b_0 y(b) + b_1 y'(b) = \beta, b_i \ge 0 \\ &a_0 + b_0 > 0 \end{aligned} \tag{5.46}$$

The related IVP is

$$\begin{aligned} &u'' = f(x, u, u'), a < x < b \\ &u(a) = a_1 s - c_1 \alpha \\ &u'(a) = a_0 s - c_0 \alpha \end{aligned}$$

where;

$$a_1 c_0 - a_0 c_1 = 1 \tag{5.47}$$

The differential equation in u and that in y are the same. The initial conditions given above are substituted in the first boundary condition at $x = a$, [Eq. (5.46a)], the equation is satisfied (the terms with s gets cancelled). The value of s is to be selected in the initial conditions such that the solution of Eq. (5.47) when substituted in the boundary condition at $x = b$ should satisfy it. That is the solution of Eq. (5.47), $u = u(x; s)$, will be a solution of Eq. (5.45) if s satisfies the other boundary condition [Eq. (5.46b)]:

$$\Phi(s) = b_0 u(b; s) + b_1 u'(b; s) - \beta = 0 \tag{5.48}$$

To carry out this procedure numerically, convert Eq. (5.47) into a first-order system:

$$\begin{bmatrix} w \\ v \end{bmatrix}' = \begin{bmatrix} v \\ f(x, w, v) \end{bmatrix} \tag{5.49}$$

with

$$\begin{aligned} w(a) &= a_1 s - c_1 \alpha \\ v(a) &= a_0 s - c_0 \alpha \end{aligned} \tag{5.50}$$

In order to find *s*, one can apply Newton's method to Eq. (5.48), giving

$$\begin{aligned} s^{[k+1]} &= s^{[k]} - \frac{\Phi(s^{[k]})}{\Phi'(s^{[k]})'}; k = 0, 1, ... \\ s^{[0]} &= \text{arbitray} \end{aligned} \tag{5.51}$$

The guess value is to be selected based on the physics of the problem. To find *Φ′*(*s*), first define

$$\xi(x) = \frac{\partial w(x; s)}{\partial s}; \quad \eta(x) = \frac{\partial v(x; s)}{\partial s} \tag{5.52}$$

Differentiation of Eqs. (5.49) and (5.50) with respect to *s* gives

$$\begin{aligned} \xi' &= \eta, & \xi(a) &= a_1 \\ \eta' &= \frac{\partial f}{\partial v}\eta + \frac{\partial f}{\partial w}\xi, & \eta(a) &= a_0 \end{aligned} \tag{5.53}$$

Solution of Eq. (5.53) allows for calculation of *Φ′* as

$$\Phi' = b_0 \xi(b; s) + b_1 \eta(b; s) \tag{5.54}$$

Therefore, the numerical solution of Eq. (5.53) would be computed along with the numerical solution of Eq. (5.49). Thus, one iteration in Newton's method in Eq. (5.51) requires the solution of two set of initial-value ODE problems [Eqs. (5.49) and (5.53)]. Once the suitable *s* value is obtained, then, the solution of *u* and *u′* for various *x* values (from *x* = *a* to *x* = *b*) will be the required result for *y* and *y′* for various *x* values.

5.4 COUPLED TWO POINT BVP ODES

Let us consider a combined mass and heat transfer problem in a tubular reactor.

Each aspect is described by a second order BVP ODE.
For example, concentration (*y*) and temperature (*z*) are described by:

$$y'' = f(x, y, y', z, z') \tag{5.55}$$

$$\begin{aligned} a_0 y(a) - a_1 y'(a) &= \alpha, a_i \geq 0 \\ b_0 y(b) + b_1 y'(b) &= \beta, b_i \geq 0 \end{aligned} \tag{5.56}$$

$$z'' = g(x, y, y', z, z') \tag{5.57}$$

$$k_0 z(a) - k_1 z'(a) = \theta \tag{5.58}$$

$$m_0\, z(a) + m_1\, z'(b) = \lambda \tag{5.59}$$

When we convert the above BVP equations to IVP ODEs, we need to use s_1 and $s_{2,}$ whose values are to be obtained by iteration. The need for solving the two nonlinear algebraic equations, representing the two BCs at $x = b$, by iteration are to be considered to select the values for s_1 and $s_{2.}$

5.5 METHOD OF PARAMETER DIFFERENTIATION

Given the nonlinear algebraic equation $f(x) = 0$

Let us write (Na, 1979):

$$f(x) = f(p)\,(1 - \tau) \tag{5.60}$$

When $\tau = 0$ we get $x = p$ (initial guess) (5.61)

When $\tau = 1$; then $f(x) = 0$ (the original problem) (5.62)

As the value of τ varies from 0 to 1, the equation goes to $f(x) = 0$. Let us derive a differential equation as τ as the independent variable. Differentiating the Eq. (5.60) with respect to τ, we get:

$$\left(\frac{\partial f}{\partial x}\right)\left(\frac{dx}{dt}\right) = -\,f(p) \tag{5.63}$$

$$\left(\frac{dx}{dt}\right) = \frac{-f(p)}{\left(\dfrac{\partial f}{\partial x}\right)} \tag{5.64}$$

Example 5.3

$$f(x) = \exp(x) - x^2 - 2x = 0 \tag{5.65}$$

Let us consider the guess value as $x = p$.

Hence,
$$\frac{f(p)}{\left(\dfrac{\partial f}{\partial x}\right)} = -\frac{[\exp(p) - p^2 - 2p]}{[\exp(x) - 2x - 2]} \tag{5.66}$$

The ODE is given by:
$$\frac{dx}{d\tau} = \frac{[\exp(p) - p^2 - 2p]}{[\exp(x) - 2x - 2]} \tag{5.67}$$

with $\tau = 0,\ x = p$ (5.68)

Integrate the above IVP ODE, by numerically (using ODE23 routine in Matlab) from $\tau = 0$; $x = 0$, and integrate up to $\tau = 1$, and the solution is x at $\tau = 1$. The above method is called the Method of parameter differentiation.

For the Eqs. (5.67) and (5.68) with $p = 0$, we get the numerical solution for x when $\tau = 1$, $x = 0.7895$. If the original nonlinear algebraic equation has multiple solutions, then we can get the solutions by assuming different initial values for x. If we assume at $\tau = 0$, $x = p = 2$, and formulate the relevant ODE, then the numerical solution obtained is $x = 2.2743$.It should be noted that Eq. (5.66) is to be solved numerically up to $\tau = 1$. Additional details of the method are given by Na (1998).

5.6 MPD FOR SIMULTANEOUS EQUATIONS

Let us consider 3 simultaneous nonlinear algebraic equations:

$$f_1(x_1, x_2, x_3) = 0; \tag{5.69a}$$

$$f_2(x_1, x_2, x_3) = 0; \tag{5.69b}$$

$$f_3(x_1, x_2, x_3) = 0; \tag{5.69c}$$

We can write the above 3 equations in a vector notation as (Na, 1979):

$$F(X) = 0 \tag{5.70}$$

where $$F = [f_1\, f_2\, f_3]^T \tag{5.71}$$

and $$X = [x_1\, x_2\, x_3]^T \tag{5.72}$$

Let us consider $$F(X) = F(P)\,(1 - \tau) \tag{5.73}$$

When $$\tau = 0;\ X = P \text{ (initial guess vector)} \tag{5.74}$$

On differentiating the equations [Eqs. (5.63a,b,and c)] with respect to τ, we get:

$$\left(\frac{\partial f_1}{\partial x_1}\right)\left(\frac{dx_1}{d\tau}\right) + \left(\frac{\partial f_1}{\partial x_2}\right)\left(\frac{dx_2}{d\tau}\right) + \left(\frac{\partial f_1}{\partial x_3}\right)\left(\frac{dx_3}{d\tau}\right) = -f_1(P) \tag{5.75}$$

$$\left(\frac{\partial f_2}{\partial x_1}\right)\left(\frac{dx_1}{d\tau}\right) + \left(\frac{\partial f_2}{\partial x_2}\right)\left(\frac{dx_2}{d\tau}\right) + \left(\frac{\partial f_2}{\partial x_3}\right)\left(\frac{dx_3}{d\tau}\right) = -f_2(P) \tag{5.76}$$

$$\left(\frac{\partial f_3}{\partial x_1}\right)\left(\frac{dx_1}{d\tau}\right) + \left(\frac{\partial f_3}{\partial x_2}\right)\left(\frac{dx_2}{d\tau}\right) + \left(\frac{\partial f_3}{\partial x_3}\right)\left(\frac{dx_3}{d\tau}\right) = -f_3(P) \tag{5.77}$$

We re-write the above equation in a matrix form as:

$$J\frac{dX}{d\tau} = -F(P) \tag{5.78}$$

where, $$J = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{bmatrix} \tag{5.79}$$

Hence $$\frac{dX}{d\tau} = -J^{-1}(x)\, F(P) \tag{5.80}$$

At $\tau = 0$; $X = P$

Solve *numerically* the above IVP ODE by ODE23 method (in Matlab) up to $\tau = 1$.

Depending upon the initial guess value of P vector, we may get the multiple solutions in case the problem has such solutions.

Example 5.4

Solve the following 2 simultaneous nonlinear algebraic equations by MPD

$$f_1\ (x_1, x_2) = x_1^{\ 2}\ x_2^{\ 2} - 2x_1 - 5x_2^{\ 0.5} + 5 = 0 \tag{5.81}$$

$$f_2(x_1, x_2) = x_1^{\ 4} - 6x_2^{\ 2}x_1 + 23 = 0 \tag{5.82}$$

We have
$$f(x) = [f_1\, f_2]^T \tag{5.83}$$

The Jacobian is obtained as:

$$J = \begin{bmatrix} 2x_2^2 x - 2 & 2x_1^2 x_2 - 2.5x_2^{-0.5} \\ 4x_1^3 - 6x_2^2 & 12x_1x_2 \end{bmatrix} \tag{5.84}$$

$$\frac{dX}{d\tau} = -\mathrm{J}^{-1}\ F(X) \tag{5.85}$$

$$p = [1\ 1]^T \tag{5.86}$$

The numerical solution of the IVP ODE for the initial conditions: p=[1 1]^T at $\tau = 1$, gives

$$X = [1.73\ 1.9859]^T \tag{5.87}$$

5.7 FINITE DIFFERENCE SCHEME METHOD FOR NONLINEAR BVP ODES

Consider the equation
$$y'' = f(y, y', x) \tag{5.88}$$

At
$$x = a,\ a_0 y' - a_1 y = \alpha \tag{5.89}$$

At
$$x = b,\ p_0\, y' + p_1\, y = \beta \tag{5.90}$$

Though the Eq. (5.88) is valid for $a < x < b$, we consider the equation at selected values of x (called grids). The objective here is to convert the nonlinear ODE to a set of nonlinear algebraic equations (at these grids).

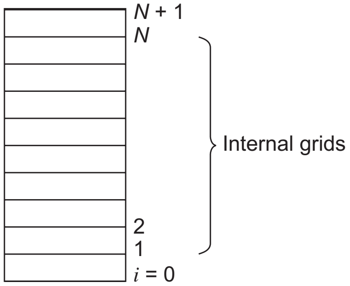


Fig. 5.1 Grids along the X-axis

Consider the N internal grid as shown in Fig. 5.1. Each grid width h is given by

$$h = \frac{(b-a)}{(N+1)} \tag{5.91}$$

$$x_i = a + ih \tag{5.92}$$

Consider the approximation for the derivatives (by central finite difference scheme)

$$\left(\frac{dy_1}{dx}\right)_i = \frac{(y_{i+1} - y_{i-1})}{2h} \tag{5.93}$$

$$\left(\frac{d^2y}{dx^2}\right)_i = \frac{(y_{i+1} - 2y_1 + y_{i-1})}{h^2} \tag{5.94}$$

Sometimes, we use a less accurate approximation particularly at the boundaries:

$$\left(\frac{dy}{dx}\right)_i = \frac{(y_i - y_{i-1})}{h} \quad \text{(Backward finite difference scheme)} \tag{5.95}$$

$$\left(\frac{dy}{dx}\right)_i = \frac{(y_{i+1} - y_i)}{h} \quad \text{(Forward finite difference scheme)} \tag{5.96}$$

Among the forward and backward schemes, the backward scheme is more stable (or we can use a large h). The above equations can be derived by Taylor series expansion of the function $y(t + h)$ or by graphical slope concepts. Central finite difference scheme for dy/dx has improved accuracy than the backward or forward schemes.

Apply the main equation at the internal grid $i = 1$ to N

at $i = 1$;

$$\frac{(y_2 - 2y_1 + y_0)}{h^2} = f\left[y_1, \frac{y_1 - y_0}{h}, x_1\right] \tag{5.97}$$

$i = 2$ to $N - 1$, we get;

$$\frac{(y_{i+1} - 2y_1 + y_{i-1})}{h^2} = f\left[y_1, \frac{y_{i+1} - y_{i-1}}{2h}, x_i\right] \tag{5.98}$$

$i = N$, we get:

$$\frac{(y_{N+1} - 2y_{N-1})}{h^2} = f\left[y_N, \frac{y_{N+1} - y_{N-1}}{2h}, x_N\right] \tag{5.99}$$

In the Eq. (5.97), we need to know y_0 and in the third equation, we need to know y_{N+1}.

Let us consider the Boundary condition (BC) 1:

$$a_0\left[\frac{(y_1 - y_0)}{h}\right] - y_0 = \alpha \tag{5.100}$$

From which we can express y_0 in terms of y_1 to be used in Eq. (5.97)

Let us consider BC 2:

$$p_0\left[\frac{(y_{n+1} - y_N)}{h}\right] + p_1\, y_{N+1} = \beta \tag{5.101}$$

From which we can get an equation for y_{N+1} in terms of y_N. Hence we get N equations in $y_1, y_2, \ldots y_N$ from Eqs. (5.97)–(5.99). Solve numerically the N nonlinear algebraic equations by using the Newton–Raphson method.

We can select the internal grid as 3. Obtain the solution and draw a profile y versus x. Then use $N = 5$ and repeat the solution method. If the profile y versus x is not changed significantly, then the solution obtained is okay. Otherwise consider $N = 7$, etc., till there is no further change in the y versus x profile.

Example 5.5

Using the finite difference scheme method, get the solution of the BVP ODE:

$$y'' + 3\,y^2 y' + y\exp(-2x) = x^2 \tag{5.102}$$

at
$$x = 0;\ -y' + y = 1 \tag{5.103}$$

at
$$x = 1\text{: } y' = 0 \tag{5.104}$$

Method: let us consider 5 internal grid on x: therefore we have grid width $h = 1/6$. We have $x_i = ih$; $i = 1,2,\ldots 6$

The grids are numbered as 0,1,2,3,4,5,6 ($x_0, x_1, x_2, x_{3,\ldots}x_6$). Here x_0 and x_6 are denoted as boundary grids for which the respective boundary conditions are to be used. The grids $x_1, x_2,\ldots x_5$ are called internal grids at which the main ODE is to be considered.

For the internal grid i, let us consider

$$y_i'' = \frac{(y_{i+1} - 2y_i + y_{i-1})}{h^2};\ y_i' = \frac{(y_{i+1} - y_{i-1})}{(2h)} \tag{5.105}$$

Hence, the ODE at the grid $i = 1$ is written as:

$$\left[\frac{(y_2 - 2y_1 + y_0)}{h^2}\right] + 3\left[\frac{y_1^2(y_2 - y_0)}{(2h)}\right] + y_1\exp(-2x_1) = x_1^{\,2} \tag{5.106}$$

We need to know x_0. Write the boundary condition at $x = 0$:

Since there is no grid below $i = 0$, let us use the forward finite difference scheme for y_i' as

$$\frac{(y_{i+1} - y_i)}{h} \text{ at } x = 0$$

Hence
$$-\left[\frac{(y_1 - y_0)}{h}\right] + y_0 = 1 \tag{5.107}$$

From which we get:
$$y_0 = \frac{(y_1 + h)}{(1 + h)}$$

$$y_0 = (y_1 + h)p \tag{5.108}$$

with
$$p = \frac{1}{(1 + h)} \tag{5.109}$$

Substitute this for y_0 in Eq. (5.106) we get

$$\left[\frac{(y_2 - 2y_i + py_i + ph)}{h^2}\right] + 3\left[\frac{y_i^2(y_2 - py_i - ph)}{(2h)}\right] + y_1\exp(-2x_1) = x_1^{\,2} \tag{5.110}$$

For the grid $i = 2, 3, 4$ we have

$$\left[\frac{(y_{i+1} - 2y_i + y_{i-1})}{h^2}\right] + \left[\frac{y_i^2(y_{i+1} - y_{i-1})}{(2h)}\right] + y_i\exp(-2x_i) = x_i^2 \tag{5.111}$$

For $i = 5$

$$\left[\frac{(y_6 - 2y_5 + y_4)}{h^2}\right] + \left[\frac{y_5^2(y_6 - y_4)}{(2h)}\right] + y_5 \exp(-2x_5) = x_5^2 \tag{5.112}$$

Since there is no grid at the forward location, at $x = 1$, let us use backward difference equation y'_i as $(y_i - y_{i-1})/h$

At grid at $i = N + 1$, we use the boundary condition $y' = 0$

$$\frac{(y_6 - y_5)}{h} = 0 \tag{5.113}$$

we get $y_6 = y_{5.}$, Eq. (5.112) cab be written as:

$$\left[\frac{(y_5 - 2y_5 + y_4)}{h^2}\right] + \left[\frac{y_5^2(y_5 - y_4)}{(2h)}\right] + y_5 \exp(-2x_5) = x_5^2 \tag{5.114}$$

The original nonlinear BVP ODE is written as the following nonlinear algebraic equations:

For the grid $i = 1$, we have

$$\left[\frac{(y_2 - 2y_1 + py_1 + ph)}{h^2}\right] + 3\left[\frac{y_1^2(y_2 - py_1 - ph)}{(2h)}\right] + y_1 \exp(-2x_1) = x_1^2 \tag{5.115}$$

For $i = 2, 3, 4$

$$\left[\frac{(y_{i+1} - 2y_i + y_{i-1})}{h^2}\right] + \left[\frac{y_1^2(y_{i+1} - y_{i-1})}{(2h)}\right] y_i \exp(-2x_i) = x_i^2 \tag{5.116}$$

At $i = 5$, we have

$$\left[\frac{(y_5 - 2y_5 + y_4)}{h^2}\right] + \left[\frac{y_5^2(y_5 - y_4)}{(2h)}\right] + y_5 \exp(-2x_5) = x_5^2 \tag{5.117}$$

The above 5 nonlinear algebraic equations for x_i ($i = 1, 2, 3, 4, 5$) at the 5 internal grids are to be solved by Newton–Raphson method. Hence, y_0 and y_6 can be obtained from $y_0 = (py_1 + ph)$ and $y_6 = y_5$.

5.8 CONVERSION OF A PDE INTO A SET OF IVP ODES

Method of Lines (MOL): The basic idea of MOL is to replace the special (boundary value) derivatives in the PDE with the algebraic approximations. Once this step is carried out, the special derivatives are no longer stated explicitly in terms of the special independent variables. Thus in effect, only the initial value variable, (typically time in a physical problem) results. With the one independent variable, we have a system of initial value ODEs approximating the original PDE. Then we can apply any standard subroutine to solve the resulting set of IVP ODEs. Schiesser and Griffiths (2009) give a good review of the work on the application of MOL to PDEs

Consider the system equation:

$$\frac{\partial c}{\partial t} = \left(\frac{1}{P}\right)\frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x} - kc^2 \tag{5.118}$$

BC 1: (at $x = 0$):

$$\left(\frac{\partial c}{\partial x}\right)_{x=0} = P(c\ (x = 0) - 1) \tag{5.119}$$

BC 2: at $x = 1$;

$$\frac{\partial c}{\partial x} = 0 \tag{5.120}$$

Initial condition:

$$c(0, x) = g(x) \tag{5.121}$$

Similar to the situation in BVP ODEs, we can consider N internal grid (Fig. 5.1) and apply the equation at each internal grid $i = 1$ to N, replacing the special derivative by the finite difference scheme. The time derivative can be kept as such (thus partial derivative will become a set of ordinary derivative equations in time).

For $i = 1$;

$$\left(\frac{dc_1}{dt}\right) = \left(\frac{1}{P}\right)\left[\frac{(c_2 - 2c_1 + c_0)}{h^2}\right] - \left[\frac{(c_2 - c_0)}{(2h)}\right] - kc_1^2 \tag{5.122}$$

For $i = 2, N - 1$,

$$\left(\frac{dc_i}{dt}\right) = \left(\frac{1}{P}\right)\left[\frac{(c_{i+1} - 2c_i + c_{i-1})}{h^2}\right] - \left[\frac{(c_{i+1} - c_{i-1})}{(2h)}\right] - kc_i^2 \tag{5.123}$$

For $i = N$,

$$\left(\frac{dc_N}{dt}\right) = \left(\frac{1}{P}\right)\left[\frac{(c_{N+1} - 2c_N + c_{N-1})}{h^2}\right] - \left[\frac{(c_{N+1} - c_{N-1})}{(2h)}\right] - kc_N^2 \tag{5.124}$$

We see that c_0 appears in Eq. (5.122) and c_{N+1} appears in Eq. (5.124).

By using the BC 1 and BC2, we can get equation for c_0 in terms of c_1 and $c_{N+1} = c_N$ (5.125)

Hence we get N ODEs with the initial condition $c(o) = g(x_i)$, where $x_i = ih$.

These IVP ODES can be solved numerically using the Runge–Kutta method (ODE23 routine in Matlab). We get the solution separately for $N = 3$, 5 and 7, till there is no further change in the profile of c versus t at each grid. Usually, the resulted ODEs will be stiff. Hence, a suitable routine (ode15s in Matlab) is to be used.

Let us look at the origin of the name: method of lines. If we consider Eqs. (5.122)–(5.124), integration of these ODEs produces the solution $c_1(t), c_3(t),..,c_n(t)$. We could then plot these functions in an $x - c(x, t)$ plane as a vertical line at x_i ($i = 1, 2, \ldots N$), with the height of each line equal to $c(x, t)$. The plot of the solution would be a set of vertical parallel lines suggesting the name *method of lines* (Schiesser and Griffiths, 2009).

Review Problems

1. Using Newton–Raphson method, set up the iterative equation for solving the followings nonlinear algebraic equation: $x - 0.333 \exp(x) = 0$. Use the guess value as $x = 0.5$
2. Using the MPD, formulate the relevant IVP ODE for the above problem. Solve the resulting equation numerically by the Runge–Kutta method.

3. Using Newton–Raphson method, set up the iterative equations for solving the following simultaneous nonlinear algebraic equations:

   $$x_1^2 + x_1x_2 - x_2 - 10 = 0$$
   $$x_2^2 + x_1x_2 - x_1 - 5 = 0$$

   Using the initial guess as $x_1 = 1$ and $x_2 = 1$, show the calculation for 3 iterations.
4. Using the MPD, formulate the relevant IVP ODEs for the above problem. Solve the resulting equations by the Runge–Kutta method.
5. Using the MPD, formulate the relevant IVP ODEs for the problem 5.5. Solve the resulting equation by Runge–Kutta method.
6. Using Newton–Raphson method, set up the iterative equations for solving the following simultaneous nonlinear algebraic equations:

   $$3x_1^3 + 4x_2^2 - 145 = 0$$
   $$4x_1^2 + x_2^3 + 28 = 0$$

   Using the initial guess as $x_1 = 1$ and $x_2 = 1$, show the calculation details for 3 iterations.
7. Given the second order IVP ODE: $8y'' - x^2 y' + 2y^3 = 0$; $y(x = 0) = 1$ and $y'(x = 0) = 0$. Convert the 2nd order ODE to two first order ODEs. Solve numerically by RKG method to get y at $x = 0.1, 0.3, 0.5, 0.6$
8. The diffusion and Chemical reaction in a spherical catalyst pellet is given by

   $$D\left(\frac{d^2c}{dr^2}\right) + \left(\frac{2}{r}\right)D\left(\frac{dc}{dr}\right) - kc = 0$$

   at $r = R$; $c = 1$ and $r = 0$; $\frac{dc}{dr} = 0$

   Give $k = 0.1\ s^{-1}$; $D = 10^{-9}\ \text{m}^2/\text{s}$; $R = 1$ cm. Using 5 internal grids, formulate the relevant algebraic equations and hence solve then by NR method.
9. Solve the above equation by the shooting method.
10. Using the finite difference scheme method, convert the following PDE into

    a system of IVP ODES. Use the number of internal grids as $N = 5$.

    $$\frac{\partial c}{\partial t} = \left(\frac{1}{P}\right)\frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial x} - \exp(-x)\, k_1 c^2$$

    BCs: at $x = 0$: $\frac{\partial c}{\partial x} = P(c(x = 0) - 1)$; at $x = 1$: $\frac{\partial c}{\partial x} = 0$; ICs: $c(0, x) = g(x)$.

    $P = 2$; $k_1 = 1$ litre/(mole. sec)
11. Jatomea et al. (2015. Chemical Engg. Sci. 138. 31–40) presented experimental study on the operation and dynamic modelling of a novel integrated anaerobic-aerobic-anoxic reactor for sewage treatment. Prepare a report on the model development and the numerical solution of the model equations.
12. Cabeza et al. (2015. Chemical Engineering Science. 138. 59–70) presented a work (experimental and modelling) on two-phase modelling and simulation of the hydrothermal fractionation of holm oak in a packed bed reactor with hot pressurized water. Prepare a report on the model development and the numerical solution of the model equations.

6

Modelling and Simulation: Case Studies

In this chapter, four detailed case studies on the development of mathematical models and their solution and analysis of the systems are given. The resulting model equations are PDEs, Variable coefficients ODEs, IVP ODEs, BVP ODES, etc.

6.1 AXIAL AND RADIAL MIXING OF CATALYST IN A BUBBLE COLUMN SLURRY CONTACTOR (BCSC)

In a bubble column slurry contactor (BCSC), the gas is disbursed in to a liquid plus catalyst solid particles in a column. The solid particles (about 50 micrometre size particles) are kept in suspension by the gas bubbling action. In present work, the solid concentration profile (as a function of radial and axial direction of the contactor) is to be calculated. The solid particles are assumed to flow by axial and radial dispersion model. The other assumptions are essentially the same as those given by Kato et al. (1972). The following notations are used.

C– concentration of solid g/cm^3

U_p = velocity of particle in downward direction

It is assumed that there is no convection in the radial direction.

Consider a hollow disc thickness Δr and height Δx.

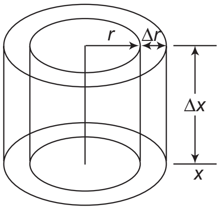


Fig. 6.1 Control element

Mass balance for the solid:

$$\text{Input} - \text{Output} = 0 \tag{6.1}$$

$$\text{(input in } x\text{-direction + input in the } r\text{-direction)} - \text{(output in } x\text{-direction + output in } r\text{-direction)} = 0 \tag{6.2}$$

$$-u_P\, C\, 3\pi r\, \Delta r \text{ (at } x) + u_P\, c 2\pi r \Delta r \text{ (at } x + \Delta x) - D_x \left(\frac{\partial c}{\partial x}\right) 2\pi r \Delta r \text{ (at } x) + D_r \left(\frac{\partial c}{\partial r}\right) 2\pi r\, \Delta r \text{ (at } x + \Delta x)$$

$$-D_r \left(\frac{\partial c}{\partial r}\right) 2\pi r\, \Delta x \text{ (at } r) + \Delta_r \left(\frac{\partial c}{\partial r}\right) 2\pi r \Delta x \text{ (at } r + \Delta r) = 0 \tag{6.3}$$

Dividing throughout by ($2\pi\, \Delta x\, \Delta r$) and making the limit $\Delta r \to 0$ and $\Delta x \to 0$, we get

$$U_p \left(\frac{\partial c}{\partial r}\right) + Dx\left(\frac{\partial^2 c}{\partial x^2}\right) + \left(\frac{D_r}{r}\right) \partial\left(\frac{r\, \partial c}{\partial r}\right) \Big/ \partial r = 0 \tag{6.4}$$

The boundary conditions are given by:

$$\left(\frac{\partial c}{\partial r}\right) \text{ (at } r = 0) = 0 \tag{6.5}$$

$$\left(\frac{\partial c}{\partial r}\right) \text{ (at } r = R) = 0 \tag{6.6}$$

At

$$x \to \infty,\ c = 0 \tag{6.7}$$

Total mass balance of solid particles in the reactor:

$$2\pi\left(\iint c\, r \partial r\, \partial x\right) = ALc_{\text{ave}} \tag{6.8}$$

The limit for x is from 0 to ∞ and r from 0 to R.

Equations (6.4)–(6.8) can be written in dimensionless form:

$$b\, \frac{\partial^2 C}{\partial Z^2} + a\, \frac{\partial C}{\partial Z} + \left(\frac{1}{y}\right) \partial\left(\frac{y \partial C}{\partial y}\right) \Big/ \partial y = 0 \tag{6.9}$$

$$\frac{\partial C}{\partial y} \text{ (at } y = 0) = 0;\ \frac{\partial C}{\partial y} \text{ (at } y = 1) = 0; \tag{6.10}$$

$$Z \to \infty,\ C = 0 \tag{6.11}$$

$$\iint Cy\, dy\, dZ\ = 0.5\ C_{\text{ave}} \tag{6.12}$$

where,

$$Z = \frac{x}{L},\ y = \frac{r}{R},\ C = \frac{c}{c_{\text{ave}}} \tag{6.13a}$$

$$Pe_Z = \frac{U_P L}{D_Z},\ Pe_r = \frac{R^2 U_P}{D_r^2};\ d = Pe_r,\ b = \frac{Pe_r}{Pe_Z} \tag{6.13b}$$

The limits in Eq. (6.12) are y from 0 to 1 and Z from 0 to 1.

The above equations are solved here by the method of separation of variables (Powers, 1972). We postulate a solution of the form:

$$C(Z, y) = \sum \varepsilon_n F_n(Z)\, G_n(y) \tag{6.14}$$

The limits for the summation are from $n = 0$ to $n = \infty$. Substituting the postulated solution for C in Eq. (6.9) and rearranging, we get

$$\left(\frac{b}{F_n}\right)\left(\frac{\partial^2 F_n}{\partial Z^2}\right) + \left(\frac{a}{F_n}\right)\left(\frac{\partial F_n}{\partial Z}\right) = -\left(\frac{1}{G_n}\right)\left(\frac{1}{y}\right)\left[\frac{\partial(y\partial G_n)}{\partial y}\Big/\partial y\right] \tag{6.15a}$$

$$= \beta_n^{\,2} \tag{6.15c}$$

where β_n is the separation constant. Equations (6.15a and b) can be separated into two equations:

$$b\left(\frac{\partial^2 F_n}{\partial Z^2}\right) + a\left(\frac{\partial F_n}{\partial Z}\right) - \beta_n^{\,2} F_n = 0 \tag{6.16}$$

$$\left(\frac{1}{y}\right)\left[d\left(\frac{ydG_n}{dy}\right)\Big/dy\right] + \beta_n^{\,2}\, G_n = 0 \tag{6.17}$$

Let us consider the Eq. (6.16). The solution for this equation is given by:

$$F_n(Z) = \gamma_1 \exp(q_n Z) + \gamma_2 \exp(-h_n Z) \tag{6.18}$$

where

$$q_n = \frac{[-a + (a^2 + 4b\,\beta_n^{\,2})^{0.5}]}{(2b)} \tag{6.19}$$

$$h_n = \frac{[-a - (a^2 + 4b\,\beta_n^{\,2})^{0.5}]}{(2b)} \tag{6.20}$$

With the boundary condition at $Z \to \infty$, $C \to 0$, we get:

$$\gamma_1 = 0 \tag{6.21}$$

since q_n is always positive. Now we have,

$$F_n(Z) = \gamma_2 \exp(-h_n Z) \tag{6.22}$$

Let us consider Eq. (6.17). The solution for this equation is given by

$$G_n(y) = \theta_1 J_0(\beta_n y) + \theta_2 Y_0(\beta_n y) \tag{6.23}$$

The Bessel function of the second kind $Y_0(\beta_n y)$ has a singularity at $y = 0$ which is forbidden in the problem at hand (at $y = 0$, c has to be finite) so that

$$\theta_2 = 0 \tag{6.24}$$

The boundary condition at $y = 1$ leads to the characteristic equation for β_n:

$$J_1(\beta_\text{n}) = 0 \tag{6.25}$$

The values of β_n satisfying Eq. (6.25) are available (Jahnke et al., 1966).

Hence, the solution for Eq. (6.14) is given by

$$C(Z, y) = \sum E_n \exp(-h_n Z)\, J_0(\beta_n y) \tag{6.26}$$

$$= E_0 \exp(h_0 Z) + \sum E_n \exp(-h_n Z)\, J_0(\beta_n y) \tag{6.27}$$

The limit for the summation term in Eq. (6.27) is $n = 1$ to ∞. Here, $h_0 = Pe_z$. Our problem is now to determine the values of E_n. Substituting Eq. (6.27) in Eq. (6.12) gives:

$$E_0 = C_{\text{ave}} \frac{h_0}{[1 - \exp(-h_0)]} \tag{6.28}$$

If we know $C(0, y)$, then E_n can be calculated by using the Sturm–Liousville theorem. Multiply both sides of Eq. (6.27) by $y\, J_0(\beta_0 y)$ and integrate from y from 0 to 1. Because of the orthogonal properties of the solution [Eq. (6.27)] it can be shown that:

$$E_n = \frac{\int C(0, y) y\, J_0(\beta_n y)\, dy}{\int y\, J_0^2(\beta_n y)\, dy} \tag{6.29}$$

The denominator can be simplified by using Eq. (6.27) (Jenson and Jeffrey, 1963) to give:

$$\int y\, J_0(\beta_n y)\, dy = 0.5\, J_0^{\,2}(\beta_n) \tag{6.30}$$

The limit for the integration term is from 0 to 1. From Eq. (6.27) we get, at $Z = 0$,

$$C(0, y) = E_0 + \sum E_n\, J_0(\beta_n y) \tag{6.31}$$

On multiplying Eq. (6.31) by y and integrating over y from 0 to 1 we get:

$$\int C(0, y)\, y\, dy = \frac{E_0}{2} \tag{6.32}$$

$$= 0.5\, C_{\text{ave}} \frac{Pe_Z}{[1 - \exp(-Pe_Z)]} \tag{6.33}$$

To calculate E_n [Eq. (6.29)] we require $C(0, y)$. That is, to calculate the $C(Z, y)$ profile from $Z > 0$, given Pe_r and Pe, we need to know $C(0, y)$ as one of the boundary conditions. In other words, given Pe and Pe_r, *a priori* knowledge of $C(0, y)$ is required to calculate $C(Z, y)$ for $Z > 0$. If the experimental data on $C(0, y)$ are known we can calculate Pe, by using Eq. (6.33), and E_n from Eq. (6.29). The values of $C(Z, y)$ (for $Z > 0$) can be calculated from Eq. (6.27) for any value of $Pe_{r.}$ By matching with the experimental data on $C(Z, y)$ we can estimate the best value of Pe_r.

For the experimental data of $C(0, y)$ reported by Pandit and Joshi (1984) (Fig. 6.1) we get the values of Pe_z as 1.58 from Eq. (6.33). By using Eq. (6.32) we get E_0 and from Eq. (6.29) we calculate the values of $C(Z, y)$ (for $Z > 0$) by assuming different values of Pe_r. By the direct search method, matching the experimental data of $C(Z, y)$at $Z = 1$ of Fig. 6.2, we get Pe_r =0.05. The concentration profiles thus calculated using these Peclet number values compare favourably with the experimental data, as shown in Fig. 6.2. It is interesting to note the Pe_r determined by matching the data at $Z = 80$ cm predicts the data adequately at other values of Z.

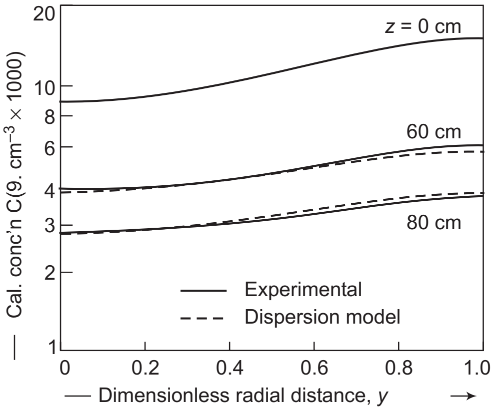


Fig. 6.2 Comparison of dispersion model with the experimental data of Pandit and Joshi (1984)

$V_G = 20$ cm/s; $d_T = 20$ cm; $d_p = 340$ um;
$L_c = 80$ cm; Gas hold up = 0.22; $L = 102.6$ cm.

It should be noted that, when there is no radial dispersion at $Z = 0$ (that is, $C(0, y) =$ constant) then from Eq. (6.29) we get $E_n = 0$ ($n = 1$ to ∞). The resulting solution for $C(Z, y)$ is given by

$$C(Z, y) = C_{\text{ave}}\, Pe_z \frac{\exp(-Pez\, Z)}{[1 - \exp(-Pe_Z)]} \tag{6.34}$$

which is a function of Z only (one dimensional model).

Conclusions: An analytical solution is given for the elliptic partial differential equation of the dispersion model describing the steady-state catalyst concentration in both the axial and radial direction in a semi-batch bubble column slurry reactor. The reported experimental data on catalyst concentration are compared with that of the proposed dispersion model.

6.2 ANALYSIS OF TRANSPORT REACTORS WITH CATALYST DEACTIVATION

6.2.1 Model equations and solution

Consider a first-order irreversible reaction which takes place in an isothermal vertical transport reactor. Assume that the entrance effect can be neglected, the gas and the catalyst particles follow the plug flow pattern, and the catalyst particles are spherical and uniform in size. The reaction is assumed to take place only on the surface of the particles. The rate of decay of catalyst activity is assumed to be proportional to the remaining activity, i.e., simple first-order decay in time-on-stream (Weekman, 1968; Wojciechowski, 1973). The steady-state material balance of the gas reactant in the gas phase and on the solid phase can be written in dimensionless form as:

$$\frac{df_1}{dZ} = -\beta\left(f_1 - f_2\right) \tag{6.35}$$

$$\frac{df_2}{dZ} = M\left(f_1 - f_2\right) - Qe^{-\lambda Z}\ f_2 \tag{6.36}$$

$$f_1\,|_{Z=0} = 1 \tag{6.37}$$

$$f_2\,|_{Z=0} = 0 \tag{6.38}$$

Combining Eqs. (6.35) and (6.36) to eliminate f_1 we get the following second-order, linear, variable-coefficient ordinary differential equation inf_2:

$$\frac{d^2 f_2}{dZ^2} + (B_0 + Qe^{-\lambda Z})\frac{df_2}{dZ} - B_1 e^{-\lambda Z}\ f_2 = 0 \tag{6.38}$$

A similar type of equation (where $e^{-\lambda z}$ appears in variable coefficient) arises in the analysis of moving or fixed bed reactors with catalyst deactivation. Only an approximate solution is reported (Lin, 1978). In the present note, an exact analytical solution of Eq. (6.38) is derived by a series-solution method (Kaplan, 1962). It is first converted into the standard form (Kaplan, 1962) by transforming the independent variables Z to Y where Y is given by $e^{-\lambda z}$ Then by substituting $f_2 = y^{\alpha}$, and equating the coefficient of y^{α}, in the resulting equation to zero, we get the following indicial roots:

$$\alpha_1 = 0 \ \text{ and } \ \alpha_2 = \frac{(M+\beta)}{\lambda} \tag{6.39}$$

The general solution of Eq. (4) is given by:

$$f_2 = \sum_{i=1}^{2} n_i \xi_i \tag{6.40}$$

where,
$$\xi_i = exp(-\alpha_i \lambda Z)\sum_{j=0}^{\infty} G_{ij}\exp(-j\lambda Z) \tag{6.41}$$

The constants n_1 and n_2 are to be found out from the initial conditions [Eqs. (6.37 a, b)] and are given by:

$$n_1 = b_3 \left. \sum\nolimits_{j=0}^{\infty} G_{2j} \middle/ b_4 \right. \tag{6.43}$$

$$n_2 = -b_3 \left. \sum\nolimits_{j=0}^{\infty} G_{1j} \middle/ b_4 \right. \tag{6.43}$$

where:
$$b_4 = \left[\sum_{j=0}^{\infty} G_{1j}\ (\alpha_1 + j)\right]\left[\sum_{j=0}^{\infty} G_{2j}\right] - \left[\sum_{j=0}^{\infty} G_{2j}\ (\alpha_2 + j)\right]\left[\sum_{j=0}^{\infty} G_{1j}\right] \tag{6.44}$$

and:
$$G_{ij} = \frac{b_2(\alpha_i + j - 1) + B_2}{(\alpha_i + j)(\alpha_i + j - 1 + b_1)} G_{i(j-1)} \tag{6.45}$$

with: $G_{i0} = 1$ $i = 1$ and 2 and $j =$ to ∞

Substituting Eq. (6.40) in Eq. (6.36) we get:

$$f_1 = \left(1 + \frac{Q}{M} e^{-\lambda Z}\right) f_2 - \frac{\lambda}{M}\sum_{i=1}^{2} n_i \sum_{j=0}^{\infty} [G_{ij} y^{\alpha_i + j}(\alpha_i + j)]. \tag{6.46}$$

Conversion at the reactor exit is given by (Fan and Hwang, 1981):

$$X = 1 - f_1\,|_{Z=1} - \frac{U_P(1-\in)f_2\,|_{Z=1}}{v_G} \tag{6.47}$$

When the catalyst activity is constant then Eq. (6.35)-(6.37) [with $\lambda = 0$] can be solved directly to get:

$$f_1 = n_3 A_0 \exp(m_1 Z) + n_4 A_1 \exp(m_2 Z), \tag{6.48}$$

$$f_2 = n_3 \exp(m_1 Z) + n_4 \exp(m_2 Z). \tag{6.49}$$

6.2.2 Hydrodynamic and mass transfer considerations

The hydrodynamic properties U_P and $\in$ needed in calculating the reactant conversions are obtained from the correlations of Yang (1973, 1977, 1978).

The mass balance for the solid particles in the reactor gives (Yang, 1974):

$$\in = 1 - \frac{4W_S}{(\rho_P - \rho_G)\pi d_T^2 U_P} \tag{6.50}$$

The particle velocity is related to the solid friction factor, f_p and the void fraction, $\in$ according to (Yang, 1974, 1978):

$$U_P = U_G - U_t\left[\left(1 + \frac{f_p U_P^2}{2gfd_T}\right)\in^{4.7}\right]^{0.5} \tag{6.51}$$

The solid friction factor, f_p can be obtained by the following empirical correlation (Yang, 1977, 1978):

$$f_p = 0.0126\frac{1-\in}{\in^3}\left[(1-\in)\frac{Re_t}{\mathrm{Re}_P}\right]^{-0.979} \quad \text{for } \frac{U_G}{U_t} > 1.5 \tag{6.52a}$$

$$f_p = 0.041\frac{1-\in}{\in^3}\left[(1-\in)\frac{Re_t}{Re_P}\right]^{-1.021} \quad \text{for } \frac{U_G}{U_t} < 1.5 \tag{6.52b}$$

The value of U_t required for the above equations is evaluated by (Yang, 1973) as:

$$U_t = 0.153\, d_p^{1.14}\, g^{0.71}\, \frac{(\rho_p - \rho_g)^{0.71}}{(\mu^{0.43}\ \rho_g^{0.29})} \quad \text{for } 2 \le \mathrm{Re} \le 1000$$

(or) $$U_t = \frac{d_P^2 g(\rho_p - \rho_g)}{(18\mu)} \quad \text{for Re} < 0.1$$

The gas film mass transfer coefficient, k_m, for suspended solid particle is obtained by the following empirical correlation (Satterfirled, 1970):

$$\frac{K_m d_p}{D_m} = 2 + 0.63\,(\mathrm{Sc})^{0.3333}\,(\mathrm{Re})^{0.5}$$

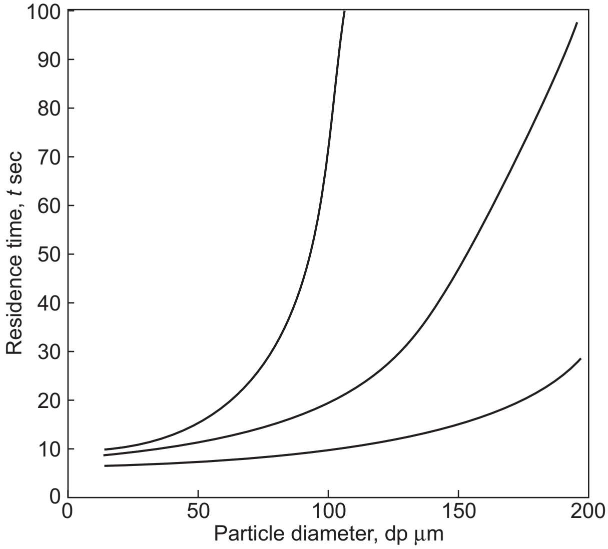


Fig. 6.3 Effect of catalyst decay velocity constant on verses behaviour υ_G = 100 cm/s; ρP = 2.5 g/cm^3(Chidambaram, 1985) Other conditions: as in Table 6.1

Now let us see what happens to X verses d_P characteristics, when the catalyst deactivation is taken into consideration. To calculate the extent of decay, we must know the residence time (t) of the catalyst particles. The residence time of the particles is given by:

$$t = \frac{L}{U_P}. \tag{6.53}$$

Figure 6.3 shows the t verses d_P behaviour. In the lower values of d_P, t increases slightly with d_P. But in the higher values of d_P, t increases steeply with d_P. This is due to the particle velocity (U_p) in the reactor with d_P as seen in Fig. 6.3.

Figure 6.4 shows the effect of catalyst decay velocity constant (λ_0) on the X verses d_P characteristics. This figure shows an interesting behaviour. As d_P increases, particle surface area increases (a), mass transfer coefficient (k_m) decreases and t increases. As t increases, the particles are much deactivated. These result in a decrease in conversion. But $\in_s$ increases as d_P increases (refer Fig. 6.3). This results in an increase in conversion. The net effect depends on the value of d_P and the level of λ_0. At the lower values of d_P (and at any value of λ_0), the decrease in the conversion [due to decrease in a, k_m, and the activity], is more than the increase in the conversion due to the increase in $\in_s$. Hence, the conversion decreases with d_P. For the higher values of d_P and the lower values of λ_0, the increase in the conversion due to increase in $\in_s$ is more than the decrease in the conversion due to the decrease in a, k_m and activity. Therefore, conversion shows an increasing trend. Hence, there is a minimum in X verses d_P behaviour. As λ_0 increases, the value of the minimum conversion decreases. For the certain intermediate values of λ_0, the conversion decreases first and then slightly increases and finally decreases with d_P. At higher values of λ_0, the conversion decreases continuously with d_P.

The above discussion clearly indicates that depending on the level of λ_0 we must choose the value of d_P to get the desired conversion. Figure 6.4 shows that the reactor can be operated with higher d_P to get the desired conversion. For lower values of λ_0 there are two values of d_P to get the same conversion. With the smaller d_P, the catalyst decay is less (because of small t) and hence the cost associated with regeneration of the catalyst is less. But the cost associated with the separation of the particles at the reactor exit is more. With higher d_P enormous saving is obtained in the separation cost. But the catalyst decay is more (because of larger t) and hence the cost associated with the regeneration of the catalyst is more. We must select d_P from the economic analysis of these two costs. For intermediate values of λ_0 and for a certain region of conversion there are three values of d_P to get the same conversion. For higher values of λ_0, there is only one level of d_P to get the specified conversion.

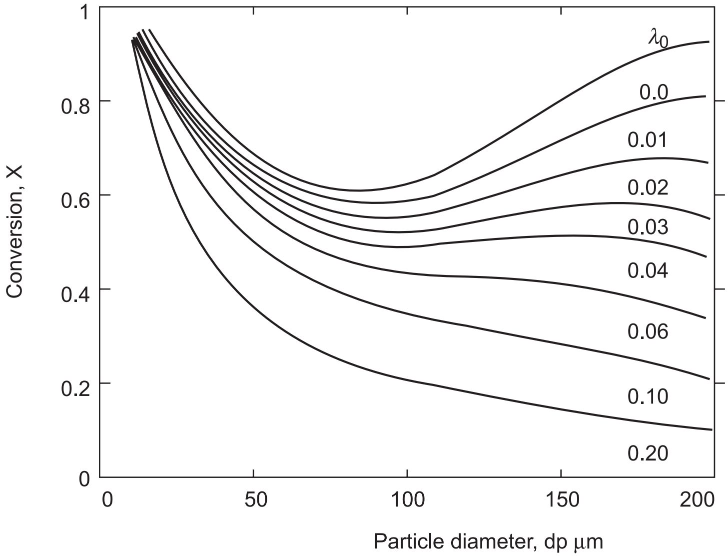


Fig. 6.4 Effect of particle diameter on the particle residence time (Chidambaram,1985) Legend: same as in Fig. 6.3

In the present study, the particle diameter is restricted to 200 micron so that for the values of the other parameters used, Thiele modulus is less than 0.4. As indicated by Pratt (1974) and Fan (1981), when the Thiele modulus is less than about 1, the resistance for intra-particle diffusion is negligibly small in the transport reactors. Thus, the model which neglects the intra-particle diffusion is justifiable for the present case studied.

In conclusion, analytical solutions are derived for the conversion of the gas reactant in a vertical transport reactor, wherein gas and catalytic particles are assumed to move by plug flow upwards and the catalyst activity deceases exponentially with time-on-stream. A particularly interesting behaviour is the minimum shown in the conversion with respect to the particle diameter. For large values of the decay constant, the conversion decreases continuously with the particle diameter.

6.3 MODELLING BCSR FOR HYDROGENATION OF α-METHYL STYRENE

Govindarao and Chidambaram (1984) have shown that the distribution of solids affects strongly the conversions in a semi-batch BCSR. The purpose of the present note is to evaluate these effects on the hydrogenation of α-methyl styrene with pure hydrogen on palladium black in a semi batch BCSR. Data on conversion of hydrogen at different levels of catalyst loading reported by Pruden and Weber (1969, 1970) are considered for this purpose. The points in Fig. 6.5 correspond to this data. At the operating conditions of this experiment the slurry-phase dispersion coefficient is estimated from the standard correlation of Kato et al. (1972) to be 26.26 cm^2/s. The corresponding concentration distribution of the particles, as seen in Fig. 6.6, is quite significant.

6.3.1 Dispersion model

For pure gas entering a semi-batch BCSR we have:

$$C_1 = 1.0 \tag{6.54}$$

The other equations of the model, those for the concentration of the diffusing component in the liquid and on the catalyst phase, and the associated boundary conditions are (Govindarao and Chidambaram,1984):

$$\frac{1}{Pe_{GL}}\frac{d^2C_2}{dZ^2} + N_1\Phi(C_1 - C_2) - M_1 f(C_2 - C_3) \tag{6.55}$$

$$M_1 f(C_2 - C_3) - QfC_3 = 0 \tag{6.56}$$

$$\left.\frac{dC_2}{dZ}\right|_0 = 0 \tag{6.57a}$$

$$\left.\frac{dC_2}{dZ}\right|_1 = 0 \tag{6.57b}$$

Solving Eqs. (6.54)–(6.57) by the analytical method of Govindarao and Chidambaram (1984) (for the general case of finite dispersion in gas and slurry phases), we get:

$$C_2 = (q_1 + v_1)\sum_{j=0}^{\infty} B_{1j} exp[-Pe_p Z(\beta_1 + j)] + (q_2 + v_2)\sum_{j=0}^{\infty} B_{2j}\exp[-Pe_p Z(\beta_2 + j)] \tag{6.58}$$

$$C_3 = \left[\frac{M_1}{(M_1 + Q)}\right] C_2 \tag{6.59}$$

$$X = \left(\frac{N_1}{m_1}\right)\int_0^1 (1 - C_2)\,dZ \tag{6.60}$$

where $$\beta_1 = \left(\frac{N_1\Phi}{G_7}\right)^{0.5};\ \beta_2 = -\beta_1 \tag{6.61a}$$

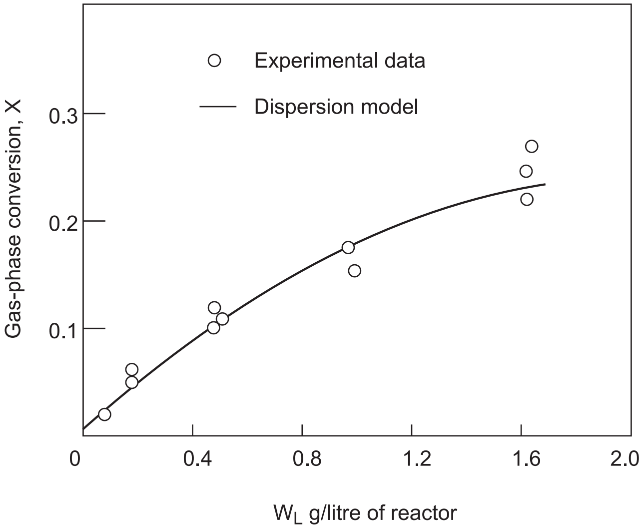


Fig. 6.5 Comparison of conversions predicted by the dispersion model with the experimental data of Pruden and Weber (1970)

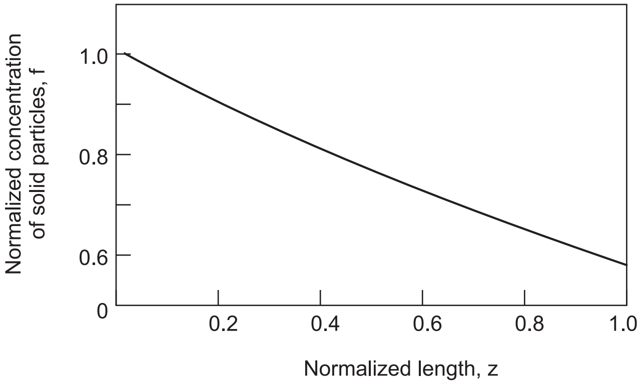


Fig. 6.6 Concentration distribution of solid particles from the dispersion model applied to the experimental conditions (Govindarao and Govindarao, 1986)

$$B_{ij} = \frac{G_8 B_{i(j-1)}}{[(\beta_i + j)^2 G_7 - N_1 \Phi]} \tag{6.61b}$$

And $$B_{i0} = 1: i = 1 \text{ and } 2 \text{ and } j = 1 \text{ to } \infty \tag{6.62}$$

6.3.2 Application to the experimental data

The model is applied to the hydrogenation of α-methyl styrene on palladium black in a semi batch BCSR, data for which are reported by Pruden and Weber (1970). The operating conditions are: $v_G = 2.13$ cm/s; $d_T = 3.82$ cm; $d_P = 6.75$ µm; gas, pure hydrogen; $T = 28°\text{C}$; pressure, 1 atm; $\rho_P = 11$ g/cm^{-3}. In the application, we assume that the reaction is pseudo first order with respect to hydrogen and zeroth order with respect to α-methyl styrene. The validity of the assumption is examined later. To calculate the conversion from Eq. (6.60) we need to know (i) dispersion coefficient, D_p, (ii) the gas-liquid and liquid-solid mass transfer coefficients (k_a and k_c) and (iii) the intrinsic rate constant, k_1.

Dispersion coefficient

The slurry phase dispersion coefficient calculated by applying the correlation of Kato et al. (1972) to the experimental data is 26.26 cm^2/s.

Mass transfer coefficients

The gas–liquid mass transfer coefficient (k_a) is calculated from the standard correlation of Calderbank and Moo-Young, (1961) as 0.038 cm/s. The liquid–solid mass transfer coefficient (k_c) is calculated from the standard correlation of Kobayashi and Saito (1965) as 0.424 cm/s.

Kinetics of the hydrogenation

Pruden and Weber (1970) assumed that the reaction was infinitely fast, based on a similar (but somewhat qualitative) observation by Sherwood and Farkas (1966). However, the argument (of fast kinetics) by Sherwood and Farkas (1966) was for a system where the size of the catalyst particles was 55 µm. At the low particle size of 6.75 µm used by Pruden and Weber (1970) the liquid–solid transfer rate increases considerably compared to the case where particles of 55 µm size are employed, and the rate of reaction becomes comparable to the rate of mass transfer. For hydrogenation of ethylene over Raney nickel particles of 5 µm size in a BCSR, Sherwood and Farkas (1966) had suggested that the hydrogenation was kinetic controlled due to the small size of the particles.

There have been several reports on the hydrogenation of α- methyl styrene, but most of these involve palladium or platinum catalysts supported on alumina or carbon. The reports of Sherwood and Farkas (1966) and Pruden and Weber (1970) are the only two reports involving palladium black catalyst. (As already pointed out, Pruden and Weber (1970) assumed the reaction to be fast, based on the suggestion made earlier by Sherwood and Farkas (1966).

In the present paper, the intrinsic kinetics is evaluated from the experimental data of Pruden and Weber (1970). An independent measurement of the kinetics will perhaps enhance the validity of the conclusions.

Order

Most reports on the hydrogenation of α– methyl styrene either indicated first order in hydrogen from the experimental determination or assumed the order to be first, based on others' reports. Since there is no direct report on the kinetics of the hydrogenation reaction with palladium black catalyst it is expected that, as with other palladium catalysts (Sakai and Ohi, 1977; Stefegle et al. 1980), the reaction is first order in hydrogen and zeroth order in α–methyl styrene. This assumption is likely to be valid for the data of Pruden and Weber (1970) because of the low level of conversions and high values of concentration of α- methyl styrene involved. Thus, first-order kinetics is assumed in interpreting the data. The close predictions obtained by the present evaluation vindicate this assumption.

Intrinsic rate constant

Pruden and Weber (1970) reported experimental conversions at five different catalyst loadings. Of these five sets one (corresponding to a catalyst loading of 0.491 g/litre) is used in estimating the hydrogenation rate constant from Eq. (6.68). The choice of this experimental data is, by and large, arbitrary. The estimated value of k_1 is 0.146 cm/s. This is about the same order of magnitude as the value of *kc,* 0.424 cm/s (estimated for the experimental data, as reported earlier), thus verifying the consideration of finite kinetics used here. This rate constant is used in evaluating the model for the other four sets of data, corresponding to four other values of the catalyst loading.

6.3.3 Evaluation

The curve in Fig. 6.5 shows the conversion versus catalyst loading characteristics predicted by the model (Eq. 6.60). As seen from the figure, the model explains the data very adequately. The largest deviation (absolute) between the experimental data and the calculated value is 0.020, which is well within the deviations observed from repeated experiments (about 0.04).

The reaction rate constant (k_1) is also estimated by assuming well-mixed slurry phase. The value estimated is 0.143 cm/s and the conversion versus catalyst loading characteristics are given by the solid line in Fig. 6.6. As seen here, both the dispersion model and the well-mixed slurry phase model predict the same behaviour. That is, the effect of the distribution of solid particles is not significant in the present experimental conditions reported by Pruden and Weber (1970) for hydrogenation of α-methyl styrene. The reaction rate constant estimated is 0.143 cm/s.

It should be noted that Pruden and Weber (1970) interpreted the experimental data by assuming the reaction to be infinitely fast, and then computed particle diameters to fit the experimental data (or what is equivalent, by assuming selective agglomeration of the particles). As discussed earlier, the assumption of fast kinetics is not valid for the conditions of their experiments, and the assumption of selective (an arbitrary) agglomeration is not tenable.

Though the present work illustrates the evaluation of the effects of solid distribution for a specific reaction system, hydrogenation of α-methyl styrene, the method presented is applicable to any reaction system when the pure gas is used and the kinetics are pseudo first order.

6.4 NON-CATALYTIC REACTIONS IN FLOW BCSR

Based on sedimentation–diffusion model for the solid particles mixing and shrinking core model for the non-catalytic reaction, analytical solutions are derived for the average conversion of the solid particles in cocurrent and countercurrent bubble column slurry reactors (BCSRs). The performance of cocurrent and countercurrent reactors are compared for identical operating conditions (Chidambaram,1984).

Bubble column slurry reactors (BCSRs) find extensive applications for gas-liquid-solid contacting where the solid is either a reactant or a catalyst. In this investigation, solids that take part in the reaction and follow the shrinking core model are analysed for flow BCSRs. The gas-liquid-solid reaction systems that follow shrinking core model are discussed by Ruether (1979) and Joshi et al. (1981). Ruether (1979) has analysed the performance of completely back mixed stirred tanks in series for the ash layer diffusion controlled mechanism. Joshi et al. (1981) have analysed the cocurrent BCSR performance based on the assumption that the residence time distribution (RTD) of solid particles is the same as that of liquid.

In the present analysis the sedimentation–diffusion model is used for the mixing characteristics of the solid particles. Analytical solutions are given for the average conversion of solid particles in isothermal cocurrent and countercurrent flow BCSRs. The effect of back mixing of the solid particles on the average conversion is analysed for the individual controlling steps of liquid-solid mass transfer, ash layer diffusion, and chemical reaction. Cocurrent and countercurrent flow BCSRs are compared for the given identical operating conditions.

6.4.1 Mathematical model and analytical solution

The assumptions made here are the same as those listed in Joshi et al. (1981) except that RTD of solid particles is different from that of liquid. In BCSRs the mixing characteristics of solid particles is given by sedimentation diffusion model Here, the longitudinal movement of the suspended solid particles is considered to be caused by longitudinal dispersion and settling of the solid particles and by the flow of the liquid. The governing dimensionless equations are

$$\frac{\partial f}{\partial \theta} = \frac{1}{Pe_P}\frac{\partial^2 f}{\partial Z^2} + \frac{\partial f}{\partial Z} \tag{6.63}$$

$$\left.\frac{\partial f}{\partial Z}\right|_0 = -\,(Pe_{PL} f_f + Pe_P f_0) \tag{6.64}$$

$$\left.\frac{\partial f}{\partial Z}\right|_1 = -\,f_1(Pe_{PL} + Pe_P) \qquad (6..65)$$

$$f = 0 \text{ at } \theta = 0 \tag{6.66}$$

where

$$\theta = \frac{U_P t}{L};\ Pe_P = \frac{U_P L}{D_P}$$

$$Pe_{PL} = \frac{U_L L}{D_P};\ f = \frac{w}{W_f} \tag{6.67}$$

$$U_P = U_S - U_L \text{ for cocurrent}$$

$$U_P = -(U_S + U_L) \text{ for countercurrent} \tag{6.68}$$

The exit age distribution of the solid particles is given by the solution of Eqs. (6.63)–(6.66) for an impulse input in feed catalyst concentration and it is given by

$$E(\theta) = a_0 \sum_{r=1}^{\infty} b_r e^{S_r \theta} \tag{6.69}$$

where

$$a_0 = 2\frac{Pe_{PL}}{Pe_P} e^{-Pe_P/2} \tag{6.70}$$

$$b_r = \frac{q_r^2}{[(q_r^2 + h_2 - h_1)\cos q_r + q_r(2 + h_1)\sin q_r]} \tag{6.71}$$

$$S_r = -\frac{1}{Pe_P}(q_r^2 + 0.25Pe_P^2) \tag{6.72}$$

and q_r is the root of the equation

$$\tan q_r = \frac{q_r h_1}{(q_r^2 + h_2)} \tag{6.73}$$

The mean residence time of the particle is given by

$$t_m = -\left(\frac{L}{U_P}\right)[\alpha_1 + \alpha_2 \exp(-Pe_P)] \tag{6.74}$$

The steps in deriving Eqs. (6.69) and (6.74) are given in the Appendix.

For the case of continuous feed of particles to a BCSR, having an exit age distribution of particles, $E(\theta)$, a mass balance gives (Levenspiel, 1972),

$$1 - X = \int_0^{\tau/\bar{t}} (1 - x)E(\theta)d\theta \tag{6.75}$$

where $E(\theta)$ is given by Eq. (6.69) and $(1 - X)$ is the fraction unreacted for a single particle. The expressions for $(1 - X)$ and τ will depend on the rate controlling step and diameter of the particle. In the following section, the individual controlling steps of liquid-solid mass transfer, ash diffusion and chemical reaction will be considered.

Case 1: Liquid–solid mass transfer controlled

For this case, the relationship between the time and fractional conversion of a single particle is given by (Levenspiel, 1972)

$$\frac{t}{\tau} = x \tag{6.76}$$

and

$$\tau = \frac{\rho_B d_p}{(6bk_{ls}c_L)} \tag{6.77}$$

Substituting Eq. (6.76) in Eq. (6.75) we get for the average conversion of solid particles in flow BCSRs

$$X_D = 1 - a_0 \sum_{r=1}^{\infty} b_r \frac{\bar{t}e^{S_r \tau/\bar{t}}}{\tau S_r^2} - \left(\frac{1}{S_r} + \frac{\bar{t}}{S_r^2 \tau}\right) \tag{6.78}$$

The fractional conversion for the case of a completely back mixed reactor can be obtained by substituting $E(\theta) = e^{-\theta}$ in Eq. (6.75) and is given by

$$X_B = \frac{t_B}{\tau}(1 - e^{-\tau/t_B}) \tag{6.79}$$

Similarly analytical solutions are derived for the individual cases of ash layer diffusion controlled and chemical reaction controlled steps and are given in Table 6.1.

Numerical evaluation

Table 6.2 shows the values of parameters used for the numerical evaluation. The dispersion coefficient D_P is calculated from the standard correlation of Kato et al. (Kato et al. 1973):

$$\frac{v_G d_T}{D_P} = \frac{13Fr}{(1+8Fr^{0.85})}(1+0.009\,\mathrm{Re}\,Fr^{-0.8}) \tag{6.80}$$

This correlation is perhaps representative of the mixing condition encountered in BCSRs in practice.

Cocurrent BCSRs

Figure 6.7 shows t_m versus d_p characteristics. For lower values of d_p, t_m increases slightly and for larger values of d_p, t_m increases steeply with d_p. As d_p increases, the dispersion coefficient D_P decreases and U_P decreases and hence the mean residence time, t_m increases. The longer the particles stay in the reactor the higher is the conversion. The value of t_m decreases with increase in v_L and d_T.

Figure 2a shows average conversion (X_D) versus d_p characteristics for the chemical reaction controlling step. Here, conversion versus d_p is plotted for two levels of mixing in the solid particles: complete back mixing and mixing corresponding to the dispersion coefficient given by the correlation of Kato et al. (1972).

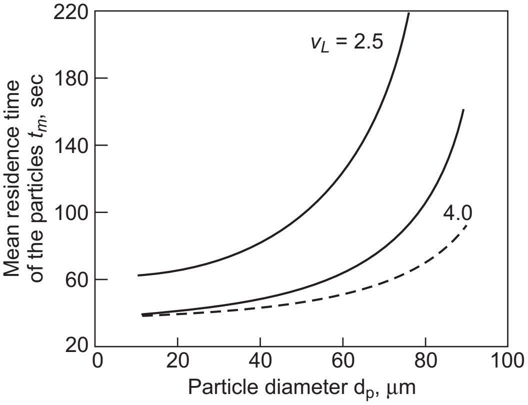


Fig. 6.7 Effect of particle diameter on the mean residence time of the particles Cocurrent flow; solid: d_T = 20 cm; dash: d_T = 40 cm. [D_P given by Eq. (6.80)].Other conditions: as in Table 6.2. (Chidambaram, 1984)

The finite dispersion curve indicates a minimum in the conversion with respect to the particle size, while the complete back mixing shows that the conversion decreases continuously with the particle size. In the latter case, an increase in d_p increases τ(the time required for complete conversion of a single particle), thus accounting for the decrease of the conversion. For this case t_m (= t_B) is the same for all d_p On the other hand, for finite dispersion of the solid particles, the effect is counter reacted by an increase in the conversion due to an increase in the mean residence time of the particles with the particle size (see Figure 6.7). As seen in Figure 6.7 for low ranges of d_p, the increase in t_m is not very significant and hence conversion continues to decrease with the particle size. For higher ranges of d_p, the increase in conversion due to increased t_m more than offsets the decrease in the conversion due to increase in τ and, therefore, conversion shows an increasing trend. Hence, there is a minimum in X versus d_p characteristics.

The discussion indicates that cocurrent flow BCSRs can be designed to give a desired conversion with relatively larger particle sizes as well. From economic point of view, operation with the higher particle size is preferable since this results in enormous savings in the investment of the particles, in the handling of the particles and the slurry, and more so in the separation of particles from the slurry, etc.

Figure 6.8a also shows that the conversion when the particles are in dispersion (X_D) is more than the conversion when the particles are completely back mixed (X_B). This enhancement in conversion is more pronounced at larger particle size. Figure 6.8b shows the similar behaviour for ash layer diffusion control. Similar type of behaviour is observed for liquid-solid mass transfer control step also.

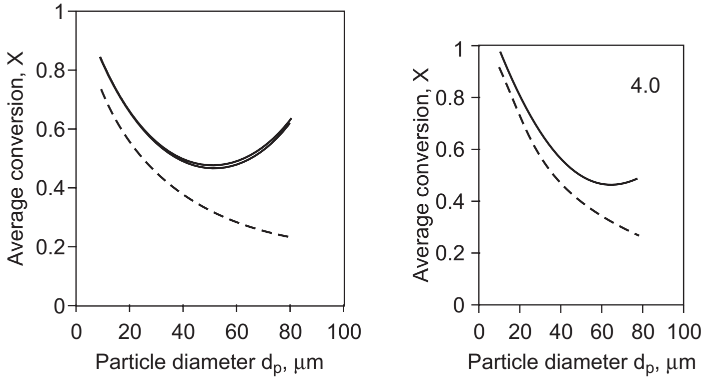


Fig. 6.8 Effect of particle diameter on the average conversion. Cocurrent flow; Upper curve: Particles finite dispersion [D_P given by Eq. (6.80)]. Lower curve: Dash: Particles completely backmixed (a) Chemical reaction controlling step; (b) Ash-layer diffusion controlling step (Chidambaram, 1984)

Figure 6.9 shows X_D versus D_P for 60 μm particle size in the case of chemical reaction control step. Conversion increases as D_P decreases. This is due to increase in t_m with decrease in D_P. Similar types of behaviours are observed for liquid-solid mass transfer control and ash-layer diffusion control steps also.

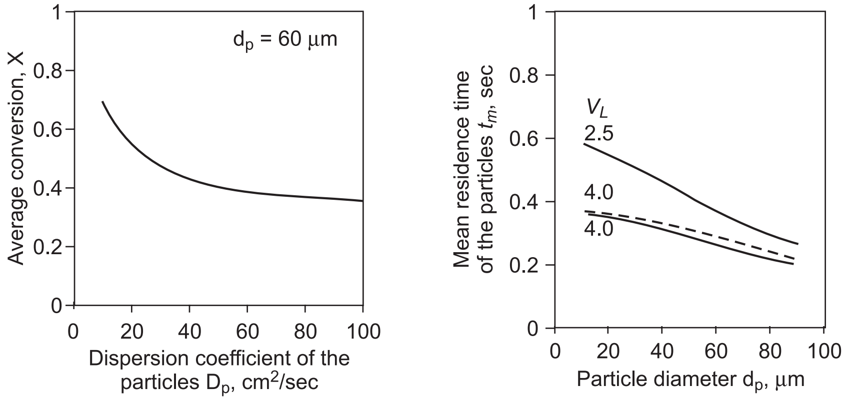


Fig. 6.9 (a) Average conversion versus particle dispersion coefficient. Cocurrent flow; chemical reaction controlling step; d_P = 60 mm; other conditions: as in Table 6.2 (b) Effect of particle diameter on the mean residence time of the particles. Countercurrent flow; —— d_T = 20 cm; .... d_T = 40 cm; [D_P given by Eq. (6.80)]; Other condition: as in Table 6.2.

Countercurrent BCSRs

Figure 6.10 shows t_m versus d_p characteristics for countercurrent BCSRs. Here t_m decreases as d_p increases, and t_m is less than t_B, the mean residence time of completely back mixed particles. The value of t_m decreases with increase in t_L and decrease in d_T.

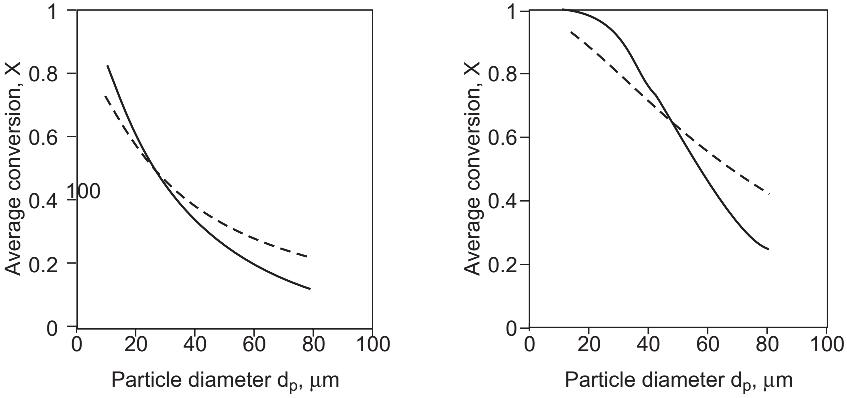


Fig. 6.10 Effect of particle diameter on the average conversion. Countercurrent flow;
____ Particles finite dispersion (DP given by Eq. (6.80))
.... Particles completely back-mixed; other conditions: as in Table 6.2.(a)
(a) Chemical reaction controlling step (b) Liquid–solid mass transfer controlling step. (Chidambaram, 1984)

Figure 6.11a shows conversion X_D versus d_p characteristics for the chemical reaction control step. As d_p increases, t_m decreases and τ increases. Hence, the conversion X_D continuously decreases with d_p. In the same figure X_B versus d_p trend is also shown. As seen in Figure 6.10, the decrease in t_m is not significant for lower range of d_p. Hence for a given d_p in this lower range, back mixed solid particles give lower conversion than with the finite dispersion.

At higher range of d_p, t_m decreases steeply with d_p. Value of t_m is significantly lower than the value of t_B . Hence for a given d_p in this range, the conversion will be higher for completely back mixed BCSRs. Figure 6.11b shows the similar behaviour for liquid-solid mass transfer control. Similar behaviour is obtained for ash-layer diffusion control also.

Figure 6.11 shows X versus D_P characteristics for 60 μm size particles when liquid-solid mass transfer is the controlling step. As D_P decreases, t_m decreases and hence X_D increases. Completely back mixed BCSRs gives the highest conversion. Similar type of behaviour is observed for ash-layer diffusion controlling and liquid-solid mass transfer controlling steps also.

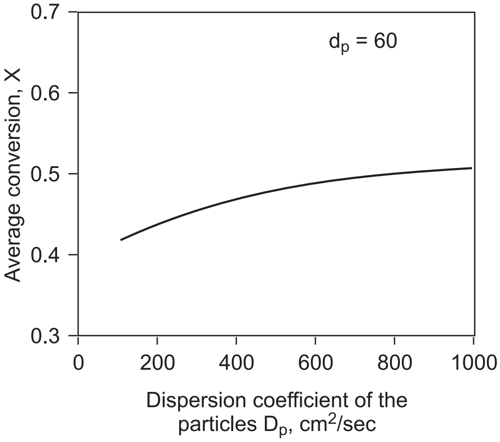


Fig. 6.11 Average conversion versus particle dispersion coefficient. Countercurrent flow; Liquid–solid mass transfer controlling step; d_P = 60 μm; Other conditions : as in Table 6.2

6.4.2 Comparison between cocurrent and countercurrent BCSRs

Figure 6.12a shows conversion X_D versus d_p characteristics for cocurrent and countercurrent BCSRs (the operating conditions are the same). Here, the chemical reaction controlling step is assumed. As seen in this figure, X_D is always higher in cocurrent BCSRs. The enhancement in the conversion is pronounced at larger particle diameter. This is mainly due to the sedimentation and diffusion of the particles and the associated increased mean residence time, t_m in the cocurrent BCSRs. Figure 6.12b shows the similar behaviour for liquid–solid mass transfer controlling step. Similar type of behaviour is observed for ash layer diffusion controlling step also.

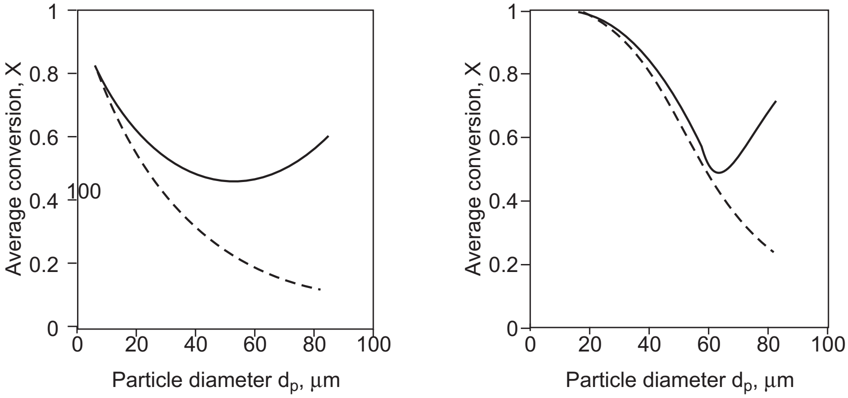


Fig. 6. 12 Comparison of average conversion of cocurrent and countercurrent flow BCSRs; solid: Cocurrent; dash: Countercurrent [D_P given by Eq. (6.80)]; Other conditions: as in Table 6.2 (a) Chemical reaction controlling step;(b) Liquid–solid mass transfer controlling step. (Chidambaram, 1984)

Conclusions Based on the shrinking core model for the gas-liquid-solid non-catalytic reaction and sedimentation-diffusion model for the solid particles mixing in BCSRs, analytical solutions are derived for the mean conversion of the solid particles for the individual controlling steps of liquid-solid mass transfer, ash layer diffusion and chemical reaction. Both cocurrent and countercurrent BCSRs are considered.

In cocurrent BCSRs, the conversion increases as dispersion of solid particles decreases. Complete back mixed BCSRs give the least conversion. A particularly interesting behaviour is the minimum shown in the conversion with respect to the particle diameter. In countercurrent BCSRs for lower d_p ranges, the conversion is the least when particles are completely backmixed. For higher particle sizes, conversion increases as dispersion of the particles increases and complete back mixed particles gives the highest conversion. Conversion decreases continuously with the particle diameter.

For the same operating conditions cocurrent BCSRs give higher conversion than countercurrent BCSRs. All these different and interesting behaviours of BCSRs are mainly due to the sedimentation and dispersion of the particles and the associated mean residence time of the particles. Thus the characteristics of mixing of the particles are the most important factor affecting the performance of BCSRs. The present analysis should be useful for the design and scale-up of BCSRs.

Table 6.1 *Analytical solutions for X_D and X_B for ash layer diffusion controlled and chemical reaction controlled steps (Chidambaram, 1984)*

For ash layer diffusion control:

$$X_D = 1 - a_0 \sum_{r=1}^{\infty} \left(\frac{2b_r \tau}{\bar{t}}\right) \int_1^0 (y - y^{2/3}) \exp\left[\frac{(1 - 3y^{2/3} + 2y) S_r \tau}{\bar{t}}\right] dy$$

$$X_B = \left(\frac{2\tau}{t_B}\right) \int_1^0 (y - y^{2/3}) \exp\left[-\frac{(1 - 3y^{2/3} + 2y)\tau}{t_B}\right] dy$$

where $\tau = \dfrac{\rho_B d_p^2}{[24 b D_e C_S]}$

For chemical reaction control:

$$X_D = 1 - a_0 \sum_{r=1}^{\infty} b_r \left[e^{S_r \tau/\bar{t}} \left(\frac{6\bar{t}^3}{\tau^3 S_r^4}\right) - \left(\frac{1}{S_r} + \frac{3\bar{t}}{\tau S_r^2} + \frac{6\bar{t}^2}{\tau^2 S_r^3} + \frac{6\bar{t}^3}{\tau^3 S_r^4}\right)\right]$$

$$X_B = 3\left(\frac{t_B}{\tau}\right) - 6\left(\frac{t_B}{\tau}\right)^2 + 6\left(\frac{t_B}{\tau}\right)^3 (1 - e^{-\tau/t_B})$$

where $\tau = \dfrac{\rho_B d_p}{(2 b k_r C_S)}$

Table 6.2 *Parameters used for numerical evaluation (Chidambaram, 1984)*

Pressure: 1 atm
Temperature, T: 298.1°K
Density of the liquid, ρ_L: 0.85 g cm^{-3}
Density of the particle, ρ_P: 3.35 g cm^{-3}
Molar density of the particle, ρ_B: 0.0335 g mole cm^{-3}
Bubble diameter: 0.28 cm
Reactor length, L: 200 cm
Reactor diameter, d_T: 20 cm
Superficial velocity of the gas, v_G: 7.5 cm sec^{-1}
Superficial velocity of the liquid, v_L: 2.5 cm sec^{-1}
Particle diameter, d_P: 10, 20, 30, 40, 50, 60, 70, 80 μm
Reaction rate constant, k_r: 0.04 cm sec^{-1}
Diffusivity through ash layer: 1.0 × 10^{-5} sec^{-1}
Liquid-solid mass transfer coefficient k_{LS}: evaluated by the equation of Brian and Hales (1969)
Fractional gas hold-up, ε: 0.25

Appendix

Here the derivation of Eqs. (6.69)–(6.73) is given. Taking Laplace transformation of Eqs. (6.63)–(6.65) with impulse δ input in the feed particle concentration gives:

$$\frac{1}{Pe_P}\frac{d^2F}{dZ^2}+\frac{dF}{dZ}-sF=0 \tag{A1}$$

$$\left.\frac{dF}{dZ}\right|_0=-(Pe_{PL}+Pe_PF_0) \tag{A2}$$

$$\left.\frac{dF}{dZ}\right|_1=-F_1(Pe_{PL}+Pe_P) \tag{A3}$$

solution of Eq. (A1) is given by

$$F=[\beta_1\cosh(mZ)+\beta_2\sinh(mZ)]e^{-(Pe_P/2)Z} \tag{A4}$$

where
$$m=\left(\frac{Pe_P}{2}\right)\left[1+\left(\frac{4s}{Pe_P}\right)\right]^{0.5} \tag{A5}$$

β_1 and β_2 are obtained by using the boundary conditions [Eqs. (A2) and (A3)] and are given by

$$\beta_1=\frac{Pe_{PL}d_1}{(md_2+m_3d_1)} \tag{A6}$$

$$\beta_2=-\frac{Pe_{PL}d_2}{(md_2+m_3d_1)} \tag{A7}$$

Now $$F\Big|_1 = e^{m3}\,\frac{[d_1 Pe_{PL}\cosh(m) - d_2 Pe_{PL}\sinh(m)]}{(md_2 + m_3 d_1)} \tag{A8}$$

Inversion of Eq. (A8) by method of residues gives Eqs. (6.69)–(6.73). We know that

$$\theta_m = \frac{\int_0^\infty \theta f_1 d\theta}{\int_0^\infty f_1 d\theta} = \int_0^\infty \theta f d\theta \tag{A9}$$

$$= \underset{s\to 0}{Lt}\int_0^\infty \theta f_1 e^{-s\theta} d\theta = \underset{s\to 0}{Lt}\left(-\frac{dF_1}{ds}\right) \tag{A10}$$

Substituting Eq. (A8) in (A10) gives

$$\theta_m = -[\alpha_1 + \alpha_2 e^{-Pe_P}] \tag{A11}$$

and hence Eq. (6.74)

$$t_m = -\left(\frac{L}{U_P}\right)[\alpha_1 + \alpha_2 e^{-Pe_P}] \tag{A12}$$

where $$\alpha_1 = a_1 a_2 a_4 - \left(\frac{Pe_{PL}}{Pe_P}\right) \tag{A13}$$

$$\alpha_2 = a_2[Pe_P a_4 a_5 - a_3(a_6 Pe_P + a_1)] - \left[\frac{(a_3 e^{Pe_P})}{Pe_P}\right] \tag{A14}$$

$$a_1 = a_3 + a_4 \tag{A15}$$

$$a_2 = \frac{Pe_{PL}}{(Pe_P a_4)^2} \tag{A16}$$

$$a_3 = Pe_P + Pe_{PL} \tag{A17}$$

$$a_4 = Pe_{PL}\exp(-Pe_P) \tag{A18}$$

$$a_5 = 1 + a_3 \tag{A19}$$

$$a_6 = -(1 + Pe_{PL})\exp(-Pe_P) \tag{A20}$$

Nomenclature (for section 6.3)

a = surface area of gas bubbles per unit volume of gas [cm^2 cm^{-3}]

a_w = surface area of particles per unit weight of catalyst [cm^2 g^{-1}]

B_{ij} = defined by Eq. (6.61b)

C = concentration of diffusing component [gmol cm^{-3}]

$C_1 = C_0 / \bar{C}_G^0$, normalized concentration in the gas phase

$C_2 = m_1 C_0 / \bar{C}_G^0$, normalized concentration in liquid phase

$C_3 = m_1 C_0 / \bar{C}_G^0$, normalized concentration of surface particles

$\bar{C}_G^0$ = concentration of the diffusing component in the entering gas phase [gmol cm^{-3}]

D = axial dispersion coefficient [cm^2 s^{-1}]

d_p = diameter of particles [cm]

d_T = reactor diameter [cm]

$f = w/(W\tau)$, normalized concentration of particles, given by exp ($Pe_P Z$)

$$G_1 = \sum_{j=0}^{\infty} B_{1j}(\beta_1 + j)$$

$$G_2 = \sum_{j=0}^{\infty} B_{2j}(\beta_2 + j)$$

$$G_3 = (v_1 G_1 + v_2 G_2)\Big|_{f=1} + \left(I_1 \sum_{j=0}^{\infty} B_{1j} \right)\Bigg|_{f=1} + \left(I_2 \sum_{j=0}^{\infty} B_{2j} \right)\Bigg|_{f=1}$$

$$G_4 = \sum_{j=0}^{\infty} B_{1j}(\beta_1 + j)\exp[-Pe_p(\beta_1 + j - 1)]$$

$$G_5 = \sum_{j=0}^{\infty} B_{2j}(\beta_2 + j)\exp[-Pe_p(\beta_2 + j - 1)]$$

$$G_6 = (v_1 G_4 + v_2 G_5)\Big|_{f=\exp(-Pe_P)} + \left(\sum_{j=0}^{\infty} I_1 B_{1j} f^{(\beta_1 + j)} \right)\Bigg|_{f=\exp(-Pe_P)} + \left(\sum_{j=0}^{\infty} I_2 B_{2j} f^{(\beta_2 + j)} \right)\Bigg|_{f=\exp(-Pe_P)}$$

$$G_7 = \frac{Pe_P^2}{Pe_{GL}}$$

$$G_8 = \frac{M_1 Q}{(M_1 + Q)}$$

H = Henry's law constant [cm^{3}atm gmol^{-1}]

$$I_1 = \frac{N_1 \Phi}{G_7 f^2 R_1}\left[\sum_{j=0}^{\infty} B_{2j} f^{(\beta_2 + j)} \right]$$

$$I_2 = -\frac{N_1 \Phi}{G_7 f^2 R_1}\left[\sum_{j=0}^{\infty} B_{1j} f^{(\beta_1 + j)} \right]$$

k = mass transfer coefficient [cm s^{-1}]

k_1 = surface reaction rate constant [cm s^{-1}]

L = length of reactor [cm]

$$M_1 = \frac{k_C a_w W L \tau}{U_G}$$

$$m_1 = \frac{H}{RT}$$

$$N_1 = \frac{k_a a L}{U_G}$$

$$Pe_{GL} = \frac{U_G L}{D_p}$$

$Pe_P = \dfrac{U_S L}{D_p}$, Pecklet number of particles

$$Q = \frac{k_1 a_w W L \tau}{U_G}$$

$$q_1 = \frac{(-G_6 - q_2 G_5)}{G_4}$$

$$q_2 = \frac{\left(-G_6 + \dfrac{G_3 G_4}{G_1}\right)}{\left(G_5 - \dfrac{G_2 G_4}{G_1}\right)}$$

R = gas constant [cm^{3}atm gmol^{-1}deg^{-1}]

$$R_1 = \sum_{j=0}^{\infty} B_{1j} f^{(\beta_1 + j)} \sum_{j=0}^{\infty} B_{2j} (\beta_2 + j) f^{(\beta_2 + j - 1)} - \sum_{j=0}^{\infty} B_{2j} f^{(\beta_2 + j)} \sum_{j=0}^{\infty} B_{1j} (\beta_1 + j) f^{(\beta_1 + j - 1)}$$

T = temperature [K]

U_G = bubble rise velocity [cm/sec]

U_S = mean settling velocity of particles [cm/sec]

v_G = superficial velocity of gas [cm/sec]

W = catalyst loading [g/cm^3]

W_L = catalyst loading, g/liter of the reactor

w = concentration of particles [g/cm^3]

X = gas-phase conversion

$Z = z/L$, normalized height from bottom of column

z = height from bottom of column [cm]

β_1, β_2 = defined by Eq. (6.61a)

$$v_1 = \int_0^f I_1 \, df$$

$$v_2 = \int_0^f I_2 \, df$$

ε = fractional hold up

ρ = density [g cm^3]

$$\tau = \frac{(U_S L / D_p)}{[1 - \exp(-U_S L / D_p)]}$$

$$\Phi = \frac{\varepsilon}{(1 - \varepsilon)}$$

Subscripts

a = gas–liquid

c = fluid–particle

G = gas phase

L = liquid phase

P = particle

S = particle surface

Nomenclature (for section 6.4)

a_0	defined by Eq. (6.70)
a_1 to a_6	defined by Eqs. (A13)–(A19), respectively
b	stoichiometry coefficient
b_r	defined by Eq. (6.71)
C	concentration of the diffusing component in the phase indicated by the subscript, g mol cm^{-3}
d_1	$m \cosh(m) + (Pe_{PL} + 0.5Pe_P)\sinh(m)$
d_2	$m \sinh(m) + (Pe_{PL} + 0.5Pe_P)\cos(m)$
d_p	diameter of the particles, cm
d_T	reactor diameter, cm
D_e	effective diffusivity in the ash layer, cm^2 sec^{-1}
D_P	axial dispersion coefficient of the particles, cm^2 sec^{-1}
$E(\theta)$	exit age distribution function of the particles for an impulse input in the feed
f	normalized solids concentration, $\dfrac{w}{W_f}$

F	Laplace transformed f
Fr	Froude number, $\dfrac{v_G}{(981 d_T)^{0.5}}$
h_1	Pe_{PL}
h_2	$\left(\dfrac{Pe_P^2}{4}\right)+\left(\dfrac{Pe_P Pe_{PL}}{2}\right)$
k_r	reaction rate constant, cm sec^{-1}
k_{ls}	liquid–solid mass transfer coefficient, cm sec^{-1}
L	length of the reactor, cm
m	$\left(\dfrac{1+4s}{Pe_P}\right)^{0.5}\left(\dfrac{Pe_P}{2}\right)$
m_3	$-\dfrac{Pe_P}{2}$
Pe_P	$\dfrac{U_P L}{D_P}$, Peclet number of the particles
Pe_{PL}	$\dfrac{U_L L}{D_P}$
q_r	roots of the Eq. (6.73)
Re	$\dfrac{d_P U_t \rho_P}{\mu}$, particles Reynolds number
S_r	defined by Eq. (6.72)
s	Laplace variable
t	time, sec
$\bar{t}$	$\dfrac{L}{U_P}$, sec
t_B	$\dfrac{L}{U_L}$, sec
t_m	mean residence time of the particles given by Eq. (A.12), sec
U_L	liquid velocity in the reactor, cm sec^{-1}
U_P	net velocity of the particles in the reactor, cm sec^{-1}
U_S	particles settling velocity, cm sec^{-1}
U_t	particles terminal velocity, cm sec^{--1}
v_G	superficial velocity of gas, cm sec^{-1}
v_L	superficial velocity of liquid, cm sec^{-1}
w	solid concentration in the reactor, g cm^{-3}
W_f	solid concentration in the feed slurry, g cm^{-3}
x	conversion of a single particle

X	average conversion of the particles
X_B	average conversion of the particles when they are completely backmixed
X_D	average conversion of the particles when they are in finite dispersion
y	$1 - x$
z	height from the slurry entering point, cm
Z	$\frac{z}{L}$, normalized height from the slurry entering point

Greek Letters

θ	$\frac{U_P t}{L}$, dimensionless time
θ_m	dimensionless mean residence time given by Eq. (A11)
τ	time required for complete conversion of a single particle
ρ_B	molar density of particles, g mole cm^{-3}
ρ_P	density of particles, gm cm^{-3}
β_1, β_2	defined by Eqs. (A6) and (A7), respectively
α_1, α_2	defined by Eqs. (A13) and (A14), respectively
ε	fractional gas hold-up
μ	viscosity of liquid

Subscripts

0 at $Z = 0$

1 at $Z = 1$

f at feed point

L liquid

S solid

Review Problems

1. Dhaouadi et al. [2008. Chemical Engg and Processing. 47. 548–556.] reported experimental and theoretical studies on gas liquid mass transfer in bubble column reactor. Prepare a report on the development of model and the experimental studies.
2. Bahena et al. [2004. Process biochemistry. 39. 2179–2182.] reported a work to validate experimentally that multiple steady-states may be achieved in a CSTR during hydrolysis of sucrose by invertase. Read the paper and prepare a report on the work studied.
3. Chidambaram (1998. Chemical Engg Commun) reported the improved yield obtained under periodic operation of an isothermal plug flow reactor for auto catalytic reactions. Write down the IVP ODEs used in the work and the method of calculating the average yield of the auto catalytic reactions.

4. Sivakumar et al. (1988. Canadian Journal of Chemical Engg. 66. 1000–1004.) reported the interpretation of the effect of particle size on heat transfer in vertical upflow of gas–solid suspension. Prepare a write on the work reported.
5. Wu and Wan (1993. Industrial and Engg Chemistry Res. 32. 2987–2990.) studied the kinetics of ethane Oxy-dehydrogenation to ethylene over AlPO-5 (molecular sieve catalyst). Prepare a write up on the work reported.
6. Chidambaram (1993. Canadian Journal of Chemical Engg. 71. 974–976.) reported the performance of isothermal plug flow reactor under feed concentration cycling for improvement in the average yield of homogeneous autocatalytic reactions. Read the paper and prepare a report on the work done, the method of solving the model equations.
7. Fan and Hwang (1981. Chemical Engg Science. 36. 1736–1740.) on a heterogeneous model for catalytic reactions in an isothermal pneumatic transport reactor with pore diffusion. Read the paper and prepare a report on the development of model equations and the analytical solution method and results obtained.
8. Chidambaram (1986. Computers and Chemical Engg. 10. 115–116) reported on the development of pde model for the transient behaviour of solid particles in flow bubble column slurry reactor. Read the paper and explain the Laplace inverse carried out by the method of residues.
9. Khilar (1983. Industrial and Engg Chemistry Fundamentals. 22. 264–266.) reported the effect of streaming potential on the permeability of sandstones. Prepare a report on the model equations developed and the results obtained.
10. Birtill (2007. Industrial and Engg Chemistry Research. 46. 2392–2398.) discusses the issues of measurement and modelling of the kinetics of catalyst decay in fixed beds: the Eurokin survey. Please read the paper and prepare a report on the work.

7

Discrimination of Mathematical Models

To develop a suitable model for a given system, usually assumptions are made in the reaction mechanism and kinetics, mixing pattern, catalyst deactivation kinetics, etc. In some cases, due to the flexibility in the assumptions and the nonlinearity of the system, there may be more than one model giving exact or very close analytical or numerical solution of the model equations. A major step is then to identify a suitable model for the system. In this chapter, three case studies are given on discriminating such mathematical models.

7.1 MODELLING DEACTIVATION DISGUISED KINETICS

Industrially important catalytic reactions often face catalyst deactivation during the course of chemical reaction. For design and optimization of reactors employing solid catalysts, knowledge of the kinetics of the primary reaction as well as of the deactivation reaction is required. Whenever the rate of deactivation is of the same order of magnitude as that of the reaction, simultaneous interpretation of the kinetics of the primary reaction and deactivation is required. In the case of a high chemical reaction rate along with a fast decay in the activity of the catalyst, it is often advantageous to have the reaction carried out in a high velocity dilute phase transport reactor.

Here the fresh catalyst is fed at the entrance of the reactor and the deactivated catalyst is removed at the reactor-exit continuously for regeneration. Usually plug flow of gas and catalyst prevails in the reactor. Both inter and intra-particle diffusion resistances are negligible because of the very small size particles used (40 to 100 μm diameter). The solid catalyst activity is defined as the ratio of reaction rate of the used catalyst and that of the fresh catalyst.

Krishnaswamy and Kittrell (1978) have shown that to interpret data obtained from an isothermal, transport reactor one may encounter the so called deactivation disguised kinetics. For example, the model A described by:

$$\frac{df}{dy} = -B_1 f^2 a \qquad \text{(main reaction)} \tag{7.1}$$

$$\frac{da}{dy} = -B_3 a \qquad \text{(deactivation reaction)} \tag{7.2}$$

and model B given by:

$$\frac{df}{dy} = -B_1 fa \tag{7.3}$$

$$\frac{da}{dy} = -(B_1 + B_3)\, fa \tag{7.4}$$

will both give identical conversion:

$$X = B_1 \frac{[1 - \exp(-B_1 y)]}{[(B_3 + B_1)(1 - \exp(-B_3 y)]} \tag{7.5}$$

Thus depending on the form of the catalyst deactivation rate equation chosen, the apparent kinetics of the primary chemical reaction can switch from second order rate expression to first order rate expression. This type of mathematical interaction between the primary reaction kinetics and the deactivation kinetics has been termed as the Deactivation Disguised Kinetics. Consequently, a kinetic model and its deactivation-disguised kinetics analog, if it exists, could fit the experimental conversion data obtained from the isothermal transport reactor equally well. Thus indeed, has been the case for the gas oil cracking and for hydrogen peroxide decomposition as discussed by Krishnaswamy and Kittrel (1978).

Lin (1980) has explored the existence of a deactivation-disguised kinetics in an isothermal steady state transport reactor. He has shown that the following model I given by

$$\frac{df}{dy} = -B_1 f^N a \tag{7.6}$$

$$\frac{da}{dy} = -B_3 f^N a^m \tag{7.7}$$

and the model II given by

$$\frac{df}{dy} = -b_1 f^h a \tag{7.8}$$

$$\frac{da}{dy} = -b_3\, f^{h_1}\, a^m \tag{7.9}$$

give identical conversion when

$$n = \left[\frac{q}{(2-m)}\right] + N \tag{7.10}$$

$$n_1 = -\left[\frac{q(m-1)}{(m-2)}\right] + N - 1 \tag{7.11}$$

$$b_1 = B_1 \tag{7.12}$$

$$b_3 = B_3 + \left[\frac{B_1 q}{(m-2)}\right] \tag{7.13}$$

where, $q = N_1 - N + 1$ and $q \neq 0$; $b_3 > 0$; and $m \neq 2$. It is interesting to note that for certain values of n, N_1 and m (e.g., $N = 1$, $N_1 = 1$ and $m = 1.5$), models I and II give identical conversion as well as identical activities. No method is reported so far to discriminate between model I and model II from the isothermal conversion data obtained in a transport reactor.

The nonlinearities of the model I and model II are different. For nonlinear systems, the laws of superposition will not hold good. That is, the response of the model for the two levels of an input will not be the same as that of the single equivalent level of the same input. The extent of deviation of the model depends on the nature of the nonlinearity of the model equations.

In the present work, transport reactor with model I and its disguised model II have been analyzed under periodic variation of inlet gas concentration (refer to Fig. 7.1) in order to discriminate between the two systems. One important class of periodic operations, as classified by Bailey (1977) is that in which the steady state condition is chosen arbitrarily and the mean value of the periodic input is same as the steady state input. Then, the time average performance of the reactor under periodic operation will be compared with that obtained under the conventional steady-state operation. The present work considers this type of operation. Periodic operation is used for the performance enhancement and to discriminate the kinetics.

Because of plug flow of both the solid and the gas streams, and the gas and catalyst particle are assumed to move at the same velocity we can solve the equation for steady state input $1/\gamma$ for the period $\gamma\tau$ and for the next part of periodic operation zero inlet concentration is used. The average concentration at the exit of the reactor is calculated as γC_e.

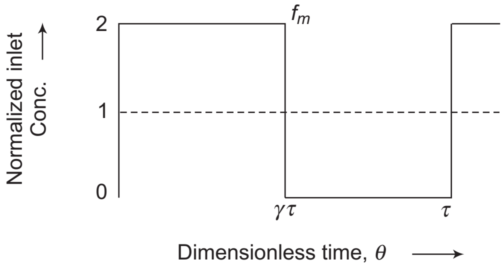


Fig. 7.1 Periodic inlet concentration function, ---- steady state, _____ periodic

The results of the simulation study are shown in Figs. 7.2 and 7.3. In both the figures, average conversion is plotted against the pulse width γ. In Fig. 7.2, the results for the system I ($N = 2$, $N_1 = 0$, $B_3 = 0.05$) and its disguised system II ($n = 1$, $n_1 = 1$, $b_3 = 1.05$) are given. These systems correspond to those proposed for the gas oil cracking and the decomposition of hydrogen peroxide, respectively (Krishnaswamy and Kittrell, 1978). $\gamma = 1$ represents the traditional steady state operation under which, of course, model I and model II are indistinguishable. As can be seen from these figures, model I can be easily distinguished from model II under periodic operation. By obtaining the conversion under periodic operation of an isothermal transport reactor, one can easily discriminate between the deactivation disguised kinetic models.

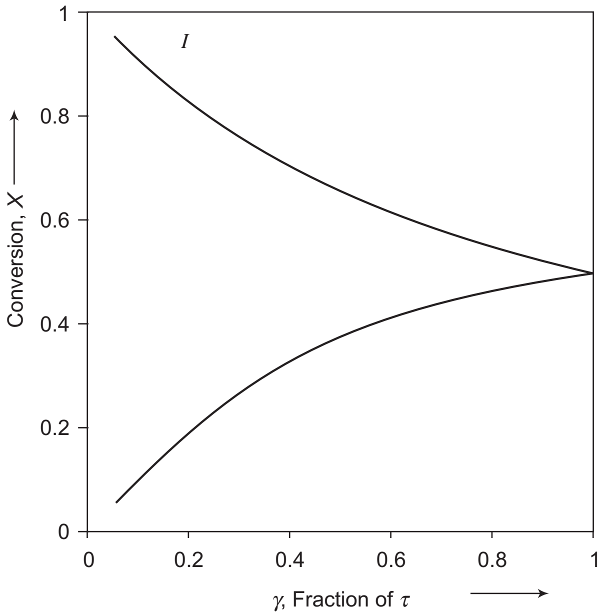


Fig. 7.2 Opposing trends shown by deactivation disguised kinetic models under periodic operation. B_2 = 1. System I: N = 2, N_1 = 0, m = 1, B_1 = 1.0 and B_3 = 0.05 System II: n = 1, n_1 = 1, m = 1, b_1 = 1.0 and b_3 = 1.05 (Sivakumar et al. 1988)

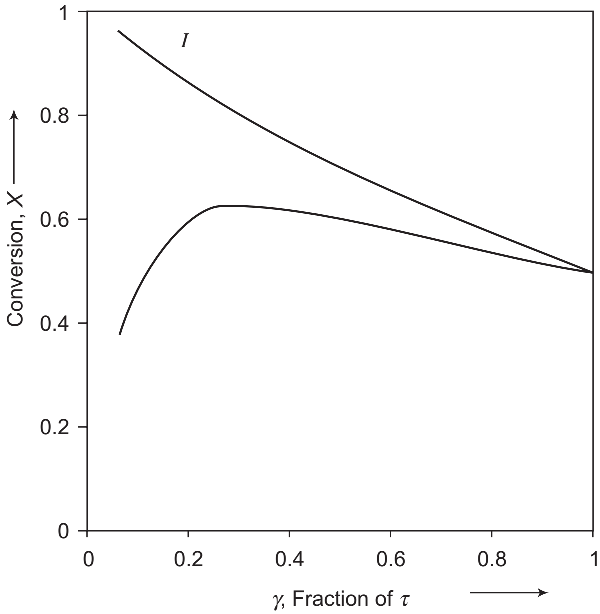


Fig. 7.3 Increasing trend for model I and resonance behaviour for model II. B_2 = 1. model I: N = 2.5, N_1 = 1, m = 1, B_1 = 1.25 and B_3 = 0.10 model II: n = 2, n_1 = 1.5, m = 1, b_1 = 1.25 and b_3 = 0.725 (Sivakumar et al. 1988)

7.2 MODELLING OF HYDRO-TREATING OF ASPHALTENES

Trejo et al. (2007) have proposed three different power-law kinetic models for the hydro-cracking of asphaltenes. Most of the heavy crude oils contain large amounts of asphaltenes formed by the association of molecules, including condensed poly-aromatic rings. Since the asphaltenes make catalytic hydro-treating (HDT) very difficult, a better understanding of their properties and the change they suffer during hydro-treating is very important for the development of technologies for the upgrading of heavy oils. According to Asaoka et al. (1981) the H/C atomic ratio of asphaltenes does not change drastically during asphaltenes hydrocracking, but V/C and S/C atomic ratios do change. Several reported works are available on the kinetic of asphaltenes isolated from the heavy crude oils. On the other hand, from the kinetic studies of the hydro-cracking of asphaltene and from other findings reported in the literature about the changes of asphaltenes properties and structural parameters during hydro-treating, it is likely that asphaltenes react by following two different paths: one easy-to-react and another hard-to-react. The resulting reaction mechanism can be similar to that reported by Kwak et al. (1992) for hydro nitrogenation (HDN) and hydro de-sulphurization (HDS) during residue conversion of bitumen and bitumen derived liquid. They adjusted the experimental data to a modified power-rate law model, in which parallel reaction schemes are considered as follows: pseudo-reaction orders greater than unity alternatively be modelled by two parallel first order reactions represented by:

$$\begin{tikzcd} & A1[=\delta A] \arrow[r, "k_1"] & B \\ A \arrow[ur] \arrow[dr] & & \\ & A2[=(1-\delta)A] \arrow[r, "k_2"] & B \end{tikzcd} \tag{7.14}$$

where A_1 and δ are the fraction of the organic compound that is more reactive and A_2 and $(1 - \delta)$ are the refractory fraction which is less reactive.

Based on the literature, Trejo et al. (2007) have proposed three different power-law kinetic models for the hydro-cracking of asphaltenes: a simple power-law model, a modified power-law model with same reaction order for more and less reactive asphaltenes and a modified power-law model with different reaction order for more and less reactive asphaltenes. Based on the absolute average deviation (AAD), Trejo et al. (2007) established that model 3 gives the best fit (AAD values are 2.79, 2.38, and 2.19). However, the values of R^2 are not different from each other (0.9988, 0.999, and 0.999). The periodic operation intentionally forces the inlet feed concentration to find the time average performance of the output (Bailey, 1977; Sivakumar et al. 1987). Let us apply the periodic operation of the reactors by simulation to discriminate the three different power-law kinetic models for asphaltenes hydro-cracking.

7.2.1 Assumptions and model equations

The model assumes isothermal plug flow with only reaction controlled mechanism and negligible mass transfer resistance and diffusional resistances. The reaction is carried out in a catalytic plug flow reactor. The rate equations are given by Trejo et al. (2007) for all three models.

Model 1

The kinetics of asphaltenes hydro-cracking is represented by a simple power-law model in both the asphaltenes and hydrogen:

$$\text{Asphaltenes} + \text{Hydrogen} \rightarrow \text{Hydrocracked products} \tag{7.15}$$

$$(-r_A) = kC_A^{\alpha}C_H^{\beta} \tag{7.16}$$

where α is the reaction order of asphaltenes, β the reaction order of hydrogen. C_A the asphaltenes concentration, C_H the hydrogen concentration, $(-r_A)$ the reaction rate of asphaltenes hydrocracking, and k is the rate constant. The steady state dimensionless equations are given by,

$$\frac{dC_A}{dZ} = -b_1 e^{-E_a/RT} C_A^{\alpha} C_H^{\beta} \tag{7.17}$$

$$\frac{dC_H}{dZ} = -b_2 e^{-E_a/RT} C_A^{\alpha} C_H^{\beta} \tag{7.18}$$

$$b_1 = \frac{k\ lC_0^{\alpha_1-1}C_1^{\beta}}{v} \tag{7.19}$$

$$b_2 = \frac{k\ lC_0^{\alpha_1}C_1^{\beta-1}}{v} \tag{7.20}$$

The parameter values are given by Trejo et al. (2007), $k = 5.65 \times 10^6$ mol/ m^3 sec, $l = 1$ m, $C_0 = 2.5818$ mol/m^3, $C_1 = 0.78$ mol/m^3, $v = 1000$ m/sec, E_{α} 10350 cal/mol, $R = 1.987$ cal/mol °K, $T = 693$ °K, $\alpha = 2.1$, $\beta = 1.28$.

Model 2

Based on the model proposed by Kwak et al. (1992) for HDS and HDN, the hydro-cracking of asphaltenes can also be represented in the following manner,

$$A\left[\begin{array}{r} A_1[=\delta A] + H_2 \xrightarrow{k_1} \\ \\ A_2\ [=(1-\delta)A] + H_2 \xrightarrow{K_2} \end{array}\right] \rightarrow \text{Hydrocracked products} \tag{7.21}$$

$$(-r_A) = \delta k_1 C_A C_H^{\beta} + (1-\delta)k_2 C_A C_H^{\beta}. \tag{7.22}$$

In this model, the reaction order of easy-to-react asphaltenes (A_1) and hard-to-react asphaltenes (A_2) are both one and for hydrogen (β), it may be differ from unity. The steady state dimensionless equations are given by,

$$\frac{dC_A}{dZ} = -(b_1 e^{-E_a/RT} C_A C_H^{\beta} + b_2 e^{-E_a/RT} C_A C_H^{\beta}) \tag{7.23}$$

$$\frac{dC_H}{dZ} = -(b_3 e^{-E_a/RT} C_A C_H^{\beta} + b_4 e^{-E_a/RT} C_A C_H^{\beta}) \tag{7.24}$$

$$b_1 = \frac{\delta k_1 l C_0^{\beta}}{v} \tag{7.25}$$

$$b_2 = \frac{(1-\delta)k_2 l C_0^{\beta}}{v} \tag{7.26}$$

$$b_3 = \frac{\delta k_1 l C_0 C_1^{\beta-1}}{v} \tag{7.27}$$

$$b_4 = \frac{(1-\delta) k_2 l C_0 C_1^{\beta-1}}{v} \tag{7.28}$$

The parameter values are given by Trejo et al. (2007) as: $k_1 = 8.95 \times 10^6$ mol/m^3.sec, $k_2 = 2.86 \times 10^7$ mol/m^3.sec, $l = 1$ m, $C_0 = 2.5818$ mol/m^3, $C_1 = 0.78$ mol/m^3, $v = 1000$ m/sec, $E_a = 10350$ cal/mol, $E_b = 9219$ cal/mol, $R = 1.987$ cal/mol.$^\circ$K, $T = 693$ $^\circ$K, $\beta = 1.28$ and $\delta = 0.4$.

Model 3

Since two types asphaltenes are assumed to react in model 2, i.e., easy-to-react and hard-to-react, both the following first-order reaction kinetics, it is also likely that each asphaltene type may have different reactivity and, consequently, different reaction orders. For this reason, the reaction order of asphaltenes, more reactive and less reactive, is considered in this model to be different than unity so that two reaction orders are supposed (α_1 for more reactive asphaltenes and α_2 for less reactive ones). The power-law model is based on reaction scheme given by Eq. (8).

$$(-r_A) = \delta k_1 C_A^{\alpha_1} C_H^{\beta} + (1-\delta) k_2 C_A^{\alpha_2} C_H^{\beta} \tag{7.29}$$

For Model 3, which considers the existence of two types of asphaltenes—one being reactive than the other one with different reaction orders—the steady state dimensionless equations are given by,

$$\frac{dC_A}{dZ} = -(b_1 e^{-E_a/RT} C_A^{\alpha_1} C_H^{\beta} + b_2 e^{-E_a/RT} C_A^{\alpha_2} C_H^{\beta}) \tag{7.30}$$

$$\frac{dC_H}{dZ} = -(b_3 e^{-E_a/RT} C_A^{\alpha_1} C_H^{\beta} + b_4 e^{-E_a/RT} C_A^{\alpha_2} C_H^{\beta}) \tag{7.31}$$

$$b_1 = \frac{\delta k_1 l C_0^{\alpha_1-1} C_1^{\beta}}{v} \tag{7.32}$$

$$b_2 = \frac{(1-\delta) k_2 l C_0^{\alpha_2-1} C_1^{\beta}}{v} \tag{7.33}$$

$$b_3 = \frac{\delta k_1 l C_0^{\alpha_1} C_1^{\beta-1}}{v} \tag{7.34}$$

$$b_4 = \frac{(1-\delta) k_2 l C_0^{\alpha_2} C_1^{\beta-1}}{v} \tag{7.35}$$

The parameter values are given by Trejo et al. (2007): $k_1 = 5.07 \times 10^6$ mol/m^3.sec, $k_2 = 3.54 \times 10^6$ mol/m^3.sec, $l = 1$ m, $C_0 = 2.5818$ mol/m^3, $C_1 = 0.78$ mol/m^3, $v = 1000$ m/sec, $E_a = 9940$ cal/mol, $E_b = 8650$ cal/mol, $R = 1.987$ cal/mol. K, $T = 693$ K, $\alpha_1 = 2.26$, $\alpha_2 = 0.93$, $\beta = 1.30$, and $\delta = 0.7$.

For all the three models, we have the initial conditions as:

at $$z = 0,\ C_A = C_{Af},\ C_H = C_{Hf} \tag{7.36}$$

7.2.2 Model description

The activation energies are similar than those obtained with model 2, but δ values and reaction orders of Model 3 are different. The fraction of the more reactive asphaltenes molecules (δ)

changed from 0.4 (model 2) to 0.7 (model 3) and the reaction order of hydrogen is almost the same (1.30 vs. 1.23).Both the models 2 and 3 differentiate between easy-to-react and hard-to-react asphaltenes, which is not possible with model 1. The activation energy calculated with model 1 is in between those determined with model 2, which seems to be the average of the easy-to-react and hard-to-react asphaltene molecules.

However, models 2 and 3 give different fraction of easy-to-react and hard-to-react asphaltenes. With model 2, the easy-to-react fraction is 0.4 and with model 3, the same fraction is 0.7. The reason for such a difference is mainly the consideration of constant and variable reaction order of asphaltene conversion, since model 2 keeps it constant as one, and for model 3 it is different than one. All the models give the same steady state conversion (refer to Figs. 7.5 and 7.6). To discriminate the models, let us study the periodic operation of the plug flow reactor similar to the one discussed in the previous case study.

7.2.3 Periodic operation

The feed concentration is assumed here as a rectangular pulse in C_{Af} as shown in Fig. 7.4a. In Fig. 7.4a, C_{Af} is the dimensionless amplitude of feed concentration pulse in asphaltenes and γ is the cycle split (i.e., pulse width expressed as a fraction of the dimensionless period, τ). The condition $\gamma = 1$ represents the conventional steady -state operation and $\gamma < 1$ represents the periodic operation.

In the type of forcing function (Fig. 7.4d), the concentration of asphaltenes is increased in the γ fraction of period in the feed whereas that of hydrogen concentration is decreased. In the remaining $(1 - \gamma)$ fraction of period, concentration of asphaltenes is decreased and that of hydrogen concentration in the feed is increased. During the first portion of the cycle, the feed concentration values are given by:

$$C_{Af} = C_A + C_A(1-\gamma) \tag{7.37}$$

$$C_{Hf} = C_T - C_{Af} \tag{7.38}$$

Let us define $(x)_{\text{out1}}$ as:

$$(C_A)_{\text{out}1} = (C_A)_{z=1} \tag{7.39}$$

In the second portion of cycling, the feed concentration is given by:

$$C_{Af} = C_A(1-\gamma) \tag{7.40}$$

$$C_{Hf} = C_T - C_{Af} \tag{7.41}$$

Let us define x_{out2} as:

$$(C_A)_{\text{out}2} = (C_A)_{z=1} \tag{7.42}$$

To evaluate the average concentration of asphaltenes and hydrogen under periodic operation, the transient equation of the tubular reactor including accumulation term in the left side of all the model equations should be considered. However, for isothermal plug flow reactors, the average conversion of asphaltenes and hydrogen can be obtained by solving steady state equation of all three model equations, for two levels of inlet concentration separately and getting the average value of outlet concentration. The steady states for two different outputs for two different inputs, i.e., one for C_{Af}

as per Eq. (7.37) and another for as per Eq. (7.40) are mixed to get the average concentration of asphaltenes at the reactor outlet. The average concentration of asphaltenes under periodic operation is calculated from Eqs. (7.39) and (7.42):

$$x_1 = \gamma(C_A)_{\text{out}\,1} + (1-\gamma)(C_A)_{\text{out}\,2} \tag{7.43}$$

Equation (7.43) is used for the inlet forcing functions shown in Fig. 7.4.

7.2.4 Results and discussions

The model equations, for the average conversion under the periodic operation, are solved numerically using the standard routines ode23 in the matlab package. The average conversion of asphaltenes is evaluated by simulation using the forcing function 7.4. Figure 7.5 shows the results. The figure shows that a distinct behaviour among the three kinetics model is obtained under periodic operation particularly when $\gamma \leq 0.5$. The present study shows by simulation of relevant equations that the kinetic models can be discriminated. However, if we carry out experimentally the periodic operation with the forcing function 7.4, then it is possible to find the most suitable kinetic model.

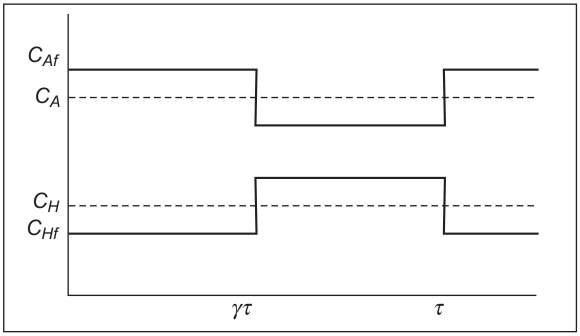


Fig. 7.4 Forcing function in the feed concentrations. solid: periodic operation, dash: steady-state operation. Periodic input cycling with increased value of asphaltenes and decreased value of hydrogen in the first part of cycling followed by reverse trend in feed concentration cycling for the second part

The present work considers the kinetics model reported in the literature. Model-A represents either the molecules containing sulphur or nitrogen. Model-B, represents the S-free and N-free products. However, it would be interesting to propose models for the reactions when basic nitrogen asphaltene constituents behave and similarly for the case of non-basic nitrogen asphaltenes. Similar situations arise for the acidic asphaltenes and amphoteric asphaletens. These situations are expected to give different yields of carbon residue and hence the different cracking patterns (Thangamani and Chidambaram, 2014).

The feed cycling with increased value of asphaltenes and decreased value of hydrogen in the first part of cycling followed by reverse trend in feed concentration cycling for the second part of pulse width gives a distinct difference in the behaviour of all the three models. All the three models kinetics can easily be discriminated under this type of feed concentration cycling mode.

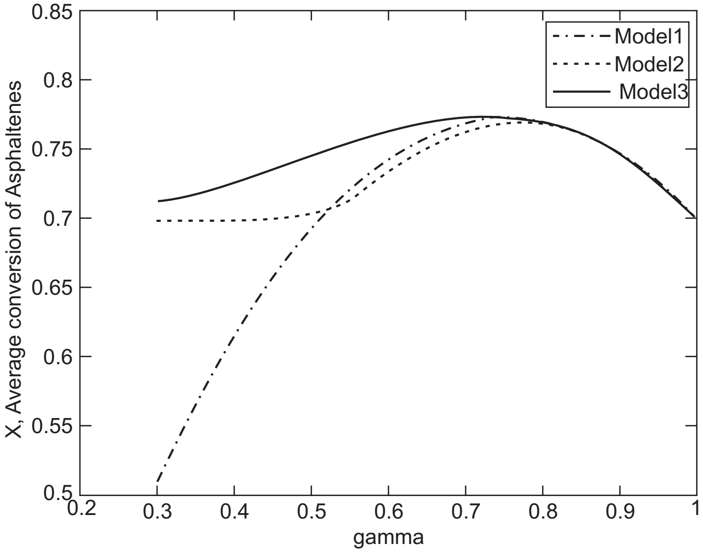


Fig. 7.5 Average conversion of asphaltenes under periodic operation (feed concentration cycling as in Fig. 1d, in C_A and CH)C_A =1, C_H = 1, C_T = 2 (Thangamani and Chidambarm, 2014)

7.3 MODELLING AUTOCATALYTIC POLYMERIZATION REACTIONS

Katime et al. (2011) have proposed different simple mechanisms for polymerization reactions (condensation polymers) with autocatalysis. It is assumed that the autocatalysis is through the activation by the product. In this reaction, common characteristics of the two mechanisms are: (a) auto catalysis should appear in all terms (Epstein and Pojman, 1998) and (b) all the kinetic equations contain the Michaelian term (Higgins, 1967). Katime et al. (2011) have assumed that the autocatalysis occurs by a dimerization between the monomer and one of its isomers, followed by the dissociation of dimeric form. Katime et. al. (2011) proposed the model with suitable model parameters and conditions to show the existence of the limit cycle behaviour of the system. However, in this work the model parameters are selected such that the system is stable. The objective of this work is to analyze the model equations under the periodic variation of inlet concentration on the average conversion and to check any difference between the models.

7.3.1 Model equations

In the polymerization reactions, the autocatalysis is due to activation by product: the polymers which will catalyze any previous step to their own production. In this work autocatalysis is achieved through the kinetic scheme (Epstein, 1989).

$$A + M \xrightarrow{\lambda} D \tag{7.44}$$

$$D \xrightarrow{\delta} 2M \tag{7.45}$$

where A is an isomer of monomer M and D is an intermediate dimeric form.

The term $-\beta x/(x+m)$, known as Michaelien type term and hence the combination of auto-catalysis and Michaelien type term $[hx - \beta x/(x + m)]$ is used in the model development. It is assumed that all the mechanisms should have: (i) appearance of autocatalysis and (ii) all kinetics equations contain the Michaelian term.

$$(?) \rightarrow G \overset{F}{\rightarrow} G \text{ disappearance} \tag{7.46}$$

$$G + M \overset{k}{\rightarrow} \text{Products} \tag{7.47}$$

(?) denotes the origin of G that will differ for both models: (i) the third compound G flows through the system and eliminates the monomer and (iii) G which eliminates the monomer can be a special adsorbent of the polymer.

All the reactions carried out in an isothermal plug flow reactor. The model equations are given by Katime et al. (2011).

Model 1

The steady state equations are given by:

$$\frac{dx}{dz} = hx - pxy - \frac{\beta x}{x+m} \tag{7.48}$$

$$\frac{dy}{dz} = \alpha x - k_{ter} y \tag{7.49}$$

Here $\beta = C/M_0$, $x = M/M_0$, $y = R/R_0$ M is the monomer and C is the initiator. The parameter values are given by: $h = 4$, $p = 2.05$, $\beta = 1$, $m = 1$, $\alpha = 1$, $k_{ter} = 1$. Here, x is the monomer dimensionless concentration and y is the concentration of dimensionless total propagators.

Model 2

The steady state model equations are given by:

$$\frac{dx}{dz} = hx - rx^2 - \frac{\beta xy}{x+m} \tag{7.50}$$

$$\frac{dy}{dz} = \alpha x - k_1 y \tag{7.51}$$

Here $x = M/M_0$, $y = U/U_0$, $\beta = k_1/M_0$, $\alpha = k_{\text{in}} M_0/R_0$, $m = F/(k_{\text{in}} M_0)$. U = polymers with first conformation. The parameter values are given by, $h = 4$, $r = 2$, $\beta = 1$, $m = 1$, $\alpha = 1$, $k_1 = 1$. For both the models, we have the initial conditions as

at $$z = 0, x = x_f, y = y_f \tag{7.52}$$

For both the models, the initiation or activation for the first propagator is first order with respect to the monomer. The autocatalysis occurs by a dimerization between the monomer and one of its isomers (A), followed by dissociation of the dimeric form. The isomerization of A into the monomer is also postulated, which leads to non-generative models.

With respect to the Michaelian term, it is present in all the models by eliminating the monomer with a substance G whose nature is diverse. In model 1, a third substance is not related to the polymerization. In model 2, the group of polymers is able to absorb/eliminate the monomer.

Monomer concentration is one of the main variables in both the models. The second variable in the model 1 is the total concentration of propagators and in model 2 is the concentration of polymer non-adsorbent of monomer. All these variables are in dimensionless form. In model-2, the value of y is also equal to that of R (Katime et al.2011).

7.3.2 Periodic operation

Let us analyze, the periodic operation of plug flow reactor for the polymerization reaction with autocatalysis. (Thangamani and Chidambaram, 2016). Several reported works are available on the periodic operation of plug flow reactors for simple reactions and as well as for the auto-catalytic reactions. The feed concentration is assumed here as a rectangular pulse in x_f as shown in Fig. 7.6. In Fig. 7.6, x_f is the dimensionless amplitude of feed concentration pulse in monomer (M) and γ is the cycle split (i.e., pulse width expressed as a fraction of the dimensionless period, τ). The condition $\gamma = 1$ represents the conventional steady-state operation and $\gamma < 1$ represents the periodic operation. If the dimensionless steady-state input is fixed as C_M, then we get on averaging the inlet pulse over period (τ) as:

$$x_f = \frac{C_M}{\gamma} \tag{7.53}$$

$$y_f = C_R \tag{7.54}$$

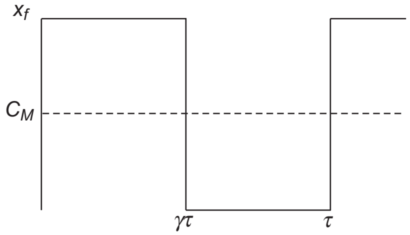


Fig. 7.6 First type of periodic input concentration of reactant in monomer (M). solid: periodic operation, dash: steady-state operation

To evaluate the average concentration of total propagators (R) under periodic operation, the transient equation of the tubular reactor including accumulation term in the left side of all the model equations should be considered. However, for isothermal plug flow reactors, the average conversion of total propagators (R) can be obtained by solving the steady state equation of all the model equations, for two levels of inlet concentration separately and getting the average value of outlet concentration.

The steady states for the two different outputs for two different inputs i.e., one for x_f as per Eq. (7.53) and another for $x_f = 0$, are mixed to get the average concentration of total propagators at the reactor outlet is given by:

$$(y)_{\text{out}} = \gamma (y)_{z=1} \tag{7.55}$$

where $(y)_{z=1}$ is the output for the input x_f as per Eq. (7.53). The average concentration of total propagators (R) is given by:

$$y_1 = (y)_{\text{out}} \tag{7.56}$$

$$y_1 = \gamma(y)_{z=1} \tag{7.57}$$

The average conversion of total propagator (*R*) is given by,

$$Y = 1 - y_1 \tag{7.58}$$

7.3.3 Results and discussions

Figure 7.7 shows the model behaviour under periodic operation in the feed concentration cycling in monomer (*M*), for the average conversion of total propagators (*R*). Figure 7.7 shows that a significant improvement in the average conversion of the total propagators (*R*) is obtained. An identical value of conversion (*Y*) under the conventional steady state operation is obtained. Model 2 gives an improved conversion compared to that of the model 1. The present study thus can be used to discriminate the models.

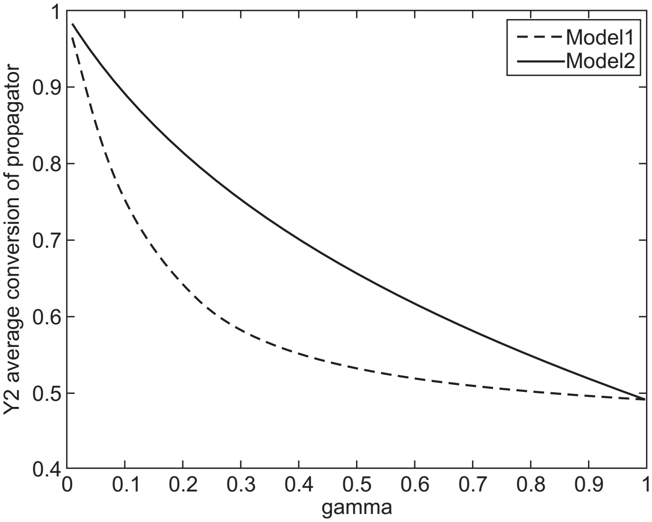


Fig. 7.7 Average conversion of total propagators (R) under periodic operation (feed concentration cycling in M.) $C_M = 0.1$, $C_R = 0.1$ (Thangamani and Chidambaram, 2016)

Nomenclature

A = isomer of M

b_1, b_2, b_3 b_4 = dimensionless variable for hydro-cracking of asphaltenes

C_0 = C_A/C_0 dimensionless concentration of asphaltenes in mol/m^3

C_1 = C_H/C_0 dimensionless concentration of hydrogen in mol/m^3

C_A, C_H = dimensionless feed concentration of asphaltenes and hydrogen steady-state operation in mol/m^3

C_T = total feed concentration of conventional steady state operation

C_M, C_R = dimensionless feed concentration of *M* and *R* at steady-state operation

D = dimer

E_a, E_b = activation energies in cal/mol

G = substance capable of eliminating M
k_1, k_2 = second order rate constant in mol/m^3.sec
l = length of transport reactor in m
M = monomer
$(-r_A)$ = reaction rate of asphaltenes hydro-cracking
R = total propagators
v = velocity in m/sec
x = M/M_0 dimensionless concentration of reactant M
x_1 = average concentration of asphaltenes
X = average conversion of asphaltenes
y = R/R_0 dimensionless concentration of product R for model 1
Z = normalized distance, z/L
z = reactor axial length
y_1 = average concentration of total propagators
Y_1 = average conversion of total propagators

Greek letters:

τ = cycle time, dimensionless
γ = pulse width expressed as a fraction of dimensionless period τ
α = reaction order of asphaltenes
β = reaction order of hydrogen
δ = reactivity of asphaltenes

Review Problems

1. What is meant by catalyst deactivation disguised kinetics in a transport reactor? Discuss a method of discriminating such models.
2. Write down the two models to be suggested for modelling of hydro-treating of Asphaltenes. Explain a method to discriminate the models.
3. Write down the two models to be suggested for modelling of auto catalytic polymerisation reactors. Explain a method to discriminate the models.
4. Bandstra and Tratnyek (2004. Industrial and Engg Chemistry Research. 43. 1615–1622) discussed the applicability of single site rate equation for reactions on inhomogeneous surfaces. Read the paper and prepare a report on the work done.

8

Sensitivity Analysis

Sensitivity analysis is concerned with the study of the effect of small (infinitesimal) changes in model parameters on the changes in the model outputs. In this chapter, methods of calculating the sensitivity are reviewed. Several examples are given.

8.1 INTRODUCTION

The sensitivity information can be used to estimate which parameters are most influential in affecting the behaviour of the system (Verma and Marbidelli, 1999). Such information is crucial for experimental design, data assimilation, reduction of complex nonlinear models, and evaluating optimization gradients and Jacobians in the setting of dynamic optimization and parameter estimation. The sensitivity analysis also plays a very important role in the dynamical systems. For example, when investigating periodic orbits, Lyapunov exponents, or other chaos indicators, and for general bifurcation analysis, computation of the sensitivities with respect to the initial conditions of the problem is a key component of the analysis.

To control a system means that by altering parameters and input variables, we can produce the desirable output. If varying a parameter does not alter system output (i.e., the system is insensitive to the parameter), then that parameter is not useful for control. Therefore, the sensitivity analysis can be used to identify which parameters have potential as control inputs.

Typically, the sensitivity analysis is carried out to the parameters of differential equations model. If some of the parameters are very sensitive on the output of our interest, then these parameters are to be estimated more precisely. When comparing with the experimental work, the effect of these parameters on the experimental results should be compared with that of the models. In the control system design problem, the variables which are very sensitive on the output variables, are to be considered as the manipulated variables. The objective in mathematical modelling of systems is to investigate a theoretical concept such as stability analysis, complex behaviour etc. Complex dynamics in difference equation or differential equations can emerge as a critical parameter is increased. At small values of the parameters, the system shows steady-state dynamics and as the parameter is increased the dynamics may change to oscillations, until, as the parameter is increased the dynamics can become extremely complex to the point of being chaotic. Interesting theoretical questions are to check which equations can show this behaviour and which parameters are responsible for it.

The methods for the sensitivity analysis are classified in to two distinct categories:

(i) Local method evaluates the local gradients in the parametric space.

(ii) Global method evaluates the effects of simultaneous, large variations of all the parameters on the output variables.

As stated earlier, the sensitivity analysis (SA) investigates how the variation in the output of a numerical model can be attributed to the variation of the input factors. Depending on whether output variability is obtained by varying the input around a reference (nominal) value, or across the entire feasible space, SA is either referred to as a local or a global. Local SA applications typically consider model parameter as varying input, and aim at assessing how their uncertainty impacts the model performance, i.e., how model performance changes when moving away from some optimal or reference parameter set. The partial derivatives or the finite differences are used as sensitivity indices in the context of local approaches. The local sensitivity can also be investigated by a method called the adjoint operator method. Examples of input factors are the parameters appearing in the model equation, and/or the initial conditions (states), and /or the boundary conditions or input forcing data of a dynamic model.

The first step of sensitivity analysis is the definition of the input factors, i.e., the neighbourhood of the nominal value $\bar{x}$ in the local SA, and the input variability space χ in the global SA. In Global SA method, the inputs are considered as stochastic variables, like variance based or density based variables, their PDFs (probability density functions) over the space χ must be defined. In the absence of specific information regarding the choice of a common approach is to assume independent, uniformly distributed inputs so that the possible results to the definition of χ only.

When the input factors x are the model parameters, feasible ranges can often be defined based on their physical meaning or from the existing literature. When the input factors are the model inputs, feasible ranges should account for the observational errors expected from the measuring devices, data pre-processing, interpolation, etc.

8.2 CALCULATION OF SENSITIVITY

As stated earlier, parametric sensitivity is the effect of variations of the input parameters on the system output variables (difference in the model output to a small change in the parameter value). The input parameters include the parameters in the model such as reaction rate constant, feed concentration, feed velocity, catalyst load, mass transfer coefficients, etc., as well as the initial conditions, operating and geometric parameters of the system. The sensitivity analysis provides effective tools to study the parametric sensitivity of systems. Let us consider a system $y(t, p_j)$. The local sensitivity of y with respect to the parameter p_j is denoted as $s(y; p_j)$ and it is defined as:

$$s(y;\, p_{\mathrm{j}}) = \frac{\partial y(t,\, p_j)}{\partial p_j} \tag{8.1}$$

$$= \lim\, (\Delta p_1 \rightarrow 0)\ \frac{[y(t,\, p_j + \Delta p_j) - y(t,\, p_j)]}{\Delta p_j} \tag{8.2}$$

The local sensitivity is also called the absolute sensitivity.

Similarly a normalized sensitivity (also called relative sensitivity) is defined as:

$$\left[\frac{\partial y(t,\, p_j)}{y}\right] \Bigg/ \left(\frac{\partial p_j}{p_j}\right) \tag{8.3}$$

$$= \frac{\partial(\ln\, y)}{\partial(\ln\, p_j)} \tag{8.4}$$

$$= \left(\frac{p_j}{y}\right) s(y;\, p_j) \tag{8.5}$$

The above equation does not depend on the units used and the level of variables used. When the sensitivity of scalar y with respect to each one of the parameters in the m vector p is considered, we get m sensitivity indices and it is a row vector defined by

$$S^T(y;\, p_j) = \left[\frac{\partial y}{\partial p_1}\, \frac{\partial y}{\partial p_2}\, \frac{\partial y}{\partial p_3} \cdots \frac{\partial y}{\partial p_m}\right] \tag{8.6}$$

$$= [s(y,\, p_1)\ s(y,\, p_2)\ s(y,\, p_3)\ ..s(y,\, p_m)] \tag{8.7}$$

If a system is described by n independent variables, y. then the column sensitivity vector is defined by:

$$\boldsymbol{s}(\boldsymbol{y};\, p_j) = \frac{\partial \boldsymbol{y}}{\partial p_j} \tag{8.8}$$

$$= [\partial \boldsymbol{y}/\partial p_1\ \partial \boldsymbol{y}/\partial p_2\ \partial \boldsymbol{y}/\partial p_3 \ldots\ \partial \boldsymbol{y}/p_{\mathrm{j}}]^{\mathrm{T}} \tag{8.9}$$

$$= [s(\boldsymbol{y};\, p_1),\ \ldots.\ s(\boldsymbol{y};\, p_m)]^T \tag{8.10}$$

If we combining all the rows and column sensitivity vector, we get a (n x m) matrix called the sensitivity matrix:

$$S(Y;P) = \begin{bmatrix} s(y_1;p_1) & s(y_1;p_2) & \cdots & s(y_1;p_m) \\ s(y_2;p_1) & s(y_2;p_2) & \cdots & s(y_2;p_m) \\ \cdots & \cdots & \cdots & \cdots \\ s(y_n;p_1) & s(y_n;p_2) & \cdots & s(y_n;p_m) \end{bmatrix} \tag{8.11}$$

We can vary only a single parameter at a time. This reduces the number of calculations, since we do not carry out all the combinations. The disadvantage is that we may ignore interactions between the parameters. The model response when p_1 and p_2 are simultaneously increased by 20% may be much greater than the response when p_1 or p_2 is increased by the same amount of change separately. In nonlinear systems, these interactions may be important.

An alternate approach is based on the fractional factorial (statistical) design. This approach treats parameter sensitivity analysis as if it were an experimental design for a statistical analysis of empirical data (ANOVA). The primary sensitivity index is not *S*, but *F* statistics is computed for the analysis of variance.

8.3 COMPUTATION ASPECTS OF LOCAL SENSITIVITY

There are three interesting methods to study: (1) Direct differential method (2) Finite difference method and (iii) Green's function method.

8.3.1 Direct differential method

Let us consider a system described by:

$$\frac{dy}{dt} = f(y, t, p) \tag{8.12}$$

initial condition: at $t = 0$; $y = a$. (8.13)

By applying the definition of the local sensitivity we can get:

$$d\left(\frac{\partial y}{\partial p_1}\right)\Big/ dt = \frac{ds(y;\, p_j)}{dt} \tag{8.14}$$

$$= \left(\frac{\partial f}{\partial y}\right)\left(\frac{\partial y}{\partial p_i}\right) + \left(\frac{\partial f}{\partial p_i}\right) \tag{8.15}$$

$$= \left(\frac{\partial f}{\partial y}\right) s\left(y;\, p_i\right) + \left(\frac{\partial f}{\partial p_i}\right) \tag{8.16}$$

Similarly, the derivative of the initial condition is also considered with respect to the parameters p_j (in case the parameters appear in the initial conditions). Similar analysis can be carried out for the multivariable systems.

$$\frac{d\boldsymbol{y}}{dt} = \boldsymbol{f}(\boldsymbol{y}, t, p);\ \text{at } t = 0;\ \boldsymbol{y} = \boldsymbol{y}_0 \tag{8.17}$$

$$\frac{d\boldsymbol{s}(\boldsymbol{y};\, p_j)}{dt} = J(t)\, s(\boldsymbol{y};\, p_j) + \frac{\partial \boldsymbol{f}}{\partial p_j} \tag{8.18}$$

where $J(t)$ is the Jacobian given by

$$\frac{\partial \boldsymbol{f}}{\partial y} = \left[\frac{\partial f_i}{\partial y_j}\right] \tag{8.19}$$

The non-homogeneous term in Eq. (8.18) is given by

$$\frac{\partial \boldsymbol{f}}{\partial p_j} = \left[\frac{\partial f_1}{\partial p_j}\, \frac{\partial f_2}{\partial p_j} \cdots \frac{\partial f_n}{\partial p_j}\right]^T \tag{8.20}$$

By solving simultaneously the model equation along with the above-formulated equations, we can get the local sensitivity. This method is called the direct differentiation method (DDM). The solution of system equations along with the equations for local sensitivity may pose computational problem when the whole set of equations become stiff. Sometimes, the formulation of sensitivity equations may be difficult because of implicit nature of appearance of the parameters in the system equations. It is important to note that for different input parameters, the sensitivity equation differs only the in the last term of Eq. (8.18), i.e., the non-homogeneous part.

8.3.2 Finite difference method

The local sensitivity is calculated using the finite difference scheme for the derivative as:

$$s(y_1; p_j) = \frac{\partial y_i}{\partial p_j} \tag{8.21a}$$

$$\approx \frac{[y_i(t, p_j + \Delta p_j) - y_i(t, p_j)]}{\Delta p_j} \tag{8.21b}$$

The model equations are to be solved once for the nominal value of p_j and second for the perturbed value of the parameter p_j. This method is called the finite difference method (FDM). In the previous method (DDM) we have to solve $2n$ equations at a time which may pose problems of solving stiff equations. The major problem in the FDM is what value of Δp_j to be used. Is it 10% of the nominal value or less? In practice, we need to take say 15% value of the nominal p_j as start-up value for Δp_j. The relevant 2 set of equations are to be solved. Then decrease the value of Δp_j to 10%. Again, the local sensitivity is to be obtained by solving the model equations and then followed by the calculation of local sensitivity. If the difference between these two set of local sensitivity is not significant, then there is no need for further computation. In case of significant difference in the local sensitivity, we need to reduce Δp_j to 5% of its nominal value.

8.3.3 The Green's function method

As noted in the previous section, for different input parameters p_j ($j = 1,2,3,\ldots n$), the m linear sensitivity [given by Eq. (8.18)] differs only in the non-homogeneous term, $\partial \boldsymbol{f}/\partial p_j$. We solve the homogeneous part first and then calculate the particular solution corresponding to each input parameter.

The homogeneous part corresponds to the Green's function problem:

$$\frac{d\boldsymbol{G}(t, \tau)}{dt} = \boldsymbol{J}(t)\, \boldsymbol{G}(t, \tau) \tag{8.22}$$

and

$$\boldsymbol{G}(\tau, \tau) = 1 \tag{8.23}$$

where $\boldsymbol{G}(t, \tau)$ is the Green's function.
The sensitivity function can be written as (Huang et al., 1978):

$$\boldsymbol{s}(y; p_j) = \frac{\partial \boldsymbol{y}(t)}{\partial p_j} \tag{8.24}$$

$$= \boldsymbol{G}(t,0)\, \delta + \int \boldsymbol{G}(t, \tau)\left[\frac{\partial \boldsymbol{f}(\tau)}{\partial p_j}\right] d\tau \tag{8.25}$$

The integration is form 0 to t,

where each element

$$\delta_k = \delta(p_j - y_k^{\,i}) \tag{8.26}$$

In the integral of Eq. (8.25), the first argument of G(t, τ), t is fixed, whereas the second one, τ, varies. This is called the Green's function method (GFM).

The DDM solves the model and the sensitivity equations (ODEs) simultaneously. The FDM solve model equations, and evaluate the local sensitivities using the finite difference approximations and the GFM solves first the homogeneous part of the sensitivity equations (the Green's function problem), and then computes the local sensitivities using the linear integral transforms.

8.4 EXAMPLES

Example 8.1

Sensitivity of the maximum yield in an isothermal batch reactor with consecutive reactions:

$$A \rightarrow B \rightarrow C$$

Each part of the reaction is first order with respect to the reactant. The reaction rate constants are k_1 and k_2. The reaction is carried out in a batch reactor with zero initial concentrations of B and C. The concentration of B exhibits a maximum (denoted as C_B^*) at a particular time t_m. Our interest is to evaluate the sensitivity of the maximum yield, Y_B^*, with respect to k_1 and separately to k_2.

The expression for Y_B* is obtained as (Levenspiel, 1972):

$$Y_B^* = \left(\frac{k_1}{k_2}\right)^h \tag{8.27}$$

where

$$h = \frac{k_2}{(k_2 - k_1)} \tag{8.28}$$

We can then derive the following expressions:

$$\frac{dY_B^*}{dk_1} = Y_B^* \, ph \tag{8.29}$$

where,

$$p = \left\{\left[\frac{1}{(k_1 - k_2)}\right]\ln\left(\frac{k_1}{k_2}\right)\right\} - \left(\frac{1}{k_1}\right) \tag{8.30}$$

$$\frac{dY_B^*}{dk_2} = Y_B^* \left[\frac{k_2}{(k_2 - k_1)}\right] p \tag{8.31}$$

The normalized sensitivity can be calculated as: $\left(\frac{k_2}{Y_B^*}\right)\left(\frac{dY_B^*}{dk_2}\right)$

The limitations of the local sensitivity analysis are:

1. Only investigate the behaviour of a model in the immediate region around the nominal parameter values. In some systems, input values are often very uncertain and cover large ranges, and cannot be investigated using the local techniques.
2. The local techniques only consider changes in one parameter at a time, with all other parameters fixed to their nominal values. In some systems, it is likely that interactions between parameters will be important.

Example 8.2

Consider the problems discussed by Meerschaert (1993):

$$p(x) = (0.65 - rx)(200 + qx) - 0.45x \tag{8.32}$$

with the nominal values of $q = 5$; $r = 0.01$

$\frac{dp}{dx} = 0$ gives the optimal solution of $x = \frac{5(13q - 49)}{(2q)} = 8$

Therefore, the absolute sensitivity of x to q is given by:

$$\begin{aligned}\frac{dx}{dq} &= \frac{245}{(2q^2)} \\ &= 4.9\end{aligned} \tag{8.33}$$

The relative sensitivity (of x to q) is given by: $\left(\frac{dx}{dq}\right)\left(\frac{q}{x}\right)$

$$= 3.0625 \tag{8.34a}$$

A 1% increase in q causes about 3% change in x.

Similarly the absolute sensitivity of x to r is given by: $\frac{dx}{dr} = -\frac{7}{(25r^2)} = -2{,}800$

The relative sensitivity (of x to r) is given by: $\left(\frac{dx}{dr}\right)\left(\frac{r}{x}\right)$

$$= (-2800)\left(\frac{0.01}{8}\right) \tag{8.34b}$$

$$= -\frac{7}{2}$$

If r goes up by 2%, then x goes down by 7%.

Example 8.3

Sensitivity analysis of a transport reactor

Consider a transport reactor carrying out catalytic reaction over the surface area of solid catalyst. The catalyst undergoes deactivation as the reaction takes place on the surface of the catalyst. We need to write two differential equations. One mass balance equation is required for the main reaction and the second equation is required for the deactivation reaction. The gas and the catalyst particle both are assumed to flow by plug flow. The reaction is assumed to take place at the surface of the catalyst.

$$\frac{dc}{dy} = -B_1 c^2 a \quad \text{(main reaction)} \tag{8.35a}$$

$$\frac{da}{dt} = -B_3 a \quad \text{(deactivation reaction)} \tag{8.35b}$$

The initial conditions are: at $y = 0$; $c = 1$ and $a = 1$. B_1 is related to the main reaction rate constant and B_3 is related to the deactivation rate constant. $Y = z/L$, where z is the axial distance and L is the length of the reactor.

The conversion at the exit of the reactor is given by:

$$X = B_1 \frac{[1 - \exp(-B_1 y)]}{[B_3 + B_1(1 - \exp(-B_3 y))]} \tag{8.36}$$

Our interest is to evaluate the sensitivity of the conversion (X) by B_1 and separately by B_3.

Taking the partial derivative of X with respect to B_1 and separately with respect to B_3, we get:

$$\frac{\partial X}{\partial B_1} = \frac{[(B_3 + B_1\alpha)\alpha + B_1\alpha^2]}{(B_3 + B_1\alpha)^2} \tag{8.37a}$$

$$\frac{\partial X}{\partial B_1} = \frac{(B_1 \exp(B_3)\,(B_3 + B_1\alpha) + B_1\alpha[1 + B_1 \exp(B_3)]}{[(B_3 + B_1\alpha)^2]} \tag{8.37b}$$

where, $\alpha = [1 - \exp(-B_3)]$ (8.37c)

The normalized sensitivity can be calculated as: $\left(\frac{B_1}{X}\right)\left(\frac{\partial X}{\partial B_1}\right); \left(\frac{B_2}{X}\right)\left(\frac{\partial X}{\partial B_2}\right)$

Assume the nominal model parameters as $B_1 = 1.0$ and $B_3 = 0.05$. Vary the values of the parameters B_1 from 0.8 to 1.20 in terms of 0.05 steps. B_3 can be varied from 0.03 to 0.08 in step of 0.01. Plot the graph of $\frac{\partial X}{\partial B_1}$ versus B_1 and separately $\frac{\partial X}{\partial B_3}$ versus B_3.

Example 8.4

Sensitivity analysis of a conical tank

The mathematical model equation, for a liquid level in a conical vessel, is given by (Ogunaike, 1986):

$$\frac{dx}{dt} = -kx^{-1.5} + \alpha u x^{-2} \tag{8.38}$$

$$\alpha = \frac{(3.14R^2)}{H^2}; k = \text{ valve coefficient}$$

R and H are the known dimensions of the conical tank. Assume $\alpha = 0.785$ and $k = 0.117$. The nominal level is $x = 40$ cm. Under the steady state condition, derive the expression of sensitivity of x by u.

At steady state condition, we have:

$$kx^{0.5} = \alpha u \tag{8.39}$$

$$x = \left(\frac{\alpha u}{k}\right)^2 \tag{8.40}$$

Taking the derivative of x with respect to u, we get:

$$\frac{\partial x}{\partial u} = 2\left(\frac{\alpha}{k}\right)^2 u \tag{8.41}$$

The normalized sensitivity is calculated as: $\left(\frac{u}{x}\right)\left(\frac{\partial x}{\partial x}\right) = 2$

A 1% increase in u causes about 2% change in x.

Example 8.5

A simplified but realistic model for waste-water treatment process is represented by a first order nonlinear equation (Goodwin and Sin, 1984):

$$\frac{dx}{dt} = \left[\frac{(c_f - x)}{\tau}\right] + k_1\, u\,(c_s - x) - k_2\alpha \tag{8.42}$$

where x = dissolved Oxygen concentration (DO), mg/l

u = air flow rate, l/h

τ = hydraulic time constant, h

c_f = inlet dissolved Oxygen concentration, mg/l

c_s = maximum dissolved Oxygen concentration (saturation limit), mg/l

k_1 = mass transfer coefficient, 1/l

k_2 = oxygen uptake rate, mg/l/h

The factor α ensures that the oxygen uptake becomes zero when the dissolved oxygen concentration falls to zero. This guarantees that x cannot become negative.

The nominal operating conditions are:

$$c_s = 9 \text{ mg}/l;\ u = 0.5,\ k_1 = 0.05\ l^{-1};\ k_2 = 2.06 \text{ mg}/l/\text{min};\ x = 2.714 \text{ mg}/l$$

Derive the expression for the sensitivity of x by u under the steady state condition.

At steady state condition, we get:

$$x_s = \frac{[-(c_f/\tau) + k_2\alpha - k_1 u\, c_s]}{[-(1/\tau) - k_1 u]} \tag{8.43}$$

Taking the derivative of x with respect to u, we get:

$$\frac{\partial x_s}{\partial u} = \frac{\{(k_1 c_s)[-(1/\tau) - k_1 u] + [-(c_f/\tau) + k_2\alpha - k_1 u\, c_s]\}}{[-(1/\tau) - k_1 u]^2} \tag{8.44}$$

The normalized sensitivity is calculated as: $\left(\frac{u}{x_s}\right)\left(\frac{\partial x_s}{\partial u}\right)$

Example 8.6

To demonstrate the usefulness of the sensitivity analysis in combustion kinetics, consider a moderate size model for the combustion of CH_4 in O_2–Ar mixture. In this system there are 13 species present and 23 rate constants; therefore, there is a total of 24 input parameters, 23 rate constants and one initial condition. Of interest is an analysis of the system near ignition, i.e., when $T = 2000$°K. The details of the reactions and the reaction rates are given by Steinfeld et al. (1999). Integrating the system of kinetic rate equations for the set of reactions given by Steinfeld et al.(1999), one can obtain the initial concentrations as:

$[CH_4] = 2.265 \times 10^{18}$ molecules/cm^3

$[O_2] = 4.530 \times 10^{18}$ molecules/cm^3

$[Ar] = 1.790 \times 10^{19}$ atoms/cm^3

$[CO_2] = [H_2] = 1$ molecule/cm^3

The concentration of all other intermediates and products are set to zero. We look at the sensitivities at $t = 2.5 \times 10^{-5}$ sec: this corresponds to the time at which most transient species in the reaction have reached their maximum values (refer to the Table given by Steibnfeld et al. 1999). Using the Green function method and solving the simultaneous differential equations, it is shown the reactions which have significant sensitivities. The conclusion that can be drawn is that reactions 1, 6, 14, and 18 are the four most important reactions for all the species. Reaction 15 is important for the production of CO_2, and some reactions of lesser significance are 10, 3, 6, 13, 2 and 5; all other reactions are insensitive. The number of reactions needed to model the process is reduced considerably. This become very useful in studying atmospheric and combustion processes, which may involve over 200 elementary reactions.

Example 8.7

Consider a thermal run away reaction of a batch reactor, with exothermic reaction A → B

The mass balance and the energy balance equations are given by:

$$\left(\frac{dA}{dt}\right) = -k\,A^n \tag{8.45}$$

$$\rho c_v \left(\frac{dT}{dt}\right) = (-\Delta H)k\,A^{\mathrm{n}} - S_v\,u\,(T - T_a) \tag{8.46}$$

$$k = k_0 \exp\left[-\frac{E}{(RT)}\right] \tag{8.47}$$

Here, ρ is the density of the fluid mixture [kg/m^3], c_v is the mean specific heat capacity of the reaction mixture, [J (kmol)$^{-1}$]; ΔH is the molar reaction enthalpy [J/mol], S_v is the surface area per unit volume [m^2/m^3], u is the overall heat transfer coefficient [J/(m^2 s K)], and T_a is the ambient temperature. The initial conditions are: at $t = 0$; $A = A_0$ and $T = T_0$.

The reactor at the explosive conditions is sensitive to small variations in, e.g., the initial temperature, while, under non-explosive conditions, the system is insensitivity to such variations. Thus the boundaries between the runaway (explosive) and non-runway [non-explosive] conditions can be identified on the basis of its sensitivity to small changes in the operating parameters. The system can also be characterized by the derivative of the maximum temperature versus the initial temperature.

Example 8.8

As discussed in Chapter 3, in the weather forecasting problem, *E.* Lorenz, a professor of Meteorology at MIT, was simulating a reduced order model of the atmosphere, which consists of 12 ODEs. He discovered a very important aspect of certain types of the nonlinear systems that of extreme sensitivity to the initial conditions. A very small difference in the initial conditions leads to different output behaviour for a long run. He pointed out that the long term prediction of certain systems (such as the weather) will never be possible.

8.5 FAST PROGRAM

The sensitivity analysis by the Global methods comprises the classical Monte Carlo method and the pattern search methods. Monte Carlo method is time consuming but involves little additional programming. Among the pattern search methods, the Fourier Amplitude Sensitivity Test (FAST) has been widely used. The method is described by Cukier et al. (1978) and the computer code of the method is discussed by McRae et al. (1982).

Essentially, the FAST method involves the simultaneous variation of all the parameters over the individual ranges of uncertainty. This variation is studied by transforming all the parameters into periodic functions of a search variable s by introducing a transformation function G_i and an associated frequency ω_i as shown below:

$$k_i = G_i \sin(\omega_i s) \tag{8.48}$$

By this transformation, the output state variables are made periodic functions of s and hence can be Fourier analyzed. The Fourier analysis of the solutions provides a measure of the effect of the ith frequency (and hence the parameter associated with that frequency) on the state variables. The Fourier coefficients thus obtained represent the average variation of the output variables over the parameter uncertainties. This variation is represented by a quantity called 'partial variance'. This is the normalized sum of squares of the Fourier coefficients of the fundamental frequency (ω_i) and its harmonics. Higher partial variances represent the higher sensitivity. The partial variations are then used to rank the parameters according to the relative influences over the output state variables.

8.6 DEPENDENCE OF THE SOLUTION OF A SET OF NONLINEAR EQUATIONS ON A PARAMETER

Sometimes in a set of nonlinear equations a parameter of physical importance appears. The goal of the computation is to find the dependence of the solution on the value of this parameter (Kubicek and Hlavcek, 1983). Kubicek and Hlavacek (1983) proposed a method. Consider a set of equations:

$$\begin{aligned} &f_1(x_1,\cdots,x_n,\alpha)=0\\ &\ldots..\\ &f_n(x_1,\ldots,x_n,\alpha)=0 \end{aligned} \tag{8.49}$$

where, α is the parameter under question. The dependence $x(\alpha)$ is required. By differentiating $f(x, \alpha) = 0$, we get $\Gamma(x, \alpha)\, dx + \left(\dfrac{\partial f}{\partial \alpha}\right) d\alpha = 0.$ Hence,

$$\frac{dx}{d\alpha} = -\Gamma^{-1}(x,\alpha)\frac{\partial f}{\partial \alpha} \tag{8.50}$$

subjected to an initial condition

$$x(\alpha_0) = x_0 \tag{8.51}$$

Here $\Gamma = \left\{\dfrac{\partial f_i}{\partial x_j}\right\}$ is the Jacobian matrix and

$$\frac{\partial f}{\partial \alpha} = \left(\frac{\partial f_1}{\partial \alpha},\cdots,\frac{\partial f_n}{\partial \alpha}\right)^T \tag{8.52}$$

It is supposed that

$$f(x_0, \alpha_0) = 0 \tag{8.53}$$

and the differential equation, Eq. (8.50), possesses a solution $x(\alpha)$ which fulfils Eq. (8.49) if $x(\alpha)$ is continuously differentiable and Γ is regular. If these conditions are not satisfied and if $x(\alpha)$ is a smooth curve in the space (x, α), a modified integration may be performed:

$$\frac{d(x', \alpha)}{dx_k} = -\Gamma_1^{-1}(x, \alpha)\frac{\partial f}{\partial x_k} \tag{8.54}$$

with an initial condition

$$x'(x_{k0}) = x'_0 \; \alpha(x_{k0}) = \alpha_0 \,, \tag{8.55}$$

where we have denoted $x' = (x_1, \cdots, x_{k-1}, x_k, x_{k+1}, \cdots, x_n)^T$ and k is fixed, $1 \le k \ge n$. The whole continuous dependence $x(\alpha)$ may be calculated by an alternated integration of Eq. (8.50) and Eq. (8.54), and the transition from Eq. (8.50) to Eq. (8.54) occurs if Γ becomes almost singular.

Example 8.9

Keesman (2011) presented an example of sensitivity analysis of a fedbatch bioreactor. The substrate concentration (S in mg/l) in a fed-batch bioreactor with Monod kinetic substrate consumption is described by:

$$\frac{dS}{dt} = -\mu\frac{S}{K_S + S} + u, \qquad S(0) = S_0 \tag{8.56}$$

where μ is the decay rate in mg/l/min, K_s is the half-saturation constant in mg/l, and u is the feed in mg/l/min. Notice that in the short-hand notation the time arguments are not explicitly shown. The Jacobi matrix is given by

$$\frac{\partial f(\cdot)}{\partial x} = -\mu\frac{K_S}{(K_S + S)^2} \tag{8.57}$$

Consequently, the parameter sensitivities are described by

$$\frac{dS_x}{dt} = \frac{d}{dt}\left[\frac{dS}{d\mu}\;\frac{dS}{dK_S}\right] \tag{8.58}$$

$$= \left[-\mu\frac{K_S}{(K_S + S)^2}\frac{dS}{d\mu} \;\; -\frac{S}{K_S + S} - \mu\frac{K_S}{(K_S + S)^2}\frac{dS}{dK_S} + \mu\frac{S}{(K_S + S)^2}\right] \tag{8.59}$$

with $S_x(0) = [0\ 0]$. Let the feed be chosen such that $u = \mu$. Then, an analytical solution of the differential equation with $S(0) = S_0$ can be found and is given by

$$S(t) = -K_S + \sqrt{K_S^2 + 2\mu K_S t + 2KS_0 + S_0^2} \tag{8.60}$$

$$= [S_0 = 0] - K_S + \sqrt{K_S^2 + 2\mu K_S t} \tag{8.61}$$

Hence, for $S_0 = 0$, the following parameter-sensitivities are found:

$$S_x(t, v) = \left[\frac{dS}{d\mu}\ \frac{dS}{dK_S}\right] \tag{8.62}$$

$$= \left[\frac{Kt}{\sqrt{K_S^2 + 2\mu K_S t}}\ \ -1 + \frac{K + \mu t}{\sqrt{K_S^2 + 2\mu K_S t}}\right] \tag{8.63}$$

The trajectories of the substrate concentration, $S(t)$, and both sensitivities, $S_x(t, v)$, for $\mu = 0.1$mg/l/min and K_S = 1 mg/l, are shown in Fig. 8.1. Basically, the feed has been chosen such that the sensitivity of S with respect to K_S (i.e., S_{K_S}) is maximized. Notice from Fig. 8.1 that both S and S_{K_S} show a monotonically increasing behaviour. Hence, for this specific choice of feed, the sensitivity of $S(t)$ with respect to K_S is increased by increasing the substrate concentration, according to a square root law. The increasing sensitivity for K_S allows subsequently a very good estimate of K_S from the fed-batch bioreactor data with $u = \mu$ and $S_0 = 0$.

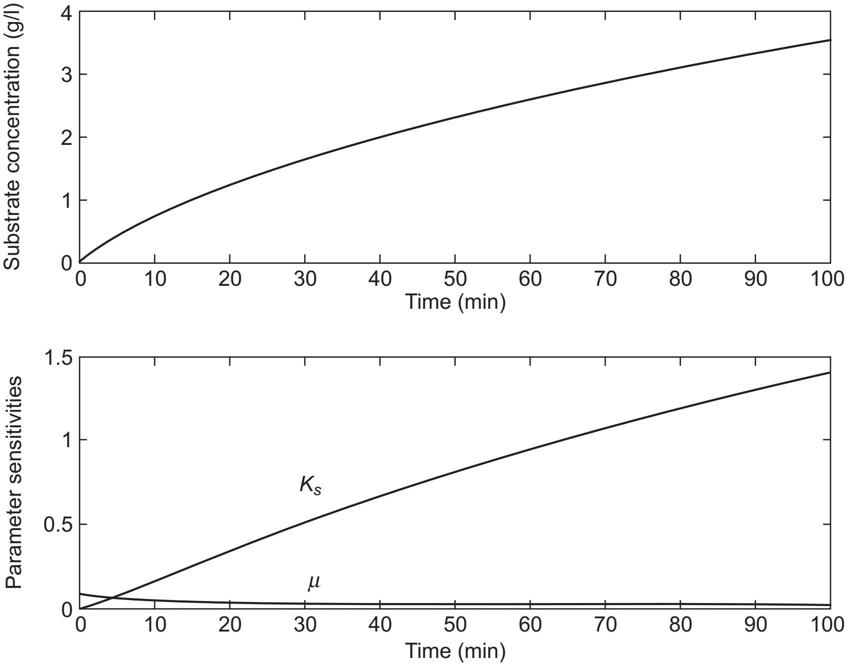


Fig. 8.1 Substrate concentration (top figure) and parameter sensitivities (indicated by K_S and μ, respectively, in bottom figure) in a fed-batch bioreactor with Monod kinetics (Keesman, 2011)

8.7 THE GENERAL PARAMETER MAPPING (GPM)

Consider a second-order differential equation (Kubicek and Hlavecek, 1983):

$$\frac{d^2y}{dx^2} = f\left(x, y\frac{dy}{dx}, \alpha\right) \quad 8.64)$$

subject to the boundary conditions

$$\alpha_0 y(0) + \frac{\beta_0 dy(0)}{dx} = \gamma_0 \tag{8.65}$$

$$\alpha_1 y(b) + \frac{\beta_1 dy(b)}{dx} = \gamma_1 \tag{8.66}$$

where, α is a physical parameter for different values of which the solution is sought. Let the unknown initial condition be denoted by A, i.e.,

$$y(0) = A \tag{8.67}$$

which can combine with the boundary condition (8.62) to give

$$y(0) = A, \; \frac{\beta_0 dy(0)}{dx} = \gamma_0 - \alpha_0 A \tag{8.68}$$

where, A is a function of the parameter α Kubicek and Hlavcek (1983) derived the differential equation governing the function $A(\alpha)$.

First, the differential equation, Eq. (8.57), and its boundary condition given by Eq. (8.61) are differentiated with respect to the parameter α, and we get

$$\frac{d^2 q}{dx^2} = \frac{\partial f}{\partial y} q + \frac{\partial f}{\partial y'} \frac{dq}{dx} + \frac{\partial f}{\partial \alpha} \tag{8.69}$$

(where, $y' = dy/dx$) subject to the boundary conditions

$$q(0) = 0, \; \frac{dq(0)}{dx} = 0 \tag{8.70}$$

where
$$q = \frac{\partial y}{\partial \alpha} \tag{8.71}$$

Next, Eq. (8.64) and its boundary conditions given by Eq. (8.65) and Eq. (8.68) are differentiated with respect to A, and we get

$$\frac{d^2 p}{dx^2} = \frac{\partial f}{\partial y} p + \frac{\partial f}{\partial y'} \frac{dp}{dx} \tag{8.72}$$

subject to the boundary conditions

$$x = 0: p(0) = 1, \; \frac{dp(0)}{dx} = -\frac{\alpha_0}{\beta_0} \tag{8.73}$$

where
$$p = \frac{\partial y}{\partial A} \tag{8.74}$$

The boundary condition at $x = b$ Eq. (8.66), can be written as

$$F(A, \alpha) = \alpha_1 y(b) + \beta_1 \left(\frac{dy(b)}{dx} \right) - \gamma_1 \tag{8.75}$$

Here y is a function of both A and α long the curve $A(\alpha)$, the following equation holds

$$\left(\frac{\partial F}{\partial A} \right) dA + \left(\frac{\partial F}{\partial \alpha} \right) d\alpha = 0 \tag{8.76}$$

from which we get:

$$\frac{dA}{d\alpha} = -\frac{\partial F}{\partial \alpha} \Big/ \frac{\partial F}{\partial A} \tag{8.77}$$

Substituting *F* from Eq. (8.75) into Eq. (8.77), we then get

$$\frac{dA}{d\alpha} = -\frac{\alpha_1 q(b) + \beta_1 \left(\dfrac{dq(b)}{dx}\right)}{\alpha_1 p(b) + \beta_1 \left(\dfrac{dp(b)}{dx}\right)} \tag{8.78}$$

which is the differential equation governing the missing initial slope *A* as a function of the physical parameter α.

The integration of Eq. (8.78) can be performed numerically, since the right-hand side of the equation can be calculated from the integration of the initial value problems defined by Eqs. (8.69), (8.70), (8.71), and (8.73). For more details on the method presented in sections 8.6, 8.7 and 8.8, the reader may refer to Kubicek and Hlavcek (1983).

8.8 SENSITIVITY ANALYSIS IN PROCESS CONTROL

In process control, for a controller to give a good disturbance rejection, the sensitivity function at the low frequency should be small. The sensitivity function (transfer function relating the error to the set point)) is given by:

$$S(s) = \frac{1}{1 + P(s)C(s)} \tag{8.79}$$

Here P(s) is the transfer function of the process and $C(s)$ Is the transfer function of the controller. The complementary sensitivity function, $T(s)$, as suggested by its name, is defined as:

$$T(s) = 1 - S(s) \tag{8.80}$$

$$T(s) = \frac{P(s)C(s)}{1 + P(s)C(s)} \tag{8.81}$$

The complementary sensitivity provides the information about the set point tracking performance of the controller. It should be as close as possible to 1. The Maximum sensitivity (Ms) function relates to the robustness measurement of the controller output $u(s)$. Using the Ms value, the gain margin and the phase margin can be determined simultaneously while these two quantities are completely independent.

The maximum sensitivity is defined as:

$$Ms = \max_{\omega} \left|S(\omega j)\right| = \max_{\omega} \frac{1}{1 + P(j\omega)C(j\omega)} \tag{8.82}$$

The shortest distance from the Nyquist curve to the critical point (–1, 0) equals 1/Ms. In order to obtain a high robustness, small values of Ms are of interest. The maximum sensitivity can be related to the phase margin (φ_m) and gain margin (A_m) as it simultaneously ensures both the following constraints:

$$A_m \geq \frac{Ms}{Ms-1}, \text{ and } \varphi_m \geq 2\sin^{-1}\frac{1}{Ms} \tag{8.83}$$

When comparing the performances of different settings of PI controllers by different methods, the method giving the lowest MS value, [which means larger gain margin and larger phase margin], is recommended.

Review Problems

1. A batch reactor is used for carrying out the auto catalytic reaction:

   $$A + B \rightarrow 2B + C$$

   For a batch reactor, the model equation is given by

   $$\frac{da}{dt} = -kab = -ka(b_0 + a_0 - a)$$

   The solution is given by

   $$\frac{a}{a_0} = \frac{1+\left(\frac{b_0}{a_0}\right)}{\left[1+\left(\frac{b_0}{a_0}\right)e^{(a_0+b_0)kt}\right]}$$

   Calculate the absolute sensitivity on 'a' to 'a_0' and separately to 'b_0' and to 'k'. Calculate the normalized sensitivity.
2. Explain the direct differentiation method calculating the sensitivity of y with respect to p of the system: $\frac{dy}{dt} = f(y, p)$ with $t = 0$; $y = y_0$
3. Explain the finite difference scheme method calculating the sensitivity of y with respect to p of the system: $\frac{dy}{dt} = f(y, p)$ with $t = 0$; $y = y_0$
4. Explain the Green's function method for calculating the sensitivity of y with respect to p of the system: $\frac{dy}{dt} = f(y, p)$ with $t = 0$; $y = y_0$
5. Explain the method of calculating the dependence of Solution of Initial Value Problem on the Initial condition.
6. Explain the method of calculating the dependence of the Solution of a Set of Nonlinear algebraic equations on a Parameter.
7. The model equation of an isothermal CSTR carrying out the following series parallel reactions are given: $A \rightarrow B \rightarrow C$; $2A \rightarrow D$

   $$\frac{dx_1}{dt} = -k_1x_1 - k_2x_1^2 + (C_{a0} - x_1)u$$

   $$\frac{dx_2}{dt} = k_1x_1 - k_2x_2 - x_2u$$

   $x_1 = C_A$; $x_2 = C_B$; $u = \frac{F}{V}$ (1/min); at $t = 0$, $x_1 = x_{10}$; $x_2 = x_{20}$;

   Calculate the dependence of the solution of above Initial Value Problem by the initial condition x_{10} and separately by the parameter k_1.

8. Perumal et al. (2013. Computers and Chemical Engg. 50. 37 – 45.) proposed dynamic sensitivities for reduction of kinetic models of alkane pyrolysis model. Read the paper and prepare a report on the work studied.

9

Optimization Methods

The optimization problem is defined as the selection of the design variables to minimize a given scalar objective function subjected to certain constraints. In this chapter, methods are given for minimizing the objective function for (i) scalar variable problems and (ii) multi-variable problems. Both the analytical and numerical methods are discussed. Table 1 gives the classification of the optimization problems.

Table 9.1 *Classification of optimization problems (Badiru, 2012)*

Characteristics	Property	Classification
No of decision variables	One	Univariate
	More than one	Multivariate
Type of decision variable	Continuous real number	Continuous
	Integers	Discrete
	Both continuous real numbers and integers	Mixed integers
	Integers in permutations	Combinatorial
Objective function	Linear function of decision variables	Linear
	Quadratic function of variables	Quadratic
	Other Nonlinear function of decision variables	Nonlinear
Constraints	No constraints	Unconstrained

Characteristics	Property	Classification
	Subject to constraints	Constrained
Decision variable realization within the optimization model	Exact	Deterministic
	Random variation	Stochastic
	Subject to fuzzy uncertainty	Fuzzy
	Subject to both random and uncertainty	Fuzzy-stochastic

9.1 OPTIMIZATION OF A FUNCTION OF A SINGLE VARIABLE

Let $f(x)$ be a function of a single variable x, defined in the range $a < x < b$ (Fig. 9.1). The system has many minima, maxima and saddle points, etc.

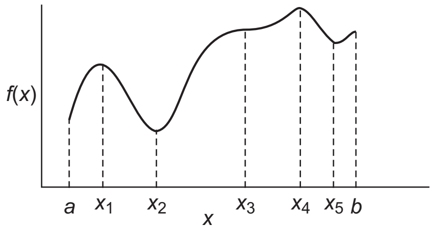


Fig. 9.1 Function of a single variable

Local maximum: the function $f(x)$ is said to have a local maximum at x_1, where it has a value higher than that at any other value of x in the neighbourhood of x_1:

$$f(x_1 - \Delta x_1) < f(x_1) > f(x_1 + \Delta x_1) \tag{9.1}$$

Local minimum: the function $f(x)$ is said to have a local minimum at x_2 and where it has a value lower than that at any other value of x in the neighbourhood of x_2:

$$f(x_2 - \Delta x_2) > f(x_2) < f(x_2 + \Delta x_2) \tag{9.2}$$

***Saddle point*:** the function has a saddle point at x_3 where the value of the function is lower on one side of x_3 and higher on the other, compared to the value of x_3:

$$f(x_3 - \Delta x_3) < f(x_3) < f(x_3 + \Delta x_3) \tag{9.3}$$

The slope of the function f at x_3 is zero.

Global maximum: The function $f(x)$ is a global maximum at x_4 in the range $a < x < b$, where the value of the function is higher than that at any other value of $f(x)$ in the defined range. Among the several local maxima, there will be one global maximum.

Global minimum: The function $f(x)$ is a global minimum at x_2 in the range $a < x < b$, where the value of the function is lower than that at any other value of $f(x)$ in the defined range. Among the several local minima, there will be one global minimum.

In Fig. 9.1 there are two local minima, two local maxima, one saddle point and global maximum at x_4^*, and global minimum at x_2^*, and a saddle point at x_3^*.

Convexity: A function is said to be strictly convex, if a straight line connecting any two points on the function lies completely above the function. If a function is strictly convex, its slope increases continuously, or $d^2f/dx^2 > 0$. For a convex function, $d^2 f/dx^2 \geq 0$. A local minimum of a convex function is also global minimum.

Concavity: A function is said to be strictly concave, if a straight line connecting any two points on the function lies completely below the function. If a function is strictly concave, it's slope decreases continuously, or $d^2f/dx^2 < 0$. For a concave function, $d^2 f/dx^2 \leq 0$. A local maximum of a convex function is also global maximum. If $f(x)$ is a convex function, then $-f(x)$ is a concave function.

The point at which a function will have a maximum or minimum is called a stationary point. $x = x_0$ is a stationary point if df/dx (at $x = x_0$) = 0. This is a necessary condition for $f(x)$ to be a maximum or a minimum at x_0. If necessary condition is not satisfied then there is no optimal value. If the necessary condition is satisfied, then there is an additional condition (sufficient condition) to be tested for checking whether the optimal point is minimum or maximum or no optimal solution (called saddle point). The sufficient condition is examined as follows:

1. If $d^2f/dx^2 > 0$ for all x, $f(x)$ is convex and the stationary point is a **global minimum**.
2. If $d^2f/dx^2 < 0$ for all x, $f(x)$ is concave and the stationary point is a **global maximum**
3. If $d^2f/dx^2 = 0$, further investigation is required. Find the first nonzero higher order derivative (say n^{th} order),. i.e, at x_0, $d^nf/dx^n \neq 0$. If n is odd, the x_0 is a ***saddle point***. If $d^nf/dx^n > 0$ at x_0, then x_0 is a local minimum. If $d^nf/dx^n < 0$ at x_0, then x_0 is a local maximum.

Given the equation for the function $f(x)$, we can plot f versus x graph and note down where the lower value of f occurs and the corresponding value of x. However, if we want the problem to be solved for different operating conditions (different f versus x curve), then a numerical optimization method may be convenient and comfortable. For multi-variables problem (say 3 variables and more), it is difficult to visualize the graphical nature of f versus x_1, x_2 and x_3. Let us consider few examples reported by Chang and Zak (2013).

Example 9.1

A 1-m long wire is made into two pieces, one in a circular shape and the other into a square as shown in Fig. 9.2. What must the individual lengths be so that the total area is a minimum?

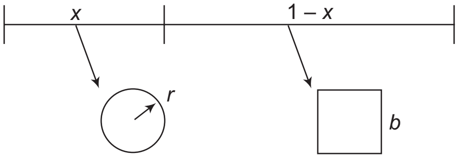


Fig. 9.2 System description for Example 9.1 (Chang and Zak, 2010)

Formulation

Set the length of first piece = x, then the area is given by $f(x) = \pi r^2 + b^2$.

Since $r = x/(2\pi)$ and $b = (1 - x)/4$, it follows that

$$f(x) = \left[\frac{\pi x^2}{(4\pi^2)}\right] + \left[\frac{(1-x)^2}{16}\right] \tag{9.4}$$

The problem, therefore, reduces to an unconstrained minimization problem:

$$\text{Minimize } f(x) = 0.1421x^2 - 0.125x + 0.0625 \tag{9.5}$$

$$\frac{df}{dx} = 0 \text{ gives } x^* = 0.4398 \text{ m} \tag{9.6}$$

and the individual lengths are $x = 0.4398$ and $(1 - x) = 0.5602$ with the area of $f(x) = 0.035$ m^2 which the minimum value.

Example 9.2

Consider the circuit in Fig. 9.3. Find the value of R such that the power absorbed by this resister is minimized.

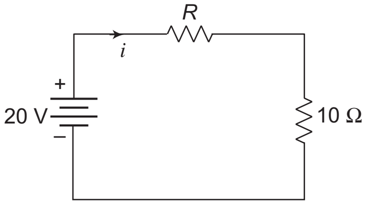


Fig. 9.3 Circuit for Example 9.2 (Chang and Zak, 2010)

Solution: The power absorbed by the register is i^2R, where

$$i = \frac{20}{(10+R)} \tag{9.7}$$

$$\text{Power} = P = \frac{400\,R}{(10+R)^2} \tag{9.8}$$

$$P'(R) = 100\,\frac{(10-R)}{(10+R)^3} \tag{9.9}$$

To make $f'(R) = 0$, we get $R = 10$. (9.10)

Example 9.3

Consider a simplified model of a cellular wireless system. The primary base station and the neighbouring base station are separate by distance Z unit. The height of the station is 1 unit. A mobile user (also called a mobile) is located at a position x unit from the primary base station. There are two base station antennae, one for the primary base station and another for the neighbouring base station. Both antennas are transmitting signals to the mobile user, at equal power. However, the power of the received signal as received from the mobile is equal to the reciprocal of the squared distance from the associated antenna (primary or neighbouring base station). Find the location of the mobile that maximize the ratio of signal to interference ratio which is ratio of signal power received from the primary base station to the signal power received from the neighbouring base station. Given $Z = 2$ unit distance.

Solution:

Let the location of the mobile is x unit.

The squared distance from the mobile to the primary antenna $= 1 + x^2$ (9.11a)

The squared distance from the mobile to the secondary antenna $= 1 + (2 - x)^2$ (9.11b)

The signal to interference ratio is given by

$$f(x) = \frac{[1 + (2 - x)^2]}{(1 + x^2)} \tag{9.12}$$

By analytical optimization method we get $x^* = 1 - \sqrt{2}$ (or) $1 + \sqrt{2}$. The values of the objective function at these two x^*, show that $x^* = 1 - \sqrt{2}$ is the optimal distance.

Example 9.4

In pure water and in dilute aqueous solutions, the following relation is valid:

$$\mathrm{K_w} = [\mathrm{H^+}]\,[\mathrm{OH^-}] \tag{9.13}$$

where $[\mathrm{H^+}] > 0$ and $[\mathrm{OH^-}]$ are the concentration of the hydrogen and hydroxide ions, respectively, and $K_w > 0$ is the autoprotolysis constant of water. Given $[\mathrm{H^+}] + [\mathrm{OH^-}]$ as a universal function and show that it has a local minimum, if $[\mathrm{H^+}] = [\mathrm{OH^-}] = K_w^{0.5}$, that is, the solution is neutral.

Solution:

The function to be studied is:

$$f(x) = x + \frac{K_w}{x} \tag{9.14}$$

where $x = [\mathrm{H^+}]$. Differentiating with respect to x , we get

$$df/dx = 1 - \frac{K_w}{x^2} \tag{9.15}$$

When the derivative is set to zero, we get

$$x_{\mathrm{opt}} = [\mathrm{H^+}]_{\mathrm{opt}} = K_w^{0.5} \tag{9.16}$$

The second derivative d^2f/dx^2 when $x = [\mathrm{H^+}]_{\mathrm{opt}}$ gives

$$2K_w/[\mathrm{H^+}]^3 \text{ which becomes } \left(\frac{2}{k^{0.5}}\right) > 0 \tag{9.17}$$

This Shows that $f(x)$ is minimum at $[\mathrm{H^+}] = [\mathrm{H^+}]_{\mathrm{min}}$.

Example 9.5

Consider the consecutive reaction $A \rightarrow B \rightarrow C$, each first order kinetics taking place in a batch reactor with an initial concentration of $C_A = C_{A0}$, $C_B = 0$ and $C_{C0} = 0$ The analytical solution for C_B (t) is given by

$$C_B = \left[\frac{C_{A0}\,k_1}{(k_1 - k_2)}\right] [\exp(-k_1 t) - \exp(-k_2 t)] \tag{9.18}$$

where k_1 is the reaction rate constant for $A \to B$ and k_2 for $B \to C$ reaction. Find the value of t_{opt} at which the maximum value of C_B is obtained and find the value of $C_{B,\,\max}$.

Taking the derivative of Eq. (9,18) with respect to t, we get:

$$\begin{aligned}\frac{dC_B}{dt} &= \left[\frac{C_{A0}\,k_1}{(k_1 - k_2)}\right][-k_2\exp(-k_2\,t_{\max}) + k_2\exp(-k_1\,t_{\max})] \\ &= 0\end{aligned} \tag{9.19}$$

Solving for $t_{\max,}$ we get:

$$t_{\max} = \left[\frac{1}{(k_1 - k_2)}\right]\ln\left(\frac{k_1}{k_2}\right) \tag{9.20}$$

Substituting this in Eq. (9.18), we get:

$$C_{B,\max} = C_{A0}\left(\frac{k_1}{k_2}\right)^q \tag{9.21}$$

where,
$$q = \left(\frac{k_2}{(k_1 - k_2)}\right) \tag{9.22}$$

9.2 OPTIMIZATION OF A FUNCTION OF MULTI-VARIABLES

Let the scalar function $f(X)$ be a function of multi-variables, $X = (x_1, x_2, \ldots, x_n)$. A necessary condition for a stationary point $X = X_0$ is that each first partial derivative of $f(X)$ should be equal to zero:

$$\frac{\partial f}{\partial x_1} = \frac{\partial f}{\partial x_2} \cdots \frac{\partial f}{\partial x_n} = 0 \tag{9.23}$$

The function $f(X)$ is a maximum or minimum or saddle at $X = X_0$ depending on the nature of the eigenvalues of its Hessian matrix (H) evaluated at X_0.

$$H(x) = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \dfrac{\partial^2 f}{\partial x_1 \partial x_2} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_n\,\partial x_2} \\ \cdots & \cdots & \cdots & \cdots \\ \dfrac{\partial^2 f}{\partial x_1\,\partial x_n} & \dfrac{\partial^2 f}{\partial x_2 \partial x_n} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \tag{9.24}$$

Since the Hessian matrix is symmetric, the eigenvalues will be only real numbers (no complex conjugate eigenvalues).

1. If *all* the eigenvalues are positive at X_0, then X_0 is local minimum.
2. If *all* the eigenvalues are negative at X_0, then X_0 is local maximum.
3. If some eigenvalues are positive and some are negative or some are zero, then X_0 is a saddle point.

The proof of the above three points is given in the books on optimization techniques.

Example 9.6

Find the optimal values of x and the nature of the optimal points for the system:

$$F(X) = 4 + 4.5x_1 - 4x_2 + x_1^2 + 2x_2^2 - 2x_1x_2 + x_1^4 - 2x_1^2x_2 \tag{9.25}$$

The stationary point can be located by setting $\nabla f(X_n) = 0$ (9.26)

$$\frac{\partial f}{\partial x_1} = 4.5 + 2x_1 - 2x_2 + 4x_1^3 - 4x_1x_2 = 0 \tag{9.27a}$$

$$\frac{\partial f}{\partial x_2} = -4 + 4x_2 - 2x_1 - 2x_1^2 = 0 \tag{9.27b}$$

The above set of nonlinear equations is solved numerically by Newton–Raphson's technique (using solve routine in Matlab) and the results are given in Table 9.2. The local minimum or global minimum can be ascertained by the values of the function.

Table 9.2 *Results for Example 6*

Stationary points (x_{1C}, x_2)*	f(X)	λ of Hessian Matrix	Classification
(1.941,3.854)	0.9855	37.03, 0.97	local minimum
(–1.053,1.028)	–0.5134	10.5, 3.5	local minimum (also global minimum)
(0.6117, 1.4929)	2.83	7.0, –2.56	saddle point

9.3 OPTIMIZATION IN MODEL REDUCTION

For design of controllers, it is often necessary to simplify a higher order (transfer function) model to a lower order model. Let the transfer function of a higher order system be

$$P(s) = (b_0 + b_1s + b_2s^2 + \dots + b_ms^m)/(a_0 + a_1s + \dots + a_ns^n) \quad m < n \tag{9.28}$$

where a_0, a_1, …, a_n, b_0, b_1,… are constants. Let the transfer function of the reduced system be expressed by

$$G(s) = (b_0 + d_1s + d_2s^2 + \dots + d_ps^p)/(a_0 + c_1s + c_2s^2 + \dots + c_qs^q) \quad p < q \cdot m \tag{9.29}$$

The values of b_0 and a_0 are to be retained in the reduced order model to keep the steady state gain the same. The problem is to determine the unknown coefficients $c_1, c_2, \dots, c_q, d_1, d_2, \dots, d_p$ in such a way that $G(s)$ represents $P(s)$ as closely as possible over a given range of frequency range $\omega_1 \le \omega \le \omega_u$. Let us select a value of ω, say ω_i. Thus letting $s = j\omega_i$ makes Eq. (9.28) as:

$$P(j\omega_i) = a(\omega_i) + jb(j\omega_i) \tag{9.30}$$

where $a(\omega_i)$ and $b(\omega_i)$ are real numbers, depending on ω_i. Similarly Eq. (9.29) becomes:

$$G(j\omega_i) = c(\omega_i) + jd(\omega_i) \tag{9.31}$$

where $c(\omega_i)$ and $d(\omega_i)$ are real numbers, depending on ω_i. We can write the objective function as the sum of error square in real part and error square as:

$$T(\omega_i) = [a(\omega_i) - c(\omega_i)]^2 + [b(\omega_i) - d(\omega_i)]^2 \tag{9.32}$$

The objective function is to minimize S which is given by:

$$S = \Sigma\ \{[a(\omega_i) - c(\omega_i)]^2 + [b(\omega_i) - d(\omega_i)]^2\} \tag{9.33}$$

The sum term is to be evaluated at N frequency values of ω_i. The model reduction problem is to choose the best values for coefficients $c_{1,}\, c_2,\ \ldots,\ c_q,\ d_{1,}\, d_2, \ldots,\ d_p$ such that the above objective function (sum of the squares of deviation) is to be minimized.

Example 9.7

Let $$P(s) = 432/[1+9.1\text{ s} + 26.08\text{ s}^2 + 30.94\text{ s}^3 + 15.76\text{ s}^4 + 2.8\text{ s}^5] \tag{9.34}$$

The initial approximate model (with the same gain as that of original system) is chosen as:

$$G(s) = 432\ \exp(d_1 s)/[1 + c_1 s + c_2 s^2] \tag{9.35}$$

By the above optimization method, we get

$$G(s) = 432\ \exp(-1.52\text{s})/(14.2\text{s}^2 + 7.54\text{s} + 1) \tag{9.36}$$

Both the original model and the reduced model match well in the Nyquist plot (real part of $G(s)$ versus imaginary part of $G(s)$ (we can use matlab command Nyquist[G]). More details on the above topic are given by Luus (1980) and Karpe et al. (1987).

9.4 OPTIMIZATION IN MODEL FITTING

Experimental data on Sh (Sherwood) number for various values of Re (Reynolds) and Sc (Schmidt) numbers are given (10 data set given)

How do you get the model parameters (a, b, c) in $\text{Sh} = c(\text{Re})^a\,(\text{Sc})^b$ (9.37)

Substituting the experimental values of Sh, Re and Sc in Eq. (9.32), we get the equation error as:

$$e_i = [\text{Sh}_i - c(\text{Re}_i)^a\,(\text{Sc}_i)^b\,] \tag{9.38a}$$

The sum of error squares is given by

$$S = \Sigma\ [\text{Sh} - c(\text{Re})^a\,(\text{Sc})^b\,]^2 \tag{9.38b}$$

The summation has to be carried out for all the N data points (substitute the experimental Re, Sc and Sh data in Eq. (9.34b). We have to select c, a and b parameters such that the sum of squares (S) is minimized.

$$\partial S/\partial a = 0;\ \partial S/\partial b = 0 \text{ and } \partial S/\partial c = 0 \tag{9.39}$$

The resulting three nonlinear algebraic equations are to be solved for the three parameters.

We can classify the optimization algorithms as per the type of information required for carrying out the optimization studies: zero order method, first order method and second order method. The simplest approach to minimize $F(x)$ is to select randomly a large number of candidates X vectors and evaluate the objective function for each of them. Methods requiring only the function values are called as zero-order methods. These methods are reliable and easy to program. They often deal with non-convex and discontinuous functions. Examples are Random search methods, Powell methods, Box's COMPLEX method, Hooke and Jeeve's method.

Methods requiring gradient or first order derivatives are called first-order methods (example: Steepest descent method, conjugate direction method), Methods requiring second derivatives of the objective function are called second order method (example: Newton's method). In general, it is not easy to guaranty that the global optimal solution obtained by the optimization method. This may be due to occurrence of multiple solutions to the problem. The ill-conditioning, occurring in setting up the problem, may result in slow convergence of the optimization algorithm. One recommended method is to use different initial guess vectors and if the optimization method gives the same solution then it may be the global optimal solution.

Computational time increases as the number of design variable increases. The methods tend to become numerically ill-conditioned. Most optimization algorithms have difficulty in dealing with discontinuous functions. Highly nonlinear problems may converge slowly or not at all.

9.5 UNCONSTRAINED OPTIMIZATION METHODS

9.5.1 Newton's method

Newton's method for solving the nonlinear algebraic equation can be modified to solve the optimization problems, because it is equivalent to finding the roots of the first order derivative, $f'(x)$, based on the stationary conditions once the objective function $f(x)$ is given. For a given function $f(x)$ which is continuously differentiable, we have the Taylor's series expansion about a known point, $X = X_n$ and $\Delta X_n = X - X_n$.

$$f(X) = f(X_0) + [\nabla f(X_n)]^T \Delta X + (1/2)\, \Delta X^T [\nabla^2 f(X_n)\,] \Delta X + \dots \tag{9.40}$$

which is written in terms of quadratic forms. This is to be minimized near a critical point when ΔX is the solution of the following linear equation:

$$\nabla f(X_n) + \nabla^2 f(X_n)\, \Delta X = 0 \tag{9.41}$$

which gives:

$$X = X_n - \mathrm{H}^{-1}\, \nabla f(X_n), \tag{9.42}$$

where $H = \nabla^2 f(X)$, is the Hessian matrix which is defined as:

$$H(x) = \begin{bmatrix} \dfrac{\partial^2 f}{\partial x_1^2} & \dfrac{\partial^2 f}{\partial x_1\, \partial x_2} & \cdots & \dfrac{\partial^2 f}{\partial x_1\, \partial x_n} \\ \dfrac{\partial^2 f}{\partial x_1 \partial x_2} & \dfrac{\partial^2 f}{\partial x_2^2} & \cdots & \dfrac{\partial^2 f}{\partial x_n\, \partial x_2} \\ \cdots & \cdots & \cdots & \cdots \\ \dfrac{\partial^2 f}{\partial x_1\, \partial x_n} & \dfrac{\partial^2 f}{\partial x_2 \partial x_n} & \cdots & \dfrac{\partial^2 f}{\partial x_n^2} \end{bmatrix} \tag{9.43}$$

which is a symmetric matrix due to $\dfrac{\partial^2 f}{\partial x_i\, \partial x_j} = \dfrac{\partial^2 f}{\partial x_j\, \partial x_i}$ (9.44)

If the iteration procedure starts from the initial vector $X^{(0)}$ (usually guessed values based on the physics of the problems), Newton's iteration formula for the nth iteration is given by:

$$X^{(n+1)} = X^{(n)} - H^{-1}(X^{(n)})\ \nabla f(X^{(n)}) \tag{9.45}$$

It is important to note that if $f(X)$ is quadratic, then the solution can be found exactly in a single step. For a general function, to speed up the convergence, the Newton's method can be modified as:

$$X^{(n+1)} = X^{(n)} - \alpha H^{-1}(X^{(n)})\ \nabla f(X^{(n)}) \tag{9.46}$$

where α is from 0 to 1. It might be time consuming to calculate the Hessian matrix at each iteration. We can use the initial Hessian matrix obtained at the initial guess condition throughout. Alternatively, We can use $H = I$ so that $H^{-1} = I$, and we have quasi-Newton method (discussed In the next section):

$$X^{(n+1)} = X^{(n)} - \alpha I\ \nabla f(X^{(n)}) \tag{9.47}$$

which is essentially the steepest Descent method.

The basic Newton method does not always perform satisfactorily. The main difficulties are:

(i) the method is not always convergent, even if x^0 is close to x^*, and

(ii) the method requires the computation of the Hessian Matrix at each iteration

9.5.2 Steepest descent method

The essence of the method is to find the lowest possible function $f(X)$ from the current point $X^{(n)}$:

$$f(X^{(n+1)}) = f(X^{(n)} + \Delta X) \approx f(X^{(n)}) + [\nabla f(X^{(n)}]^T\ \Delta s \tag{9.48}$$

where $\Delta X = X^{(n+1)} - X^{(n)}$ is the increment vector. Since we try to get a lower (better) approximation to the objective function, we require the second term on the right hand side negative. We get

$$f(X^{(n)} + \Delta s) \approx f(X^{(n)}) = (\nabla f)^T\ \Delta s < 0 \tag{9.49}$$

From the vector analysis, we know the inner product $\mathbf{u}^T\mathbf{v}$ of two vectors u and v is the largest when they are parallel but in opposite direction. $(\nabla f)^T\ \Delta s$ becomes the smallest when

$$\Delta X = -\alpha \nabla f(X^{(n)}) \tag{9.50}$$

where $\alpha > 0$ is the step size. This is the case when the direction Δs is along the steepest descent in the negative gradient direction. The choice of step size α is important. A small step size means slow movement towards the minimum, while a large step may overshoot and subsequently makes it move far away from the local minimum. Therefore the step size $\alpha(\alpha^{(n)})$ should be different at each iteration step and to be selected so that it minimizes the objective function $f(X^{(n)}) = f(X^{(n)}, \alpha^{(n)})$. The steepest descent method can be written as:

$$X^{(n+1)} = X^{(n)} - \alpha^{(n)}\ [\nabla^2 f(X^{(n)})]\ \nabla f(X^{(n)}) \tag{9.51}$$

In each iteration the gradient and step size will be checked. Again, good initial guess values of both the starting point and the step size are to be used.

9.5.3 Levenberg–Marquardt algorithm

If the Hessian matrix H is not positive definite, then the search direction may not point in a descent direction. A simple technique to ensure that the search direction is a descent direction is to introduce the Levenberg–Marquadrt modification of Newton's algorithm:

$$X^{(k+1)} = X^{(k)} - [H(x^{(k)}) + \mu_k I]^{-1} g^{(k)} \tag{9.52}$$

where $\mu_k \geq 0$.

Consider asymmetric matrix H, which may not be positive definite. Let λ_1, λ_2,.. λ_n be the eigenvalues of H with the corresponding eigenvectors v_1, v_2, $\ldots v_n$. The eigenvalues are real (due to symmetry of matrix H), but may not all be positive. Consider now the matrix $H + \mu I$, where $\mu \geq 0$. It can be verified that G has also the same eigenvector with the eigenvalues $(\lambda_i + \mu)$. Therefore, if μ is sufficiently large, then all the eigenvalues of G are positive and G is positive definite. By letting $\mu_k \to 0$, then the LM method approaches to that of Newton method. If $\mu_k \to \infty$, then the LM algorithm approaches the pure gradient method with a small step size. In practice, a small value of μ_k is used to start with and the value is increased slowly until we find the iteration is descent, $f(x^{k+1}) < f(x^k)$.

9.6 CONSTRAINED OPTIMIZATION

9.6.1 The method of Lagrange multipliers

Consider a single equality constraint:

$$\text{minimize } f(\mathbf{x}) = 0 \tag{9.53a}$$

$$\text{Subject to } h(\mathbf{x}) = 0 \tag{9.53b}$$

For f to have a stationary value, meaning a minimum, maximum, or saddle point, we need

$$df = \left(\frac{\partial f}{\partial x_1}\right) dx_1 + \left(\frac{\partial f}{\partial x_2}\right) dx_2 + \cdots + \left(\frac{\partial f}{\partial x_n}\right) dx_n = 0 \tag{9.54a}$$

while the violation of the constraint equation gives:

$$dh = \left(\frac{\partial h}{\partial x_1}\right) dx_1 + \left(\frac{\partial h}{\partial x_2}\right) dx_2 + \cdots + \left(\frac{\partial h}{\partial x_n}\right) dx_n = 0 \tag{9.54b}$$

If there were no constraint then each dx_i is independent and Eq. (9.54a) would yield the optimality condition $\partial f/\partial x_i = 0$ for each i. This however, is not the case because of the constraint Eq. (9.54b). We would use Eq. (9.54b) to eliminate dx_n by writing it in terms of the order dx_i, substituting into Eq. (9.43a), and obtain an unconstrained variation involving dx_1, dx_2, …, dx_{n-1} to give us the optimality condition. Lagrange suggested a different approach: it is obviously permissible to multiply Eq. (9.54b) by some unconstrained factor λ and add it to Eq. (9.54a). Hence we obtain

$$\sum \left[\left(\frac{\partial f}{\partial x_i}\right) + \lambda \left(\frac{\partial h}{\partial x_i}\right) \right] dx_i = 0 \tag{9.55}$$

The summation index is from $i = 1$ to $i = n$.

Now rather eliminating dx_n, we can choose λ such that

$$\left[\left(\frac{\partial f}{\partial x_i}\right)+\lambda\left(\frac{\partial h}{\partial x_i}\right)\right]=0\,. \tag{9.56}$$

This dispenses the task of eliminating dx_n. The sum in Eq. (9.55) is then reduced to only $(n - 1)$ terms:

$$\sum\left[\left(\frac{\partial f}{\partial x_i}\right)+\lambda\left(\frac{\partial h}{\partial x_i}\right)\right]dx_i=0 \tag{9.57}$$

The summation index is from $i = 1$ to $i = n - 1$.

Now dx_i in Eq. (9.57) are independent since we have already accounted for the restriction imposed by the constraint. Thus, each coefficient in this equation shall vanish:

$$\left[\left(\frac{\partial f}{\partial x_i}\right)+\lambda\left(\frac{\partial h}{\partial x_i}\right)\right]=0 \tag{9.58}$$

Equation (9.55) together with Eq. (9.57), lead to the conclusion that each coefficient in (9.56) vanishes just as if all variations dx_i , were unconstrained. Lagrange method can be viewed as follows: consider the function (call it as 'Lagrangian') $L = f + \lambda h$. The optimality conditions for f to have a stationary value are $\partial L/\partial x_i = 0$ for I = 1, 2, … n. These n equations along with the constraint $h = 0$, give us an $n + 1$ equation for the $n + 1$ unknown $x, \ldots, x_n$ and λ.

We may generalize, the method for p constraints as follows:

$$\text{Minimize } f(\mathbf{x}) \tag{9.59a}$$

$$\text{Subject to } h_j(\mathbf{x}) = 0, \quad j = 1, 2, \ldots p. \tag{9.59b}$$

Form the Lagrangian:

$$L = f + \Sigma\, \lambda_j h_j \tag{9.60}$$

The summation is form $j = 1$ to p.

If **x*** is a stationary point (maximum, minimum, or a point of inflection), then it is necessary that the following conditions are satisfied:

$$\frac{\partial L}{\partial x_i}=\frac{\partial f}{\partial x_i}+\sum\lambda_i\left[\frac{\partial h_i}{\partial x_i}\right]=0,\ \ i=1,2\ldots n. \tag{9.61a}$$

The summation is from $j = 1$ to p.

$$h_j(\mathbf{x}) = 0, \quad j = 1, 2, \ldots p. \tag{9.61b}$$

Equations (9.61a) and (9.61b) can be written as $\nabla_X L = 0$ and $\nabla_\lambda L = 0$ and can be used to verify a given point x^* is a minimum point. However, if we plan to use them to determine all the candidate points that satisfy the Eq. (9.60) and then compare the function values and pick the minimum point, if this was what we desire 'sufficiency' conditions.

9.7 THE MATHEMATICAL PROGRAMMING

Minimize $f(X)$

$$\text{subject to } h_i(X) = 0; \quad i = 1, 2, \ldots m \tag{9.63a}$$

$$g_j(X) \geq 0 \quad j = 1, 2, \ldots l \tag{9.63b}$$

If the above functions $f(X)$, $h_i(X)$ and $g_j(X)$ all are linear then, we have the linear programming problem. Otherwise, it is called nonlinear programming. If inequality constraints are present, the optimization problem can be converted into an unconstrained problem. To simplify the optimization procedure, we need to (i) transform an inequality constrained problem in to equality constrained problem, and (ii) transform the equality constrained problem in to an unconstrained problem.

Inequality constraint: An inequality constraint can be converted to equality constraint by introducing an additional variable on the left side of the constraint. $G(X) \leq 0$ is converted as $g(X) + s^2 = 0$ where s^2 is a nonnegative variable (being square of s). Similarly, a constraint $g(X) \geq 0$ can be as $g(X) - s^2 = 0$. For each inequality constraint, there will be one additional variable (s_i). The solution is found by the Lagrange multiplier method, treating each s_i as an additional in each inequality constraint. When the Lagrange of $f(X)$ is formed with either type of constraint, equating the partial derivative with respect to s gives:

1. If $\lambda > 0$, $s = 0$. This means that the corresponding constraint is an equality constraint (active constraint)
2. If $s^2 > 0$, $\lambda = 0$. This means that the corresponding constraint is inactive or redundant.

The equality constrained optimization problem can be converted in to unconstrained problem by (i) Elimination method, (ii) by Lagrange method and (iii) by penalty function method.

Example 9.8

Select x_1 and x_2, so as to minimize $f(x) = x_1^2 + x_2^2 + 4x_1x_2$

subject to the constraint $x_1 + x_2 = 8$.

By (i) elimination method, (ii) by Lagrange multiplier method and (iii) penalty function method.

a) Elimination method

From the constraint $x_1 + x_2 = 8$ we can express x_1 in term of x_2
As $x_1 = 8 - x_2$. Substituting this equation in the objective function, we get:

$$f(x) = (8 - x_2)^2 + x_2^2 + 4(8 - x_2)x_2 \tag{9.64a}$$

$$= -2x_2^2 + 16x_2 + 64 \tag{9.64b}$$

Hence, $\partial f/\partial x_2 = 0$ gives

$$-4x_2 + 16 = 0$$

$$x_2 = 4$$

And hence x_1 from $x_1 + x_2 = 8$ gives $x_1 = 4$.

The optimal solution set is given by $x_1 = 4$ and $x_2 = 4$. To check whether this corresponds to minima or maxima, take one more derivative $\partial^2 f/\partial x_2^2$,we get this value as positive using the optimal value of x. Hence, the optimal solution corresponds to the minimum condition. In case, it is not possible to express one variable in terms of the other variable, we need to use Lagrange multiplier method discussed in the next section.

b) Lagrange multiplier method

The new objective function is written as:

$$\varphi = f(x) + \lambda\, g(x) \tag{9.65}$$

$$= x_1^2 + x_2^2 + 4x_1\, x_2 + \lambda(x_1 + x_2 - 8)$$

Hence, for optimality conditions we get:

$$\partial\varphi/\partial x_1 = 2x_1 + 4x_2 + \lambda = 0 \tag{9.66a}$$

$$\partial\varphi/\partial x_2 = 2x_2 + 4x_1 + \lambda = 0 \tag{9.66b}$$

$$\partial\varphi/\partial\lambda = x_2 + x_1 - 8 = 0 \tag{9.66c}$$

From the above first two equations we get:

$$x_1 = x_2 \tag{9.67}$$

Substituting this relation in the constraint equation we get: $x_1 = 4$

Substituting the values of $x_1 = 4$ and $x_2 = 4$ in the first condition gives: $\lambda = -24$

Hence, using the constraint and $x_1 = x_{2,}$ we get $x_1 = 4$ and $x_2 = 4$ (9.68)

The Hessian matrix for φ with respect to x_1 and x_2 can be checked for minimum or maximum condition.

c) Penalty function method

The new objective function is written as:

$$\varphi = f(x) + P\,[g(x)]^2 \tag{9.69}$$

where P is considered as a large value.

$$= x_1^2 + x_2^2 + 4x_1x_2 + p(x_1 + x_2 - 8)^2 \tag{9.70}$$

The optimality conditions are:

$$\partial\varphi/\partial x_1 = 2x_1 + 4x_2 + 2P(x_1 + x_2 - 8) = 0 \tag{9.71a}$$

$$\partial\varphi/\partial x_2 = 2x_2 + 4x_1 + 2P(x_1 + x_2 - 8) = 0 \tag{9.71b}$$

For assumed large value for P, we can solve these equations to get

$$x_1 = 4 \text{ and } x_2 = 4 \tag{9.72}$$

9.8 CONVERTING INEQUALITY CONSTRAINT TO EQUALITY CONSTRAINT

Example 9.9

$$\text{Select } x_1 \text{ and } x_2 \text{ to Min } (x_1^2 + 2x_2^2) \tag{9.73}$$

$$\text{subject to } x_1 + 3x_2 + 11 \le 0 \tag{9.74}$$

The inequality constraint can be converted into an equality constraint by introducing an auxiliary variable α^2:

$$x_1 + 3x_2 + 11 + \alpha^2 = 0 \tag{9.75}$$

Then we can formulate the Lagrange function:

$$L(x_1, x_2, \alpha^2) = x_1^2 + 2x_2^2 + \lambda(x_1 + 3x_2 + 11 + \alpha^2) \tag{9.76}$$

$$\frac{\partial L}{\partial x_1} = 2x_1 + \lambda = 0 \tag{9.77a}$$

$$\frac{\partial L}{\partial x_2} = 4x_2 + 3\lambda = 0 \tag{9.77b}$$

$$\frac{\partial L}{\partial \lambda} = x_1 + 3x_2 + 11 + \alpha^2 = 0 \tag{9.77c}$$

$$\frac{\partial L}{\partial \alpha} = 2\lambda\,\alpha = 0 \tag{9.77d}$$

We get

$$\alpha = 0; \quad x_1 = -\lambda/2; \quad x_2 = -3\lambda/4 \tag{9.78}$$

Substituting these values in Eq. (9.77c)

$$x_1 + 3x_2 + 11 + \alpha^2 = 0 \text{ gives } \lambda = 4 \tag{9.79}$$

Hence, we get:

$$x_1 = -2 \quad \text{and} \quad x_2 = -3 \tag{9.80}$$

Example 9.10

A firm's weekly output is given by the production function $q(k, l) = k^{0.75}\, l^{0.25}$.

The unit costs for capital and labour are respectively 1 and 5 per week. Find the maximum cost of producing weekly output of 5000 and the corresponding values of k and l.

Solution:

The problem can be formulated as an optimization problem as:

$$\text{Minimize } k + 5l \tag{9.81}$$

$$\text{Subject to } k^{0.75}\, l^{0.25} = 5000 \tag{9.82}$$

The Lagrange function for the problem is

$$L = k + 5l - \lambda(k^{0.75}\, l^{0.25} - 5000) \tag{9.83}$$

The optimal values of k and l are the solution to the three equations:

$$\frac{\partial L}{\partial k} = 1 - 0.75\,\lambda k^{-0.25}\,l^{0.25} = 0 \tag{9.84a}$$

$$\frac{\partial L}{\partial l} = 5 - 0.25\,k^{0.75}\,l^{-0.75} = 0 \tag{9.84b}$$

$$k^{0.75}\,l^{0.25} = 5000 \tag{9.84c}$$

The first two equations above, Eqs. (9.84a and b), give l = k/15. Substitution of this in Eq. (9.84c) gives:

$$k = 5000(15)^{0.25} \tag{9.85}$$

Hence, $l = 5000\,(15)^{-0.25}$ (9.86)

Hence, the minimum cost is given by

$$k + 5l = 13120. \tag{9.87}$$

Example 9.11

Solve the following programming problem:

$$\text{Select } x_1 \text{ and } x_2 \text{ to Min } f(X) = x_1^2 + x_2^2$$

$$\text{Subject to } 3x_1 + 2x_2 - 6 \geq 0$$

$$x_1 \geq 0,\ x_2 \geq 0$$

Solution:

We rewrite the problem as

$$\min f(X) = x_1^2 + x_2^2 \tag{9.88}$$

Subject to $g_1(X) -3x_1 - 2x_2 + 6 \leq 0$ (9.89a)

$$g_2(X) = -x_1 \leq 0 \tag{9.89b}$$

$$g_3(X) = -x_2 \leq 0 \tag{9.89c}$$

We will use the exterior penalty method.

$$P(X) = x_1^2 + x_2^2 + p_1(-3x_1 - 2x_2 + 6)^2\,u_1(g_1) + p_2(-x_1)^2\,u_2(g_2) + p_3(-x_2)^2\,u_3(g_3) \tag{9.90}$$

Since x_1 x_2 are in the first quadrant, $u_2 = 0$ and $u_3 = 0$. Since the constraint $g_1 \leq 0$ is not satisfied, we set $u_1 = 1$. The optimality conditions, $\partial P/\partial x_1 = 0$ and $\partial P/\partial x_2 = 0$, give

$$x_1(p_1) = 36p_1/(2 + 26p_1) \tag{9.91}$$

$$x_2(p) = 24p_1/(22 + 6p_1) \tag{9.92}$$

when p_1 → large (∞), we get

$$x_1 = 18/13;\ x_2 = 12/13 \tag{9.93}$$

9.9 KUHN–TUCKER CONDITIONS

There is a counterpart of the Lagrange multipliers for nonlinear optimization with inequality constraints.

$$\text{Select } x \text{ to Minimize } f(x)$$

$$\text{subject to } h(x) = 0$$

$$g(x) \le 0.$$

The Modified Lagrange equation is written as:

$$L_M(x, \lambda, \mu) = f(x) + \lambda h(x) + \mu g(x) \tag{9.94}$$

There exists λ^* (Lagrange multiplier vector) and μ^* (*KT* multiplier vector) such that the following conditions, called KT conditions are satisfied:

$$\mu^* \ge 0 \tag{9.95}$$

$$Df^* + \lambda^{*T} Dh(x^*) + \mu^{*T} Dg(x^*) = 0 \tag{9.96}$$

$$\mu^* g(x^*) = 0 \tag{9.97}$$

Here

$$Df(x) = \nabla^T f(x) \tag{9.98}$$

$$Dh(x) = [\nabla h_1(x) \ldots \nabla h_m(x)] \tag{9.99}$$

$$Dg(x) = [\nabla g_1(x) \ldots \nabla g_P(x)] \tag{9.100}$$

The point x^* is known as the KT point. This is a generalized method of the Lagrange multipliers. However, there is a possibility of degeneracy when $\mu = 0$ under certain conditions.

Example 9.12

$$\text{Select } x_1 \text{ and } x_2 \text{ to min } (x_1^2 + 2x_2^2) \tag{9.101}$$

$$\text{Subject to } 2x_1 - 2x_2 = 1 \tag{9.102}$$

$$x_1^2 + 2x_2^2 \le 5 \tag{9.103}$$

we have $f(x) = x_1^2 + 2x_2^2$; $\quad \nabla f(x) = (2x_1\ 4x_2)$

$h(x) = 2x_1 - 2x_2 - 1$; $\quad \nabla h(x) = (2, -2)$

$g(x) = x_1^2 + 2x_2^2 - 5$; $\quad \nabla g(x) = (2x_1\ 4x_2)$ (9.104)

The KT reduces to

$$\frac{\partial f}{\partial x_i} + \lambda \frac{\partial h}{\partial x_i} + \mu \frac{\partial g}{\partial x_i} = 0; \quad j = 1, 2 \tag{9.105}$$

$$\mu \geq 0 \tag{9.106}$$

$$\mu(x_1^2 + 2x_2^2 - 5) = 0 \tag{9.107}$$

along with

$$2x_1 + 2\lambda + 2\mu x_1 = 0 \tag{9.108}$$

$$4x_2 + 2\lambda + 4\mu x_2 = 0 \tag{9.109}$$

and along with

$$2x_1 - 2x_2 - 1 = 0 \tag{9.110}$$

When $\mu = 0$, we get from Eqs. (9.105) and (9.106) as

$$x_1 = -\lambda \text{ and } x_2 = -\lambda/2 \tag{9.111}$$

Substituting these values in Eq. (9.107), we get: $\lambda = -1/3$.

Hence,
$$x_1 = 1/3 \quad \text{and} \quad x_2 = -1/6. \tag{9.112}$$

$\mu \neq 0$ does not satisfy the KKT condition.

Example 9.13

Estimate the value of parameters k_1 and k_2 of the yield expression

$$y = [k_1/(k_1 - k_2)]\,[\exp(-k_2 t) - \exp(-k_1 t)] \tag{9.113}$$

given the experimental data at $t = 0.5$; $y = 0.323$; at $t = 1$; $y = 0.455$; at $t = 1.5$; $y = 0.548$.

Substituting the output y and input variable t in the model Eq. (9.113), we get the equation error (e_i). The objective function may be stated as select the values of k_1 and $k_{2,}$ such that the objective function S is minimized.

$$\text{Min } S = \sum \left\{ y - \left[\frac{k_1}{k_1 - k_2}\right]\left[\exp(-k_2 t) - \exp(-k_1 t)\right]\right\}^2 \tag{9.114}$$

The summation is over the given three experimental data points. The optimality conditions are:

$$\frac{\partial S}{\partial k_1} = 0 \quad \text{and} \quad \frac{\partial S}{\partial k_2} = 0 \tag{9.115}$$

Two nonlinear algebraic equations are formed which are numerically solved for k_1 and k_2. Otherwise, we can use the any numerical optimization method: We can use the *fminsearch* routine (given in the next chapter) with the initial guess as $k_1 = 0.3$ and $y_2 = 0.4$ to get the optimal value for k_1 and k_2 as: $k_1 = 0.669$ and $k_2 = 0.1546$.

Example 9.14

Given the expression $\mu = \mu_m\, s/(c + s)$ and the 5 experimental data s = [19 8.286 4.17 3.68 2.11] and μ = [0.38 .29 .205 .19 .13], obtain the optimal values for μ_m and c.

The expression for the equation error is formulated (by substituting experimental *s* and *c* in the model equation) as

$$e_i = \left[\mu_i - \left\{\frac{s_i}{(c + s_i)}\right\}\right] \tag{9.116a}$$

The objective function may be stated as

$$S = \sum \left[\mu_i - \left\{\mu_m \frac{s_i}{(c + s_i)}\right\}\right]^2 \tag{9.116b}$$

The summation is over the given 5 experimental data points ($i = 1, 2, \ldots, 5$).

By taking $\partial S/\partial c = 0$ and $\partial S/\partial \mu_m = 0$, we get two nonlinear algebraic equations in c and μ_m. Numerical solution of the two equations will give the values of c and μ_m. Otherwise, we can use the numerical optimization method to get the optimal values of the parameters. Using the matlab routine *fminsearch* given in the next chapter, using the initial guess values $\mu_m = 1$ and $c = 1$, we get the optimal solution as: $\mu_m = 0.5$ and $c = 6$.

9.10 MULTI-OBJECTIVES OPTIMIZATION PROBLEM

Multi-objective optimization is concerned with the minimization of a vector objective function.

Select $(x_1, x_{2,\,x}x_3, \ldots, x_n)$ to minimize $F(X)$

where
$$F(X) = [f_1, f_2 \ldots f_n] \tag{9.117}$$

subject to
$$g_i(X) = 0 \quad i = 1, 2, \ldots\ n_e \tag{9.118}$$

$$g_i(X) \le 0 \quad i = n_{e\,+\,1} \ldots.m \tag{9.119}$$

$$x_{i,\,\text{low}} \le x \le x_{i,\,\text{high}}$$

Here $F(X)$ is a vector, so it is difficult to get the solution for the multi-objective optimization problem as such.

Therefore we are converting the multi-objective optimization problem in to a scalar objective optimization problem: (i) weighted sum of squares strategy method (ii) ε-constraint method and (iii) goal attainment method.

a) Weighted sum of squares method

We consider a new objective function which is a weighted sum of squares of all the objectives,

$$\text{Min } F(X) = \sum w_i\, f_1^2 \tag{9.120}$$

$$\sum w_i = 1 \tag{9.121}$$

Since it is a scalar objective optimization method, this problem can be solved as discussed in the earlier sections. How to select w_i (the weighting factors)? We can use $w_i = 1/n$. The weighting factor can also be selected based on the physics of the problem. If the function f_i are already positive value (say e^2), then f_i can be used in Eq. (9.120), rather than f_i^2.

b) ε-constraint method

This involves in selecting the most important objective as the objective function as the scalar objective function and the other objectives are kept as a realistic inequality constraints

$$\text{Mini } f_p(X) \tag{9.122}$$

$$\text{subject to } f_j(X) \leq \varepsilon_i \quad i = 1, 2, \ldots m \; i = 1, 2, \ldots \; m \; i \neq p \tag{9.123}$$

How to select the realistic values for ε_i? The resulted scalar objective function can be solved by any suitable method.

c) Goal attainment method

The method involves expressing a set of design goals, $f^* = \{f_1^*. f_2^*, \ldots f_n^*\}$, which is associated with a set of objectives, $f(X) = \{f_1(X), \ldots f_m(X)\}$. The problem formulation step allows the objectives to be under- or over-achieved, enabling the designer to be relatively imprecise about the initial design goals. The relative degree of under-or-over achievement of the goals is controlled by a vector of weighting coefficients $w = \{w_1, w_2, \ldots w_n\}$ and it is expressed as a standard optimization problem using the following formulation

$$\text{Minimize } \gamma \tag{9.124}$$

$$\text{subject to } F_i(X) - w_i \gamma \leq f_i^* \; i = 1, 2, \ldots m \tag{9.125}$$

The term $w_i \gamma$ introduces an element of slackness into the problem, which otherwise imposes that the goals by rigidly met. The weighting vector, w, enables the designer to express a measure of the relative trade-off between the objectives.

9.11 RANDOM SEARCH OPTIMIZATION TECHNIQUES

For complex systems, the conventional optimization techniques are rather difficult and time consuming as the objective function may not be continuous and also due to large number of state variables, the initial guess may not be nearer to the optimum values. The conventional method is deterministic (no randomness in the algorithm), well-established and benchmarked ones. The disadvantage is that the method may get trapped in local optimum and hence no guarantee to get optimum. What is required is that randomness makes sure that it can ‘jump’ out of local optimum.

For such complex problems, the random search techniques are the recommended methods. Sarma (1990) considered random optimization technique, where the search is uniformly distributed over the admissible region and he has reported that even an enormous of number of function evaluations did not yield convergence to the optimum unless the search domain was chosen to be immediate vicinity of the optimum. Spaans and Luus (1992) have overcome the problem by applying the method of Luus and Jaakola (1979), which employs a systematic reduction of the search domain after every iteration. Luus (1993) has also applied this method to an optimization of heat exchanger network and has shown that the method requires lesser computational time. Conley (1981, 1984, 1987) has proposed a multi-stage random search technique, called the multi-stage Monte Carlo method, and shown that the method is easy to program and gives reliable results on several complex optimization problems. Anand and Chidambaram (1994) have applied the technique to an optimization of redundancy allocation of a pressurized water reactor cooling loop. In the present work, the performance of the random search techniques of Luus and Jaakola and Conley are evaluated and compared on two complex examples.

9.11.1 Luus and Jaakola (L–J) method

The method consists of the following steps:

(i) Take initial values for the stat variables $x_{1,}\ x_{2,\ \ldots.x}x_n$ and an initial range for each variable; denote these by x_1^*, x_2^*, … x_n^* and by $r_1^{(0)}$,' $r_2^{(0)}$,…., $r_n^{(0)}$. Set the iteration index j to 1.

(ii) Read in a sufficient number of random numbers (example 2000 numbers) between –0.5 and +0.5. Denote these by y_{k_1}.

(iii) Take pn random numbers from the step (ii) and assign these to $x_1, x_2, \ldots, x_n$, so that we may have p sets of values, each calculated by

$$x_1^{(j)} = x_1^{*(j-1)} + y_{ki}\,\mathrm{r}_1^{(j-1)}\ i = 1, 2, \ldots n; \quad k = 1, 2, \ldots, p \tag{9.126}$$

(iv) Test whether all the constraints are met and calculate the value of the objective function (F) with each admissible set.

(v) Find the set which minimizes (i.e., optimizes) the value of F and the corresponding x_1^{*j}, $i = 1, 2, \ldots, n$. increment j to $(j + 1)$

(vi) If the number of iterations has reached the maximum allowed, end the problem. For example, we may choose 200 to be the maximum number of iterations.

(vii) Reduce the range by an amount $\varepsilon(\varepsilon > 0)$

$$r_i^{(j)} = (1 - \varepsilon)\, r_i^{(j-1)}\,, \tag{9.127}$$

Typical value of ε may be 0.05.

(viii) Go to step (ii) and continue

In most of the cases Luus has considered the values of the number of iterations as 201 and the number of random points per iteration about 9.

9.11.2 Conley method

Conley method consists of evaluating a function at a large number of randomly chosen points in the feasible domain to find maxima (or minima). During repeated optimization of the same function it becomes obvious, that some variable consistently fall in the same region while others are widely distributed. One way for an improved result is to write an indefinite number of programs, each time restricting the appropriate variables to a smaller region where the distribution is high. Another way is to write a program which would automatically focus around the region of the optimal. This is carried out by the multi-stage Monte Carlo method. The method consists of a 'n' dimensional 'rectangular' inside the bounds $x_{\min} < x_i < x_{\max}$ for $i = 1, 2, 3, \ldots, n$.

Here p sample numbers are drawn. The values of the objective function at these sample points are evaluated and the best results stored. Then the bounds of the rectangular are reduced by a factor in each of the n dimension and the 'rectangle' is selected at the new best result so far. The p more sample numbers are drawn and the best result so far is stored. The bounds are reduced by the same factor and the process is repeated with p more samples drawn each time. This focusing with small rectangular each time is repeated q times. Conley has applied this method to several problems and usually 8 to 16 stages and with each stage about 1000 random numbers are used.

To compare these two methods, let us consider the same number of total number of random numbers. For application of Luus and Jaakola method, the number of iterations per step used is 201 and hence the corresponding (random) number per iteration is used. Whereas for the Conley method the number of stages used is 12 or 16 and hence the corresponding (random) number per stage is used.

9.11.3 Simulation results

Example 9.15

The optimization problem on heat exchanger network is considered here. The computer program listing (in FORTRAN) is given by Luus for the method of Luus and Jaakola. The objective function (to be maximized) is given by:

$$C = 2700\ (Q_1/\Delta T_1) + 7200\ (Q_2/\Delta T_2) + 240\ (Q_3/\Delta T_3) + 900\ (Q_4/\Delta T_4) \tag{9.128}$$

subject to the constraints:

$$Q_1 = 5.555\ (T_1\text{-}395);\ Q_2 = 1000 - Q_1;\ T_2 = 398 + (Q_2/3.125);\ Q_3 = 5.555\ (575\text{-}T_1)$$

$$T_3 = 365 + (Q_3/4.545);\ Q_4 = 3.125(718 - T_2);\ T_4 = 358 + (Q_4/3.571);\ \Delta T_1 = 0.5\ (T_1\text{-}305)$$

$$\Delta T_2 = 0.5(T_2 - 302);\ \Delta T_3 = 0.5(T_1 - T_3 + 210);\ \Delta T_4 = 0.5(T_2 - T_4 + 360)$$

$$T_i \geq 405;\ T_2 > 405;\ T_1 \leq 575;\ T_2 \leq 718;\ T_3 \geq 365;\ T_4 \geq 358;\ \Delta T_1 \geq 5;\ Q_1 \geq 0 \text{ for } i = 1, 2, \ldots, 4 \tag{9.129}$$

Here T_1 is chosen as a free variable. Queseda and Grossman (1993) have shown that G versus Q_1 has a local minimum around $Q_1 = 168.4$ and a global minimum at $Q_1 = 978.1$ kW. These corresponds to $T = 425.9$ K and $T_1 = 571.1$ K respectively. Luus has considered the middle value of the ranges of T_1 (i.e., middle point of 405 and 575) as the initial guess and an initial region size of 170 is used to cover the entire range. The region reduction factor $(1 - \varepsilon)$ is chosen as 0.95, since this value appears to be good one to use for a variety of problems. Luus has used 201 iterations and 9 random points per iteration. The program can be run on PC. The multi-stage Monte Carlo method of Conley is also applied to this problem. The computer program listing is given in Appendix. The number of stages is considered as 16 and the number of random points per stage is considered as 113. The total number of random numbers for these two methods is almost the same. A value of $\phi = **$ is used. The results show that both the methods give similar value of objective function (36162) and $T_1 = 571.08$ with close computational time (2 secs). The FORTRAN program for the Conley method for example 1 is given in the appendix

Example 9.16

Consider the problem given by Spaans and Luuus (1992):

$$\text{Minimize } f(X) = (L_1 + L_2)\ (x_1 + x_2 + x_3) + (L_3 + L_4)\ (x_1 + 1.57\ x_2 + x_4) \tag{9.130}$$

$$L_1 = 0.0204\ x_1x_4;\ L_2 = 0.0607\ x_1x_4x_5^2$$

$$L_3 = 0.0187\ x_2x_3;\ L_4 = 0.0437\ x_2x_3x_6^2$$

subject to the constraints:

$$x_i > 0, \quad i = 1, 2, \ldots, 6$$

$$x_1x_2x_3x_4x_5x_6 = 2.07\times10^3$$

$$1 - Ax_5^2 - Bx_5^2 > 0$$

where $$A = 0.00062\ x_1x_4(x_1 + x_2 + x_3) > 0$$

$$B = 0.00058\ (x_1 + 1.57x_2 + x_4)\ (2.07)^2\ x10^6/(x_1^2\, x_2\, x_3\, x_4^2) > 0$$

$$[[1/(2A)] + C]\ x_5^2 > [1/(2A) - C]$$

$$C = [1/(2A)]\ [1 - 4AB]^{0.5}$$

$$AB < 0.25;\ x_4 > [(x_1 + x_2 + x_3\ ) + (x_1 + 1.57x_2)]/D$$

$$D = Kx_1x_2x_3 - (x_1 + x_2 + x_3)$$

$$x_3 > (x_1 + x_2)/(Kx_1x_2 - 1)$$

$$x_2 > [1/(Kx_1)]$$

$$K = 0.16225 \tag{9.131}$$

Spaans and Luus (1992) have used 201 iterations and 50 random numbers per iteration. The initial guess for the state variables are 5.5, 5.5, 10, 12 and 1. The multi-stage Monte Carlo method of Conley is also applied to this problem with 12 stages and 150 random numbers per stage. Luus and Jaakola (*L* – *J*) method gives the final optimum values of x_1 = 5.34418, x_2 = 4.54235, x_3 = 11.65543; x_4 = 11.13610; x_5 = 0.76448; x_6 = 0.85936 with the final objective function value as *f* = 135.35424; whereas Conley method gives x_1 = 5.51855, x_2 = 4.55616, x_3 = 11.33190; x_4 = 11.04488; x_5 = 0.75605; x_6 = 0.87301 with the final objective function value as *f* = 135.29079. The computation time is 7.03 sec for *L* – *J* method and 6.15 for Conley method.

9.12 LINEAR LEAST SQUARE CURVE FITTING

Given the experimental data output *y* versus *x* (*N* data points) and from the plot of *y* versus *x* and the trend may show that a straight line can be fitted. The objective function may be defined as:

$$S = \sum e_i^2 = \sum [y_i - (mx_i + c)]^2 \tag{9.132}$$

Here e_i is called the equation error. The summation is over all the experimental data points (*N*). We need to select the parameters *m* and *c* so that the value of *S* can be minimal. Taking the partial derivative of *S* with respect to *m* and separately with respect to *c*, we get:

$$\frac{\partial S}{\partial m} = 2\sum [y_i x_i - (mx_i^2 + cx_i] = 0 \tag{9.133}$$

$$\frac{\partial S}{\partial c} = 2\sum [y_i - (mx_i + c] = 0 \tag{9.134}$$

The above two equations can be written as:

$$m\sum x_i^2 + c\sum x_i = \sum (y_i x_i) \tag{9.135a}$$

$$m\sum x_i + c\,N = \sum y_i \tag{9.135b}$$

From the given N data set y_i versus x_i , we can calculate $\sum x_i$, $\sum x_i^2$, $\sum x_i y_i$ and $\sum y_i$. Using these summation values, the above two linear algebraic equations can be solved to get the values for the model parameters, m and c. The above equation, Eq. (9.135a), can be written from the model equation [$y = mx + c$], by multiplying the model equation by the coefficient of m in the model equation (x_i) and taking the sum over all the data points. Similarly Eq. (9.135b) can be obtained by multiplying the model equation [$y = mx + c$] by the coefficient of c in the model equation (in this case 1) and taking the sum over all the points. For example, if the model selected is of the form: $xy = mx + c$, then the normal equations can be written as:

$$\sum x_i^2 y_i = m \sum x_i^2 + c \sum x_i \tag{9.136a}$$

$$\sum x_i y_i = \sum x_i^2 + cN \tag{9.136b}$$

If there are two independent variable x and z and the output is y. The model equation is given by

$y = m_1 x + m_2 z + c$. Then the normal equations can be written (by multiplying separately the coefficient of m_1, coefficient of m_2 and by the coefficient of c) as:

$$\sum (y_i x_i) = m_1 \sum x_i^2 + m_2 \sum (x_i z_i) + c \sum x_i \tag{9.137a}$$

$$\sum (y_i z_i) = m_1 \sum (x_i z_i) + m_2 \sum z_i^2) + c \sum z_i \tag{9.137b}$$

$$\sum y_i = m_1 \sum x_i + m_2 \sum z_i + Nc \tag{9.137c}$$

From the given data y_i versus x_i and z_i, we can calculate all the summation terms given in the above three equations. The resulting three linear algebraic equations can be solved to get the values for the constants m_1, m_2 and c. As a general guideline, the number of data points (N) should be at least five times the number of parameters in the model to be fitted. The data points to be collected so that uniformly the x variables are covered in the entire range.

Example 9.17

Suppose that we are given two types of concrete. The first type contains 30% cement, 40% gravel, and 30% sand (all percentage of weights). The second type contains 10% cement, 20% gravel, and 70% sand. How many pounds of each type of concrete should we mix together so that we get a concrete mixture that has as close as possible to a total of 5 pounds of cement, 3 pounds of gravel, and 4 pounds of sand?

Given

$$Y = Ax \tag{9.138}$$

where

$$A = \begin{bmatrix} 0.3 & 0.1 \\ 0.4 & 0.2 \\ 0.3 & 0.7 \end{bmatrix} \tag{9.139}$$

$$Y = [5 \quad 3 \quad 4]^T$$

where the decision variable $X = [x_1\ x_2]$ and x_1 and x_2 are the amounts of concrete of the first and second type, respectively.

$$\text{error } E = (y - Ax)^T (y - Ax) \tag{9.141}$$

$$= 0.5\, x^T (2A^TA)x - x^T(2A^Ty) + y^Ty \tag{9.142}$$

Select x to minimize E ,we get

$$x_{\text{opt}} = (A^TA)^{-1} A^TY \tag{9.143}$$

[we can remember the above equation by pre-multiplying $Y = Ax$ by A^T to get $A^Ty = A^TAx$; hence $x_{\text{opt}} = (A^TA)^{-1} (A^Ty)$]. Substituting the numerical values for A and y, we get

$$X = [10.6\ 0.961]^T \tag{9.144}$$

9.13 VARIABLE TRANSFORMATION TO GET A LINEAR EQUATION

Example 9.18

The trend in data set y versus x is shown in Fig (9.4). The trend shows that there is a maximum in the behaviour of y versus x. The data can be fitted by a model:

$$y = cx \exp(-dx) \tag{9.145}$$

As x is increased, initially the output y increases and the term $\exp(-dx)$ will decrease, the overall effect is towards increase in y. As the value of x is increased, the overall effect is towards decrease in y. Hence, there is a maximum in the y versus x data. To get the values of the model parameters c and d, we have to use an appropriate variable transformation to get a linear equation in the transformed variables: We can recast the model equation:

$$y/x = c \exp(-dx) \tag{9.146}$$

where $X = c \exp(-x)$ and $Y = y/x$. (9.147)

By taking logarithms both sides, we get

$$\ln(Y) = \ln(c) - dx \tag{9.148}$$

This equation represents a straight line: $p = C + mq$, where $p = \ln(y/x)$ and $C = \ln c$; $q = x$, $m = -d$. The new variables p and q can be obtained from the data set on y versus x. Using the data set p versus q, we can obtain the values of m and C. Hence, we can get the values of c and d for the original model $y = cx \exp(-dx)$.

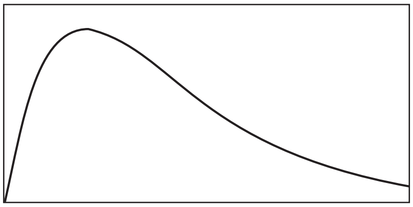


Fig. 9.4 y versus x for Example 9.18. $y = Cxe^{-Dx}$; $C = 12, D = 1$

Example 9.19

The trend in data set y versus x is shown in Fig. 9.5. The trend shows that there is a saturation in the output for the large value of x. The data can be fitted by a model: $y = L/[1 + c\exp(-dx)]$. The final value reached is noted and set as L. To get the values of the model parameters c and d, we have to use an appropriate variable transformation to get a linear equation in the transformed variables: We can recast the model equation as:

$$(L/y) = (1 + c\exp(-dx)] \tag{9.149}$$

i.e.,

$$(L/y) - 1 = c\exp(-dx) \tag{9.150}$$

By taking logarithms both sides, we get $\ln[-1 + (L/y)] = \ln c - dx$. This equation can be rewritten as

$$p = C + mq \tag{9.151}$$

where $p = \ln[-1 + (L/y)]$; $C = \ln c$; $q = x$ and $m = -d$.

In the new variables p and q, we can get a linear fit for the given data set y versus x and hence we can estimate the model parameters.

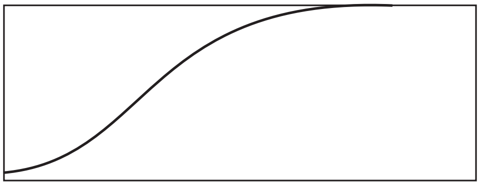


Fig. 9.5 y versus x for Example 9.19 with $L = 5$, $C = 20$, $A - 2$

Example 9.20

Let us consider the model given by:

$$y = b\,x^{a} \tag{9.152}$$

By taking Laplace transform of the equation, we get:

$$\ln y = \ln b + a\ln x \tag{9.153}$$

By using the variables $Y = \ln y$, $X = \ln x$, $C = \ln b$ and $m = a$, we can write a linear equation: $Y = C + mX$. The value of the parameters, m and C, and hence the parameters b and a of the original model, can thus be obtained.

Example 9.21

Let us consider the model:

$$y = c\exp(-dx) \tag{9.154}$$

By taking Laplace transform of the equation, we get:

$$\ln y = \ln c - dx \tag{9.155}$$

By using the variables $Y = \ln y$, $X = x$, $C = \ln c$, $m = -d$, we can write a linear equation:

$Y = C + mX$. The value of the parameters m and C and hence the parameters c and d of the original model, can be obtained.

Using the data on Nu (Nusselt number) versus Re (Reynolds number) and Sc (Schmidt number), we can fit a correlation for heat transfer coefficient as

$$\mathrm{Nu} = 2 + b\,\mathrm{Re}^{m}\mathrm{Sc}^{n}. \tag{9.156}$$

Similarly for the mass transfer problem:

$$\mathrm{Sh} = 2 + b_1\,\mathrm{Re}^{m2}\,\mathrm{Sc}^{m2} \tag{9.157}$$

By suitable variable transformation, we can get a linear model as $y = mx + c$

Example 9.22

The reaction rate (v) of the photosynthesis in a green plants can be approximated by the following expression: $v = \alpha/[I + (\beta/I)]$; where I is the light intensity, and α is the maximum rate, and β is the affinity. The experimental data set on v for different values of I are as follows:

$$I = 10, 20, 30, 40 ,50;$$

$$v = 15.2\ 20, 22.5\ 24, 25$$

Find the optimal values of α and β.

Solution:

The nonlinear relation of I on v is rewritten as:

$$(1/v) = (1/\alpha) + (1/I)\,(\beta/\alpha) \tag{9.158}$$

This is a linear equation in $(1/v)$ versus $(1/I)$

$$y = mx + c$$

where $$y = 1/v\ ;\ x = 1/I;\quad m = (\beta/\alpha);\ c = (1/\alpha) \tag{9.159}$$

By linear least square method, we get $\alpha = 30$ and $\beta = 10$

9.14 SET-POINT WEIGHTED PI/PID CONTROLLERS

For design of controllers, the dynamics of many processes are described adequately by first order plus time delay transfer function models $[\Delta y(s)/\Delta u(s) = K_P \exp(-Ls)/(\tau s + 1)]$. A method for tuning PI/PID controllers for stable first order plus time delay systems is given by Ziegler and Nichols (1942) and review of the methods is given by Astrom and Hagglund (1995). The response by Ziegler–Nichols method is good for regulatory problems whereas a significant overshoot is present for servo problems. Astrom and Hagglund (1995) have shown that use of set point weighting reduces the overshoot for servo problems. Hang et al. (1991) have selected the set point weighting for the stable system by a numerical optimization search method to reduce the overshoot. An optimization method is proposed here for the selection of the weighting parameter for stable first order plus time delay systems.

The set-point weighting PI/PID controller is given by (Astrom and Hagglund, 1995):

$$u(t) = k_c \left[e_p + (1/\tau_t) \int_0^t e\,dt - \tau_D (dy/dt) \right] \tag{9.160}$$

where
$$e_p = (by_r - y) \tag{9.161}$$

$$e = (y_r - y) \tag{9.162}$$

Here y is the system output, y_r is the set point for y and b is the set-point weighting parameter. For stable systems, Astrom and Hagglund (1995) have shown by simulation, for the parameters of the stable first order plus time delay systems considered, that $b = 0.5$ gives less overshoot. However as stated earlier, there is no systematic method given for the selection of the parameter b. Let us consider a PI controller (Eq. 1) for the stable system $k_p \exp(-Ls)/(\tau_s + 1)$. The transfer function relating y to y_r is given by

$$y/y_r = \frac{k_p k_c [b + (1/\tau_I s)][\exp(-Ls)/\tau s + 1)]}{1 + k_p k_c [1 + (1/\tau_I s)]/[\exp(-Ls)/(\tau s + 1)]} \tag{9.163}$$

Using the approximation $\exp(-Ls) = 1 - Ls$, in the denominator, Eq. (9.106) can be written as

$$y/y_r = \frac{(b\tau_I s + 1)\exp(-Ls)}{(\tau_e s^2 + 2\tau_e \zeta s + 1)} \tag{9.164}$$

where
$$\tau_e^2 = \frac{\tau_I (\tau - k_c k_p L)}{(k_c k_p)} \tag{9.165}$$

$$2\tau_e \zeta = \frac{[\tau_I + k_c k_p (\tau_I - L)]}{(k_c k_p)} \tag{9.166}$$

From the Eqs. (9.108) and (9.109) we get,

$$\tau_I = \frac{(-\tau_e^2 + \tau L + 2\tau_e \zeta)}{(\tau + L)} \tag{9.167}$$

$$k_c = \frac{\tau \tau_I}{(\tau_e^2 + \tau_I L)} \tag{9.168}$$

Once the effective time constant (τ_e) and the damping coefficient (ζ) for the closed loop system are specified, then the controller settings k_c and τ_I can be calculated from Eq. (9.167) and (9.168) The settling time of the closed loop is related to τ_e and ζ by $t_s = 5/\zeta\omega_n$. Hence, $\omega_n = 5/(\zeta t_s)$. Usually ζ and t_s are specified. That is, by specifying ζ and t_s, we are indirectly assigning the closed loop dominant poles. Let us discuss how to select the set-point weighting parameter (b).

The step response of Eq. (9.107) for unit step change in the set point is given by

$$y(t) = \left[1 - d \exp\left(-\frac{\zeta\theta}{\tau_e} \right) \sin(E\theta + \phi) \right] \tag{9.169}$$

where
$$\theta = t - L \tag{9.170}$$

$$d = \left[1 - 2\zeta\left(\frac{b\tau_I}{\tau_e}\right) + \left(\frac{b\tau_I}{\tau_e}\right)^2\right]^{0.5} \Big/ q \tag{9.171}$$

$$q = \left|(1-\zeta^2)\right|^{0.5} \tag{9.172}$$

$$E = q/\tau_e \tag{9.173}$$

$$\phi = \tan^{-1}\{q/[\zeta - (b\tau_I\tau_e)]\} \tag{9.174}$$

The time to reach the first peak (θ_1) in the response is obtained by taking partial derivative of y and equating the expression to zero to get:

$$\theta_1 = \left[\tan^{-1}\left(\frac{q}{\zeta}\right) + \pi - \phi\right]\tau_e / q \tag{9.175}$$

at $\theta = \theta_1$, we can simplify the term sin ($E\theta + \phi$) as:

$$\sin(E\theta_1 + \phi) = -q \tag{9.176}$$

Hence, from Eq. (9.112) we get,

$$y(\theta_1) = [1 + F\exp(-\zeta\theta_1/\tau_e)] \tag{9.177}$$

where

$$F = \left[1 - 2\zeta\left(\frac{b\tau_I}{\tau_e}\right) + \left(\frac{b\tau_I}{\tau_e}\right)^2\right]^{0.5} \tag{9.178}$$

The parameter b can now be selected in order to minimize the first overshoot in y. To minimize the overshoot, we must set $\partial F/\partial b = 0$. Then we get,

$$b = \frac{\tau_e\zeta}{\tau_I} \tag{9.179}$$

With this value, we can show that the second derivative of F with respect to b becomes $2q$ which is positive. Thus b given by Eq. (9.179) ensures a minimum value in F. Equation (9.179) shows that the set-point weighting parameter (b) depends on ζ, L and τ_e. We already seen that by specifying ζ and τ_e, we can calculate the PI controller settings k_c and τ_I. By Eq. (9.179) we can now calculate b.

By using Eq. (9.110) and Eq. (9.111) in Eq. (9.112), we get the weighting parameter b for a PI controller in terms of the controller settings and the model parameters as:

$$b = \frac{[\tau_I + k_c k_p(\tau_I - L)]}{(2k_c k_p \tau_I)} \tag{9.180}$$

For the PI controllers settings by Ziegler–Nichols method ($k_c k_p = 0.9/\varepsilon$; $\tau_I = 3.33\text{L}$, where $\varepsilon = L/\tau$) Eq. (9.180) becomes:

$$b = 0.35 + 0.556\varepsilon \tag{9.181}$$

That is, the value of b varies for Ziegler–Nichols method from 0.35 to 0.906 as ε varies from 0 to 1.0. In case, we calculate the PI controller settings k_c and τ_I, by any other method other than specifying ζ and τ_e then Eq. (9.181) is used to calculate the set point weighting parameter b. Let us assume $k_p = 1$, $\tau = 1$ and $L = 0.5$. The PI controller settings, by Ziegler–Nichols open loop tuning method, are given by $k_c = 1.8$, $\tau_I = 1.665$.

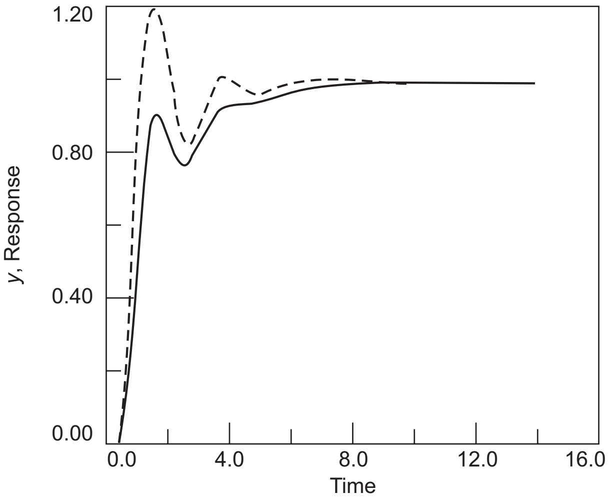


Fig. 9.6 The response (solid) with b = 0.63 and (- -) with b = 1 (Chidambaram, 2000)

The response for a unit step change in the set-point without and with set-point weighting (PI controller) $k_p = 1$, $L = 0.5$, $\tau = 1$; $k_c = 1.8$, $\tau_I = 1.665$, $b = 1$; $b = 063$ is shown in Fig. 9.6. The set-point weighting reduces the overshoot significantly (from 0.2 to 0.0).

Set Point Weighting Parameter for PID Controller

Let us consider the selection of b for PID controllers. In deriving Eq. (9.107) from Eq. (9.106), we have assumed exp(–Ls) = 1 – Ls. However, without making the assumptions also, we can still get similar to Eq. (9.106). For PID controller (9.106) the numerator of Eq. (9.107) is the same and the denominator is given by

$$1 + \left[K + \frac{K_I}{s} + K_p s\right]\left[\exp\left(\frac{(-Ls)}{(\tau s + 1)}\right)\right] = 0 \tag{9.182}$$

where $K = k_c k_p$; $K_I = K/\tau_I$; $K_D = K\tau_{D.}$ The method is applicable to higher order systems by reducing the higher system to a first order plus time delay system.

C Program for multi stage Monte Carlo optimization (example 9.16)

```
      IMPLICIT DOUBLE PRECIION(A-H,O-Z)
      REAL*4 YFL
      DIMENSION B(10), N(10), L(10), AU(10), X(10), A(10)
      REAL B,N,L,AU
      OPEN(UNIT=50, FILE: 'MSMCO1.OUT')
      READ(*,*) IX
      READ(*,*)NST,NPT
```

```
      WRITE(50,5)IX,NST,NPT)
5     FORMAT(2X,3(2x,I5))
      PMIN = 1.D20
C FOCUSING FACTOR
      F=2
      NV=1
      DO I K=1,NV
      B(K) =405
      A(K) = 490
1           N(K) = 575
                  CALL GETTIME(ih,im,is,i100)
      SSTIME = i100+100*is+6000*im+360000*ih
C NST rectangles of ever decreasing size
      DO 19 J=1,NST
      Q=F**J
      NCN =1
      DO 30 I=1,NPT
      DO 4 K=1,NV
      IF(NCN.EQ.0) GO TO 1109
      IF(A(K)-N(K)/Q.LT.B(K)) GO TO 50
      GO TO 60
50    K(K) = B(K)
      GO TO 65
60    L(K) = A(K) -N(K)/Q
65    IF(A(K)+N(K)/Q.GT.N(K)) GO TO 80
      GO TO 90
80    AU(K)=N(K)-L(K)
      GO TO 100
90    AU(K) =A(K)+N(K)/Q-L(K)
1109  CONTINUE
      CALL RANDU(IX,IY,YFL)
      RAND=DBLE(YFL)
      IX=IY
100   X(K) = L(K) +AU(K)*RAND
```

```
4     CONTINUE
C THE FUNCTION
      T(1) =X(1)
      IF(T1.LT.405.D0) GO TO380
      IF(T1.GT.575.D0)GO TO 30
      Q1=5.555D0*(T1-395.0D0)
      Q2=1000.D0-Q1
      IF(Q2.LT.0.0D0) GO TO 30
      T2=Q2/3.125D0+398.0D0
      IF(T2.LT.405.D0) GO TO 30
      IF(T2.GT.718.D0) GO TO 30
      Q3=5.555D0*(575.0D0-T1)
      T3=365.D0+Q3/4.545D0
      IF(T3.LT.365.D0) Go TO 30
      Q4=3.125D0*(718.D0-T2)
      T4=358.D0+Q4/3.571D0
      IF(T4.LT.358.D0)O TO 30
      DT1=0.5D0*(T1-305.D0)
      IF(DT1.LT.5.0D0)GO TO 30
      DT2=0.5D0*(T2-302.D0)
      IF(DT2.LT.5.0D0)GO TO 30
      DT3 = 0.5D0*(T1-T3+210.D0)
      IF(DT3.LT.5.D0)GO TO 30
      DT4= 0.5D0*(T2-T4+360.0.D0)
      IF(DT4.LT.5.D0)GO TO 30
      P=2.7D3*Q1/DT1+7.2D3*Q2/DT2+2.4D2*Q3/DT3+9.0D2*Q4/DT4
      NCN=0
C THE COMPARISION STATEMENT TO FIND OUT THE BEST ANSWER SO FAR
      IF(P.LT.PMIN) GO TO 200
      GO TO 30
C THE STORAGE SPACE WHICH ALSO CONTROLS and CENTRES THE EVER CHANGING
C RECTANGLES
200   PMIN=P
      NCN=1
      DO 201 IN=1,NV
```

```
201    A(IN) = X(IN)
30     CONTINUE
C      THE ANSWER
       WRITE(50,402)J,A(1),PMIN
402    FORMAT(5X,I4,2X,F11.3,3X,F15.3)
19     CONTINUE
       CALL GETTIME(Ih,I,is,i100)
       endtime = i100+100*is+6000*im+360000*Ih)
       TIME = (endtime-sattim)*0.01
       WRITE(50,197)time
197    FORMAT(1X,'CPU TIME'=',f12.5,1X,'secs')
       STOP
       END
C
C RANDOM NUMBER GENERATION
       SUBROUTINE RANDU(IX,IY,YFL)
       IY=IX+65539
       IF(IY)5,5,6
5      IY=IY+2147483647+1
6      YFL = IY
       YFL = YFL*0.4656613E-9
       RETURN
       END
```

Review Problems

1. Find the values of x in order to minimize $f(x) = x^4 - 5x^3 - 10x^2 + 2$ and determine if the stationary points correspond to maxima, minima, or saddle points by using the necessary and sufficient conditions of optimality.
2. Given $f = 6x_1^2 + x_2^3 + 6x_1x_2 + 3x_2^2$, find the stationary points and classify them by calculating the eigenvalues of the corresponding Hessian matrix.
3. Given $y = a_0 + a_1 x_1 + a_2x_2 + a_3 x_1x_2$ and a set of 20 data sets on y versus x_1 and x_2 , write down the normal equations to estimate the parameters a_0, a_1, a_2 and a_3.
4. Find the stationary points and their local nature of:

   $dx_1/dt = 2x_1 \{ 1 - [(x_1 + 3x_2)/400]\}$; $dx_2/dt = x_2 \{ 1 - [(3x_1 + x_2)/400]\}$

   Get the phase plane diagram by using ODE23 routine using various initial conditions.
5. Sketch the plots of commonly occurring functions $y(x)$. Give the suitable transformation of variables so to recast the equation as linear in the parameters.

6. Select x_1 and x_2 to minimize $f(X) = 7x_1^2 + 4x_1x_2 + 2x_2^2 - 8x_1 + 8$

   Subject to the constraints $x_1 + x_2 - 2 = 0$

   Convert the constrained optimization problem into an unconstrained optimization problem and get the solution by (i) elimination method (ii) Lagrange's multiplier method and by (iii) penalty function method.

7. Determine the optimum operating pressure and recycle ratio for a process where the hydrocarbon feed is mixed with a recycle stream and compressed before passed in to catalytic reactor. The product and un-reacted materials are separated by distillation, and the un-reacted material is recycled. The feed is brought up to pressure at an annual cost of \$1,000 P, mixed with the recycle stream, and fed to the reactor at an annual cost of $\$4 \times 10^9/(PR)$. The product is removed in a separator at a cost of $\$10^5$ R per year and the un-reacted material is recycled in a re-circulating compressor which consumes $\$1.5 \times 10^5$ per annum. Determine the annual cost and show it is a minimum.

8. In the above problem, it is necessary to maintain the product of the pressure and recycle ratio equal to 9,000 psi. Determine the optimal pressure and recycle ratio and the minimum cost within by (i) the Lagrange multiplier method (ii) by direct substitution method and (iii) By the penalty function method.

9. Convert the inequality constrained optimization method in to an equality constrained optimization method and then solve the resulting problem:

   $$\underset{x_1,\, x_2}{\text{Min}}\ f(X) = x_1^3 - 3x_1x_2 + 4$$

   subject to $5x_1 + 3x_2 \geq 18$

10. Given the over determined systems of algebraic equations, formulate the problems as an optimization problem and hence get the values of x_1 and x_2:

    $2x_1 + 3x_2 = 9$; $3x_1 + 5x_2 = 12$; $7x_1 + 12x_2 = 33$

11. Given the systems of linear algebraic equations

    $4x_1 - x_2 + 3x_3 = 6$; $-3x_1 + 7x_2 + 9x_3 = 13$; $8x_1 + 3x_2 - 5x_3 = 6$;

    Formulate an optimization problem by least square method to find the values of x_1, x_2 and x_3.

12. State the multi-objectives optimization problem. Discuss the methods of converting into a scalar objective optimization problem

13. By least square method, write down the normal equation for estimating the model parameters of:

    a) $y = a_1x_1 + a_2x_2 + a_3\, x_1x_2$; 20 data set on y versus x_1 and x_2 available.

    b) use appropriate variable transformation to get a linear least square problem for $y = ax^b$

14. For the gas phase reaction $A \rightarrow B \rightarrow C$ over a solid catalyst , the input data on P_A, P_B and P_C , and the corresponding output data on the rate of reaction $(-r_A)$ for the component

    A are noted and there are 10 such experimental data are available. The theoretically

    derived expression for $(-r_A)$ is given by $(-r_A) = kP_AP_B/[1 + K_AP_A + K_CP_C]$

    By use of transformed variables, convert the above rate equation in to a linear equation:

    $y = a_1x_1 + a_2x_2 + a_3x_3$. Explain the steps to estimate the values of k, K_A and K_C.

15. Consider the enzymatic conversion of a substrate S to a product P in a batch bioreactor. The mole balance on the substrate in a batch bioreactor with m gram of enzyme is given by $dS/dt = -m/(\alpha V_R)\ V_m\, S/[k_m + S + k_s^2]$

    [For simulation purpose use: $V_m = 200\ \mu\text{mol/(min/mg)}$; $k_m = 0.201$ M and $k_m = 0.5616$ M].

The reactor volume V_R is 100 ml , m =10 mg α = 10^6. The concentration of substrate as a function of time is obtained at various time, starting from an initial concentration of 2 M. Using the experimental data and the model equation, get the estimates of V_m, k_m and k_{st}. Use the objective function as $F = \sum(S_{\text{mod}} - S_{\text{expt}})^2$; The summation is over the nine experimental data points.

Experimental data Time = [30 60 90 120 180 240 300 315 330]; S = [1.87 1.73 1.58 1.43 1.07 0.63 0.12 0.04 0.01]. Use *fminsearch* or *fminunc* routine to obtain the parameters.

16. Zhu et al. (1997. Ind. Eng. Chem. Res. 36. 2897–2902) discussed the kinetic parameters estimation for 3-hydroxypropanal hydrogenation over $Ni/SiO_2/Al_2O_3$ catalyst. Read the research paper and give a write-up on the optimization method used for the estimation of parameters.
17. Linga et al. (2006. Ind. Eng. Chem. Res. 45. 4716–4725) presented a study on comparison of the Luss–Jaakola optimization and Gauss–Newton Methods for parameter estimation in ODEs models occurring in four different examples. Give a write up of the work.

10

Simulation Using Matlab/Scilab

In this Chapter, applications of Matlab and Scilab packages are explained for solving numerically nonlinear algebraic equations, nonlinear IVP ODES, BVP ODEs, optimization problems, and nonlinear PDEs, etc.

10.1 MATLAB (MATrix LABoratory)

It provides computing, visualization and application specific tool boxes for solving mathematical equations arising in modelling. A matrix oriented language is used which incorporates many features of C. It has built-in set of commands for standard algorithms involving numerical computations. It has interactive 2-D, 3-D graphical capabilities for analysis, transformation and visualization of data. Matlab has interactive mathematical software. It contains powerful sets of commands that the user enters, to click on an icon. Immediately the response is shown on the screen. Programming time is less since there is no compile-link-execute cycle. The user spends less time worrying about formalisms and syntax. Matlab is available on wide range of computers: PCs, Workstations. More than 20 tool boxes for specific applications are available: Signal & image processing, Control system design, identification, Neural networks, fuzzy logic, optimization, Communications, Financial Time series, etc. As with any software program, there are a few 'rules' and 'codes' which must be followed.

The structure of matlab consists of two separate files, te 'M-file' and an execution file which we call the 'command file'. Simply put, the M-file is the file where you identify the equations you want to solve and the command file is the file that establishes the initial conditions, identifies the solution methodology and dictates the particular output that is desired. Because these two file must be linked, it is important to establish a 'file path' to the location where the M file is saved.

The command file

Within the command file, you can establish the initial condition, solve the set of equations and manipulate the data. To solve a set of differential equations where the independent variable is t, and the dependent variable is a vector, y, the following statement is used:

[t, y] = ode45('probl1',tspan,y0)

where tspan is the initial time and the final time during which the equations are to be integrated. For example

tspan = [0 10];

y0(1) = 1.0;

y0(2) = 2.0;

Here ODE45 is the name of the differential equation solver you want to use for the solution. Probl1 is the name of the function you define in the M-file.

Non stiff solver	ode45, ode23, ode113
Stiff solvers	oder15s, ode23s, ode113t

The numbers associated with the names indicates the 'order' of the numerical method, the 's' indicates a stiff algorithm and the 't' indicates an implementation of the trapezoidal rule.

The main routine for solving the nonlinear algebraic equations **f(x) =0** is **fsolve**

X = fsolve (funmane, x0, Options,p1,p2)

Funname is the name of the routine:

Function f = funmane(x,p1,p2)

That returns the function vector for input x for the system under consideration. x0 is the initial guess, and p1, p2, are optional parameters. Options is a data structure managed by optimset that controls the operation of fsolve. To start with, we need not use options. Fsolve is part of the optimization toolkit and so is not available in all installations of Matlab. For a single nonlinear algebraic equation, fzero can be called:

X = fzero(funname, Options,p1,p2)

The **fmincon** solves constrained optimization problems with the structure

Minimize F(x)

Subject to the constraints (linear and nonlinear)

$$A\mathbf{x} \le \mathbf{b} \quad \mathbf{A}^{(eq)}\,\mathbf{x} = \mathbf{b}^{(eq)};\ c(\mathbf{x}) = 0 \text{ and } c^{eq}(\mathbf{x}) = 0$$

And the upper and lower bounds $LB_j \le x^j \le UB_j$

The routine is called with the syntax

[x.F,exitflag, output, grad, Hessian] = fminunc

(funmane,x0,A,b,Aeq,beq,,LB,UB,nonlcon, Options,P1,P2,) Fun is the name of the function that returns the objective function

Function F – fun(x,p1,p2,)

If constrain is not present, use [ ] as a place holder. The vectors of lower bounds for each parameter are LB and UB.

10.2 TYPES OF ODES SOLVERS

Nonstiff Problems: There are three solvers designed for nonstiff problems:

`ode45`	Based on an explicit Runge–Kutta (4,5) formula, the Dormand–Prince pair. It is a *one-step* solver- in computing $y(t_n)$, it needs only the solution at the immediately preceding time point, $y(t_{n-1})$. In general, `ode45` is the best function to apply as a "first try" for most problems.
`ode23`	Based on an explicit Runge–Kutta (2,3) pair of Bogacki and Shampine. It may be more efficient than `ode45` at crude tolerances and in the presence of mild stiffness. Like `ode45`, `ode23` is a one-step solver.
`ode113`	Variable order Adams-Bashforth-Moulton PECE solver. It may be more efficient than `ode45` at stringent tolerances and when the ODE function is particularly expensive to evaluate. `ode113` is a *multistep* solver—it normally needs the solutions at several preceding time points to compute the current solution.

10.2.1 Stiff problems

Not all difficult problems are stiff, but all stiff problems are difficult for solvers not specifically designed for them. Solvers for stiff problems can be used exactly like the other solvers. However, you can often significantly improve the efficiency of these solvers by providing them with additional information about the problem. There are four solvers designed for stiff problems:

`ode15s`	Variable-order solver based on the numerical differentiation formulas (NDFs). Optionally it uses the backward differentiation formulas, BDFs (also known as Gear's method). Like `ode113`, `ode15s` is a multistep solver. If you suspect that a problem is stiff or if `ode45` failed or was very inefficient, try `ode15s`.
`ode23s`	Based on a modified Rosenbrock formula of order 2. Because it is a one-step solver, it may be more efficient than `ode15s` at crude tolerances. It can solve some kinds of stiff problems for which `ode15s` is not effective.
`ode23t`	An implementation of the trapezoidal rule using a "free" interpolant. Use this solver if the problem is only moderately stiff and you need a solution without numerical damping.
`ode23tb`	An implementation of TR-BDF2, an implicit Runge–Kutta formula with a first stage that is a trapezoidal rule step and a second stage that is a backward differentiation formula of order 2. Like `ode23s`, this solver may be more efficient than `ode15s` at crude tolerances.

10.3 MATLAB PROGRAMS WITH EXAMPLES

Problem 10.1

Find the roots
Fine the value of root near x = 0 of $x^2 - 2x - 3 = 0$

M File

```
function y = nitt1(x)
y=x^2-2*x-3;
```

Command window

```
% (initial guess:x0=0)
>> x0=[0];
>> z=fzero('nitt1',x0)
```

Solution

```
z = -1
% (initial guess:x0=2)
>> x0=[2];
>> z=fzero('nitt1',x0)
```

Solution

```
z = 3
```

Problem 10.2

Find the roots
Find all the roots of $x^2 - 2x - 3 = 0$

Command window

```
c=[1 -2 -3]';
>> roots(c)
```

Solution

```
ans =
     3.0000
    -1.0000
```

Problem 10.3

Solution linear algebraic equation Ax = b

```
A = [ 1 1 1
      2 1 3
      3 1 6 ]
```

```
and b =[4 7 2]ᵀ
A = [1 1 1; 2 1 1; 3 1 6];
B=[4; 7; 2];
X = A\b
X =
   19.00
     7.00
    -8.00
```

Problem 10.4

To find the roots of the nonlinear algebraic equation: $e^x - x^2 - 2x = 0$ for two different initial guess values by using **fsolve** routine.

Solution:

Main Program with Function in one m-file: *tutprob1main.m*

```
function tutprob1main
a = [0 2];
for i=1:2
    x0=a(i);
    z=fsolve(@tut_prob1,x0);
    x0
    z
end
end
function f = tut_prob1(x)
f = exp(x) - x^2 - 2*x;
end
```

Output: For initial guess `x0=0` and `x0=2`

```
x0 =      0
z =    0.7895
x0 =      2
z =    2.2743
```

Problem 10.5

Solve a set of nonlinear algebraic equation

Write a matlab program to solve the following nonlinear algebraic equations:

$$x_1 - 4x_1^2 - x_1x_2 = 0$$

$$2x_2 - x_2^2 + 3x_1x_2 = 0$$

M file

```
function f=nitt3(x)
f(1)=x(1)-4*x(1)*x(1)-x(1)*x(2);
f(2)=2*x(2)-x(2)*x(2)+3*x(1)*x(2);
```

Command window

```
>> x0=[1 1]';
>> x=fsolve('nitt3',x0)
```

Solution

```
x =    0.2500    0.0000
```

Write a Matlab program to solve the following simultaneous nonlinear algebraic equations:

$$x^2y^2 - 2x - 5y^{0.5} + 5 = 0$$

$$x^4 - 6y^2x + 23 = 0$$

M-file

```
function f = proble (x)
f(1) = (x(1)^2)*x(2)^2 - 2*x(1) - 5*x(2)^0.5 + 5;
f(2) = x(1)^4 - 6*(x(2)^2)*x(1) + 23;
end
```

Command Window:

```
>> x0  = [1 1] ;
>> z = fsolve('probe', x0)
```

Solution

```
    z  =      1.0171       1.9860
```

Problem 10.6

Solve Nonlinear IVP ODEs

Write a matlab program to solve the following IVP ODES:

$$dx_1/dt = x_2;\ dx_2/dt = x_2\,(1-x_2^{\,2}) - x_1 \text{ at } 0;\ x_1 = 0.25;\ x_2 = 1.0$$

M file

```
function xdot=nitt4(t,x)
xd(1)=x(2);
xd(2)=x(2)*(1-x(1)^2)-x(1);
xdot=[xd(1) xd(2)]';
```

Command window

```
tspan=[0 20];
```

```
x0=[0.25 1]';
[t,x]=ode23('nitt4',tspan,x0);
plot(t,x(:,1),':',t,x(:,2));
xlabel('time,sec')
ylabel('response in x1,x2')
```

Solution

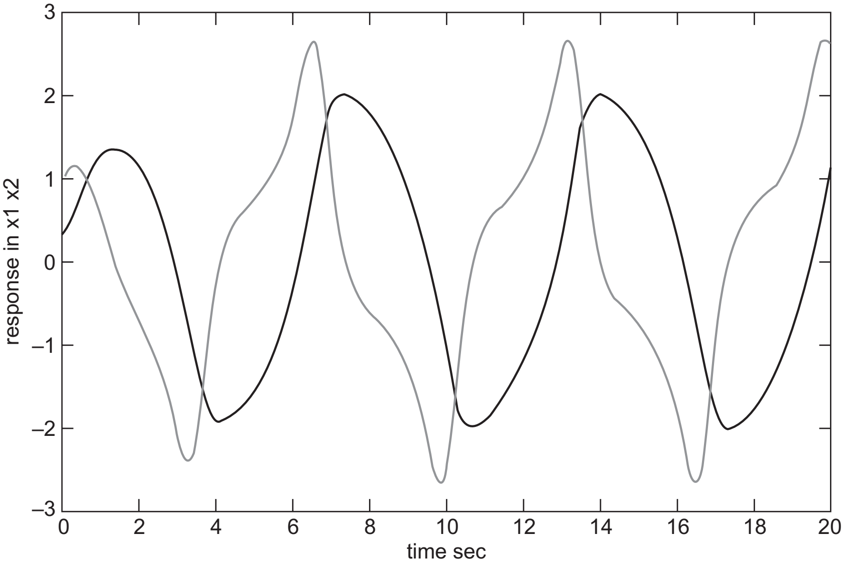


Fig. 10.1 Output for problem 10.6.

Problem 10.7

Method of parameter differentiation

By the method of parameter differentiation (MPD), find the root of $e^x - x^2 - 2x = 0$ near x = 0 and separately at x = 2.

For initial guess x0=0

<u>Function</u>: tutprob3.m

M-file

```
Function xdot= tutprob3(t,x)
xdot==-1/(exp(x)-2*x-2);
End
-----------------------------------------------------
```

Command window

```
Clear all
Tspan=[0 1];
```

```
x0=0;
[t,x]= ode23('tutprob3', tspan,x0);
[r c] = size(x);
z=[x(r)]
```

Output:

```
z = 0.7895
-----------------------------------------------------
For initial guess x0=2
Function: tutprob3.m
```

M File*:*

```
-----------------------------------------------------
Function xdot= tutprob3(t,x)
xdot==-0.6109/(exp(x)-2*x-2);
End
-----------------------------------------------------
```

Command window

```
Clear all
Tspan=[0 1];
x0=2;
[t,x]= ode23('tutprob3', tspan,x0);
[r c] = size(x);
z=[x(r)]
Output:
z = 2.2743
-----------------------------------------------------
```

Problem 10.8

MPD for simultaneous algebraic equations

By the method of parameter differentiation (MPD), solve the following simultaneous nonlinear algebraic equations:

$$x^2y^2 - 2x - 5y^{0.5} + 5 = 0;$$

$$x^4 - 6y^2x + 23 = 0$$

with an initial guess x = 1 and y = 1.

M-file

```
Function xdot = tutprob4(t,x)
  FP= = [-1  18]';
```

```
J11 = 2*x(1)*x(2)^2-2;
J12 = 2*x(1)^2*x(2) – 2.5*x(2)^(-0.5);
J21 = 4*x(1)^3 – 6*x(2)^2;
J22 = -12*x(1)*x(2);
J = [J11 J12 ; J21 J22];
F = -inv(J)*FP;
xdot = [f(1) f(2)]';
end
```

Command window

```
clear all;
tspan = [0 1];
x0 = [ 1 1];
[t,x] = ode23('tutprob4',tspan,x0);
z = x(size(x,1)
Output
z =
           1.0173    1.9859
-------------------------------------------------------
```

Problem 10.9

Minimise the function
Select x_1 and x_2 to minimize $f(x_1,x_2) = \exp(x_1)\ [4x_1^2 + 2x_2^2 + 4x_1x_2 + 2x_2 + 1]$

Given the initial guess $x_1 = –1$; $x_2 = 1$

M file

```
function f=nitt5(x)
f=exp(x(1))*(4*x(1)^2+2*x(2)^2+4*x(1)*x(2)+2*x(2)+1);
```

Command window

```
x0=[-1 1];
x=fminunc('nitt5',x0)
```

Solution

```
x =   0.5000   -1.0000
```

Problem 10.10

Phase plane diagram
Draw the phase plane diagram for the system:

$$dx_1/dt = x_1\ [1- \{(x_1 + 2x_2)/300\}];$$

$$dx_2/\ dt = x_2[1-\{(2x_1+x_2)/300\}]$$

Function File

```
function f=plane(t,x)
f(1)=x(1)*(1-(x(1)+2*x(2))/300);
f(2)=x(2)*(1-(2*x(1)+x(2))/300);
f=[f(1) f(2)]';
```

Main File

```
x1=[0.5 1  10 50 100 150 200 250 300 350 400 450 500];
x2=[0.5 1  10 50 100 150 200 250 300 350 400 450 500];
for i=1:13
for j=1:13
[t,x]=ode23s('plane',[0 20],[x1(i),x2(j)]);
plot(x(:,1), x(:,2));
hold on;
end
end
>> xlabel('x(1)');
>> ylabel('x(2)');
```

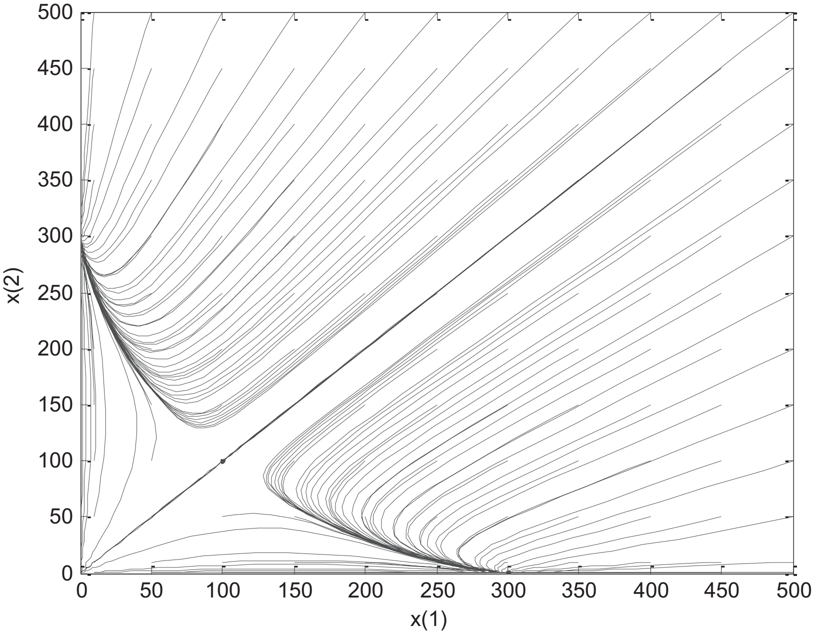


Fig. 10.2 Output for problem 10.10

Problem 10.11

Solution of a delay differential equation
Consider the differential equation:

$$dx/dt = r\ x(t)\ [1 - \{(x(t\text{-}T)/K\}]$$

where T represents the time delay between increased death and the resulting decrease in population reproduction. The above equation is known as a differential difference equation or differential delay equation. Matlab has a built in routine for dealing with such equations, dde23, similar to ode45 for solving ODEs. The values of parameters assumed are r=2.0; K=100; T=1, initial condition x(t=0) = 50. The oscillatory response is shown in the following figure. The matlab listing is given in the following listing.

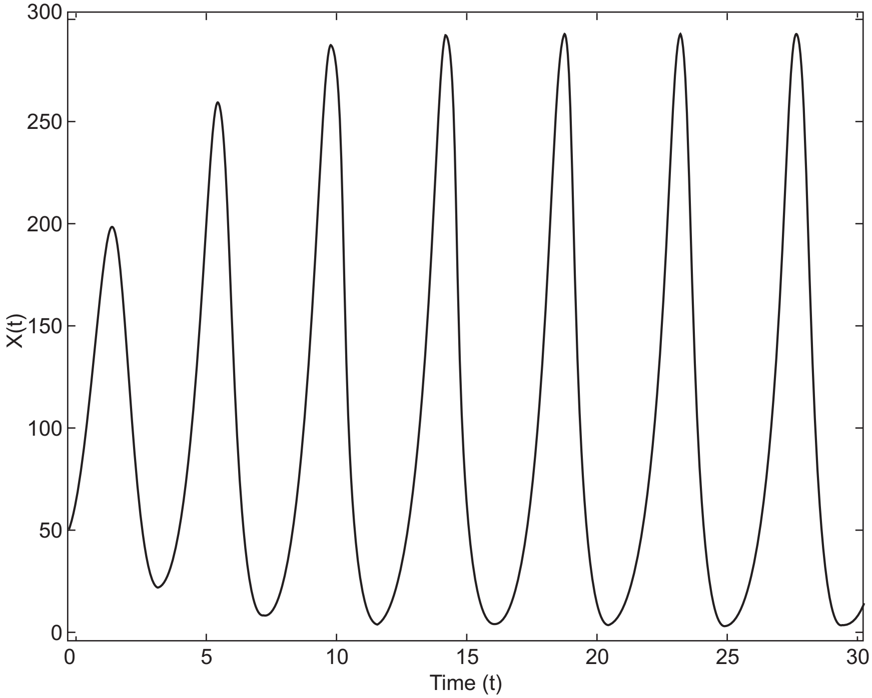


Fig. 10.3 Solution of the delayed logistic equation with initial population X(0)=50, and with parameter values r=2.0, K=100

```
%--------------Logistic_eq.m-----------%
clc
clear all

global r K tau;
r=2.5;      K=150;
```

```
tau=1.0;    % delay amount
t_end=30;    % end tine
X0=60;      % Initial value
sol=dde23(@rhs,tau,X0, [0 t_end]);
plot(sol.x,sol.y);
xlabel('Time(t)', 'FontSize',10);
ylabel('X(t)', 'FontSize',10);
%--------------rhs.m----------------%
function Xdot=rhs(t,X,Xlag)
global r K;
    Xdot=r*X*(1-Xlag/K);
end
```

Problem 10.12

Solution of BVP ODE (Using NonLinear Algebraic Equ Solver)
By shooting method solve the following BVLP ODEs

$$y'' = -(y')^2/y; \quad y(0)=1;\ y(1)=2$$

NBVP.m:

```
function f = nbvp(x)
ya = 1;   yb = 2;  a = 0;   b = 1;
tspan = [a, b];
x0 = [ya, x, 0, 1]';
[t,z] = ode23('fnlode', tspan, x0);
[n,nn] = size(z);
f = z(n,1) - yb;
```

FNLODE.m:

```
function dz = fnlode(t,z)
dz = [z(2),
      -(z(2)^2)/z(1),
      z(4),
      z(3)*(z(2)/z(1))^2-2*z(4)*z(2)/z(1)]';
```

INFL.m (main program):

```
x0 = 0;
x = fsolve('nbvp', x0);
ya = 1;   yb = 2;  a = 0;   b = 1;
tspan = [a, b];
```

```
x0 = [ya, x, 0, 1]';
[t,z] = ode23('fnlode', tspan, x0);
plot(t, z(:,1));
```

Command prompt :

```
>>INFL.m
```

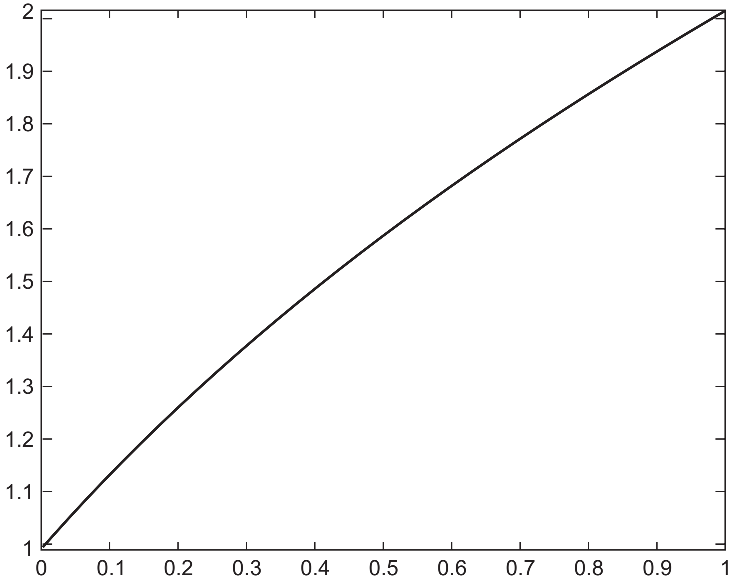


Fig. 10.4 Output for problem 10.12 via algebraic equation solver (z versus time)

Problem 10.13

Solution of BVP ODE (using ODE Solver)

F_NS_NEWT.m:

```
function dz = f_ns_newt(x,z)
dz = [z(2),
      -(z(2)^2)/z(1),
      z(4),
      z(3)*(z(2)/z(1))^2-2*z(4)*z(2)/z(1)]';
```

NL_SHOOTING.m (main program):

```
ya = 1;   yb = 2;  a = 0;   b = 1;
max_it = 5;  tol = 0.00001;
 t(1) = 0;   test = 1;
i = 1;    tspan = [a,b];
```

```
while(test>tol)&(i<=max_it)
    z0 = [ya, t(i), 0, 1];
    [x,z] = ode23('f_ns_newt', tspan, z0);
    [n,nn] = size(z);
    m(i) = z(n,1) - yb;
    test = abs(m(i));
    t(i+1) = t(i) - m(i)/z(n,3);
    i = i+1;
end
plot(x, z(:,1));
```

Command prompt :

```
>>NL_SHOOTING.m
```

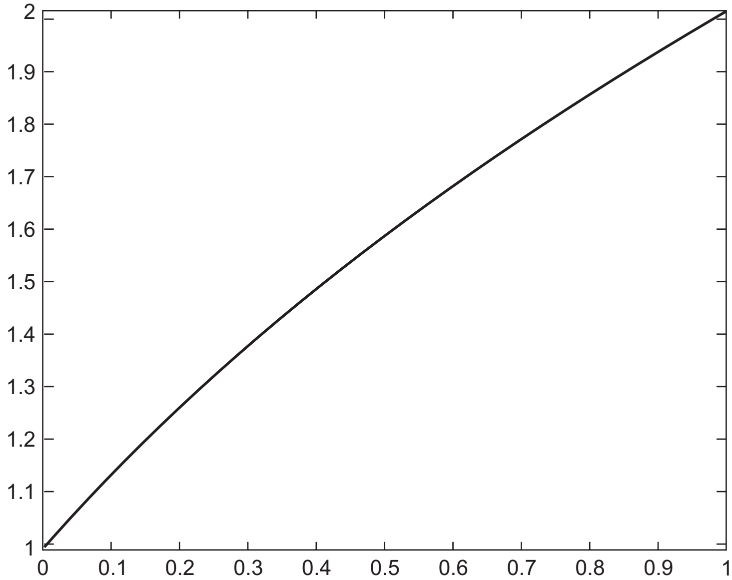


Fig. 10.5 Output for problem 10.13 via ODE solver (z versus time)

10.4 PARAMETER ESTIMATION

Problem 10.14

Estimation of parameters

Estimate the model parameters k, n and m from

$$R = k\, p_a^{\,n}\, p_b^{\,m}$$

Using the following data of R for various values of p_a p_b.

```
  pa=[0.1044 0.1049 0.1030 0.2582 0.2608 0.2407 0.3501 0.3437 0.3494
0.4778 0.4880 0.5014];
  pb=[0.1036 0.2871 0.5051 0.1507 0.3100 0.4669 0.0922 0.1944 0.5389
0.1017 0.2580 0.5037];
  rate1 =[0.5051 0.6302 0.6342 1.3155 1.5663 1.5981 1.6217 1.8976
2.1780 2.1313 2.7227 3.1632];
  function value=para(parameters)
  k=parameters(1);
  n=parameters(2);
  m=parameters(3);
  pa=[0.1044 0.1049 0.1030 0.2582 0.2608 0.2407 0.3501 0.3437 0.3494
0.4778 0.4880 0.5014];
  pb=[0.1036 0.2871 0.5051 0.1507 0.3100 0.4669 0.0922 0.1944 0.5389
0.1017 0.2580 0.5037];
  rate1 =[0.5051 0.6302 0.6342 1.3155 1.5663 1.5981 1.6217 1.8976
2.1780 2.1313 2.7227 3.1632];
  value=0;
  for i=1:12
      rate2(i)=k*(pa(i)^n)*(pb(i)^m);
      value=value+(rate1(i)-rate2(i))^2;
  end
  value=value/12;
  end


  Main File
  feval(@para,[2 3 4])
  fminsearch(@para,[1 1 1])
  ans =
      3.3819
  ans =
      6.9776    0.9561    0.1957
  ------------------------------------------------------
```

Problem 10.15

Estimate the model parameters C and μ_m in $\mathbf{\mu = \mu_m S/(C+S)}$
From the given data set:

s = [19; 8.286 ;4.17; 3.68;2.11;1;2.8];

μ = [.38; .29; .205; .19; .13;.0714;.159];

Initial values

```
Mu=0.38 .29 .205 .19 .13
S=19 8.286 4.17 3.68 2.11
Relation :
Mu= (Mum *S)/C+S
By newton-gauss
clear all
clc
s=[19; 8.286 ;4.17; 3.68;2.11;1;2.8];
mu=[.38; .29; .205; .19; .13;.0714;.159];
y=mu;
n=length(s);
para=[10 ;20];
%gauss increment and weight factor
delta=[1 ;1];
lamda=1;
while(abs(delta)>[.0001 ;.0001])
    for i=1:n
        b1=(para(2)*s(i,1));
        b2=s(i,1)+para(1);

        %fuction to be evaluated fun

        fun(i,1)=b1/b2;

        %differentials of the functions
        %w.r.t I
        dfun(i,1)=-(b1/b2.^2);
        %w.r.t ks
         dfun(i,2)=b1/(b2*para(2));
         end
       error=y-fun;
       [Q,R]=qr(dfun);
       w=Q'*error;
```

```
    delta=inv(R'*R)*R'*w;
    para=para+lamda*delta;
end
mum=para(1)
kl=para(2)
```

Command Window

```
Mum =
  6.0059
K1 =
   0.5001
------------------------------------------------------
```

Problem 10.16

Use of fminsearch routine
By fminsearch

```
function f=parang(parameter)
c=parameter(1);
u=parameter(2);
s=[19; 8.286 ;4.17; 3.68;2.11;1;2.8];
n=length(s)
for i=1:n
fun(i,1)=u*s(i,1)/(s(i,1)+c)
end
mu=[.38; .29; .205; .19; .13;.0714;.159]
f=0;
for j=1:n
    f=f+(fun(j,1)-mu(j,1))^2;
end
end
```

Command Window

```
>> fminsearch (@parang, [1  1])
ans =
    6.0059   0.5001
------------------------------------------------------
```

Problem 10.17

Estimatie rate constants in a series reactions A→B→C, each of first order kinetics. Given the data on concentration of A, B and C at selected times.

```
  function rate = basicdeter(parameter)
  global k1 k2
  k1 = parameter(1);
  k2 = parameter(2);
  global x1 x2 x3
  x1=1;
  x2=0;
  x3=0;
  % experimental values at t= 0.000 0.263 0.526 0.789 1.053 1.316
  experimental = [1.0000000  0.0000000 0.0000000;
                  0.59096447 0.3555550 0.05348051;
                  0.34923934 0.4834497 0.16731099;
                  0.20638798 0.4958219 0.29779013;
                  0.12172441 0.4543303 0.42394528;
                  0.07193491 0.3925423 0.53552284];
  calculated = zeros(6,3);
  % calculated values
  [T, calculated]= ode45(@bsicodesol,[0.000 0.263 0.526 0.789 1.053
1.316],[x1 x2 x3]);
  %m= number of components to be minimised
  %n = number of parameters
  rate = 0;
  m=3;
  n=6;
  %error calculation
  for i=1:m
      for j=1:n
          rate= rate+(experimental(j,i)-calculated(j,i))^2;
      end
  end
  end
  function dx=bsicodesol(t,x)
```

```
  global k1 k2
  dx = zeros(3,1);
  dx(1) = -k1*x(1);
  dx(2) =  (k1*x(1))-(k2*x(2));
  dx(3) =  k2*x(2);
  end
  >>[parameters,objectivefunc,exit,out]=fminsearch(@basicdeter,
[0 0])
  parameters =
      2.0000    1.0000
  objectivefunc =
     1.3590e-10
  exit =
       1
  out =
      iterations: 69
       funcCount: 136
       algorithm: 'Nelder-Mead simplex direct search'
         message: 'Optimization terminated:
   the current x satisfies the termination criteria ...'
```

[**Note:** For the above linear ODEs, analytical solution for C_A, C_B and C_C can be derived. The numerical solution of ODEs may not be required. However, for situations where the nonlinear ODEs are to be considered, the above matlab program with suitable modifications can be used].

10.5 CONSTRAINED OPTIMIZATION PROBLEM

```
 [x,fval] = fmincon (@objfn,x0,A,b,Aeq,beq,lb,ub,@confun,options);
```

Nonlinear constraints equations are to be defined in confun routine (first inequality and then equality constraints).

The linear constraints (equality A_{eq} $x=b_{eq}$ and inequality $Ax < b$ are to be defined in the main program.

The lower bound and the upper bound for the vector x are to be defined in the main program.

Problem 10.18

Find the vector x to minimize $f(x) = \exp(x_1)[4x_1^2 + 2x_2^2 + 4x_1x_2 + 2x_2 + 1)$
Subjected to

$$x_1x_2 - x_1 - x_2 + 1.5 \leq 0$$

$-x_1x_2 -10 \le 0$

$-x_4 + 0.1\ x_5 \le 0$

$x_4 - 0.5x_5 \le 0$

$x_3 + 0.9\ x_4 \le 0$

$x_1 - 0.3\ x_2 = 0$

Step 1: Write M file confun.m for the nonlinear constraints

```
% Nonlinear inequality constraints
function [c, ceq] = confun(x)
c = [1.6 + x(1)*x(2) – x(1) – x(2); -x(1)*x(2) – 9];
% nonlinear equality constraints
ceq = [];
```

Step 2: Write the objective function objfun file

```
function = objfun(x)
f = exp(x(1))*(4*x(1)^2 + 2*x(2)^2 + 4*x(1)*x(2) + 2x(1) + 1);
```

Step 3: Call constrained optimization routine.

```
x0 = [1; 4; 5;  2; 5];   % initial guess for the solution
lb = [-inf; -inf; 0; -inf; 1];
ub = [ Inf; Inf; 20];
Aeq = [1 -0.3  0 0 0];
Beq = 0;
A = [0 0 0 -1 0.1
         0 0  1 -0.5
         0 -1 0 0.9];
b = [0; 0; 0];
opts = optimset('algorithm', 'sqp')
[x,fval] = fmincon (@objfn,x0,A,b,Aeq,beq,lb,ub,@confun,options)
------------------------------------------------------
```

10.6 PDE SOLVER IN MATLAB

Problem 10.19

Prepare MATLAB code to solve the following PDE

$$\frac{1}{x}\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}(\sqrt{u+1}\,\frac{\partial u}{\partial x}) + xt$$

Initial Conditions $u(x, 0) = 1$

Boundary conditions:

$$u(0,t) + 2\frac{\partial u}{\partial x} = 0; \quad u(1,t) + 2\frac{\partial u}{\partial x} = 0$$

PDE solver

`Syntax:` sol = pdepe(m,pdefun,icfun,bcfun,xmesh,tspan)

Basic function:

$$c\left(x, t, u, \frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^m f\left(x, t, u, \frac{\partial u}{\partial x}\right)\right) + s\left(x, t, u, \frac{\partial u}{\partial x}\right).$$

Initial condition

$$u(x, t_0) = u_0(x).$$

Boundary condition

$$p(x, t, u) + q(x, t) f\left(x, t, u, \frac{\partial u}{\partial x}\right) = 0.$$

Matlab program for problem 10.19:

```
clear all
clc
m=0;
x = linspace(0,1,20);
t = linspace(0,2,5);
sol = pdepe(m,@eqtn,@ic,@bc,x,t);
u = sol(:,:,1);
figure;
surf(x,t,u);
xlabel('Distance x');
ylabel('Time t');
%----------------------------%----------------------------%
function [c,f,s] = eqtn(x,t,u,DuDx)
c = 1/x;
f = (sqrt(u+1))*DuDx;
s = x*t;
end
%----------------------------%----------------------------%
function u0 = ic(x)
u0 = 1;
end
```

```
%--------------------------%--------------------------%
function [pl,ql,pr,qr] = bc(xl,ul,xr,ur,t)
pl = ul;
ql = 2;
pr = ur;
qr = 2;
end
```

10.7 SCILAB

Scilab (http://www.scilab.org) is a free open-source software package for scientific computation. It includes hundreds of general purpose and specialized functions for numerical computation, organized in libraries called toolboxes that cover areas such as simulation, optimization, systems and control, and signal processing. These functions reduce considerably the burden of programming for scientific applications. There exist two categories of general scientific software: computer algebra systems that perform symbolic computations, and general purpose numerical systems performing numerical computations and designed specifically for scientific applications. The best examples in the first category are Maple, Mathematica, Maxima, Axiom, and MuPad. Scilab and Matlab belong to this second category, Scilab being open source software.

10.7.1 Development of Scilab

Scilab was originally named Basile and was developed at INRIA as part of the Meta2 project. Development continued under the name of Scilab by the Scilab group, which was a team of researchers from INRIA Metalau and ENPC. Since 2004, Scilab development has been coordinated by a consortium. The Scilab can be used as a scripting language to test algorithms or to perform numerical computations. Now it has taken over the market of programming language, and the standard Scilab library contains around 2000 Scilab coded functions. The Scilab syntax is simple, and the use of matrices, which are the fundamental object of scientific calculus, is facilitated through specific functions and operators. These matrices can be of different types including real, complex, string, polynomial, and rational. Scilab programs are thus quite compact and most of the time, are smaller than their equivalents in C, C++, or Java.

Scilab is mainly dedicated to scientific computing, and it provides easy access to large numerical libraries from such areas as linear algebra, numerical integration, and optimization. It is also simple to extend the Scilab environment. Now Scilab/Scicos is gaining ground in industrial environments and is widely used at universities and engineering schools. This is due in part to the creation of an international consortium in 2003 that a number of large and small companies have joined. The consortium is responsible for providing well-tested and documented releases for various platforms and coordinates the development of the core product and toolboxes, which is done by research groups, in particular, at INRIA1 and ENPC.2 Currently there are over 10,000 monthly Scilab downloads from www.scilab.org alone. Scilab includes a full user's manual, which is available with search capabilities in a help window. All commands, their syntax, and simple illustrative examples are given but it does not address how to use several of these commands together in the solution of a technical problem.

10.7.2 Functions of Scilab

One can easily import new functionalities from external libraries into Scilab by using static or dynamic links. It is as well possible to define new data types using Scilab structures and to overload standard operators for new data types. Numerous toolboxes that add specialized functions to Scilab are available on the official site. Scilab provides many visualization functionalities including 2D, 3D, contour and parametric plots, and animation Graphics can be exported in various formats such as Gif, Postscript, Postscript-Latex, and xg. Scilab is a large software package containing approximately 13,000 files, more than 400,000 lines of source code (in C and Fortran), 70,000 lines of Scilab code (specialized libraries), 80,000 lines of online help, and 18,000 lines of configuration files. These files include

- Elementary functions of scientific calculation;
- Linear algebra, sparse matrices;
- Polynomials and rational functions;
- Classic and robust control, LMI optimization;
- Nonlinear methods (optimization, ODE and DAE solvers, Scicos, which is a hybrid dynamic systems modeller and simulator);
- Signal processing;
- Random sampling and statistics;
- Graphs (algorithms, visualization);
- Graphics, animation
- Parallelism using PVM
- MATLAB-to-Scilab translator
- A large number of contributions for various areas.

10.7.3 ODE package in Scilab

The primary simulation tool for ordinary differential equations is ode. In order to simulate a differential equation, the least that can be given to the integrator is the initial time t0, the initial value y0, and a formula for evaluating f(t,y). When we do this, the software picks the method and the error tolerances and adjusts the step size to try to meet the error tolerances which can be altered by the options tool. The standard calling sequence is

$$y = ode(t0,\ y0,\ tspan,\ function);$$

where $t0$ is the initial time

$y0$ is the value of the integral at time $t0$

tspan is a set of points provided for integration

function is the differential function of the form

$dy/dt = f(y,\ t)$

Examples are given in appendix A.

10.8 OPTIMIZATION PROGRAMS IN SCILAB

10.8.1 Optim

The general optimization utility in Scilab is optim. This algorithm allows the user to have some control of the optimization process. It can accept bound constraints. optim needs to know the gradient. If the gradient is unknown, or too complicated to code, then a utility is provided to enable optim to proceed using only the function to be minimized. This utility is ND cost, which stands for numerical differentiation of the cost. It approximates the gradient using finite differences.

10.8.2 Fsolve

Another optimization tool is fsolve, which finds zero of a system of n nonlinear functions in n variables. Fsolve implements a modification of the powell hybrid method to solve the problem. Jacobian may be provided. For some starting points and some equations system, the fsolve method can fail. The fsolve method is a local search method. So, to have a good chance to find a solution to your equations system, you must give, a good starting point to fsolve.

Problem 10.20

Ode solver in scilab:
Given the prey (x_1)-predator (x_2) system:

$$dx_1/dt = 0.25\ x_1 - 0.01\ x_1x_2$$

$$dx_2/dt = -x_2 + 0.01\ x_1x_2$$

with the initial conditions: x_1 (t=0) =80 & x_2(t=0)=30

`plot` x_2`(t) versus` x_1`(t) from t=0.0 to 20.`

`Use scilab routine ode.`

```
--------------------------------------------------------
get (“Predat.sci”)
x0= [80 ,30]’; t0=0; T=0:0.1:20; T=T’
results = ode(x0,t0,T,predat)
clf();
plot2d(T,results’)
xset(‘window’, 1)
plot2d(result(2,: ),result(1,:) )


function  xder = predate(t,x)
xder(1) = 0.25*x(1) - 0.01*x(1)*x(2);
xder(2) = -x(2)+0.01*x(1)*x(2);
--------------------------------------------------------
```

Problem 10.21

Problem solving using scilab routines

```
dy/dx= -y + sin(t)
given at x=0; y=0
plot y versus x form x=0 to x=20.

function ydot = f(t,y)
  ydot = -y + sin(t);
endfunction


x0=0.0
t0=0.0
tt=0:0.01:20;
y = ode (x0,t0,tt,f);
plot (tt,y)
```

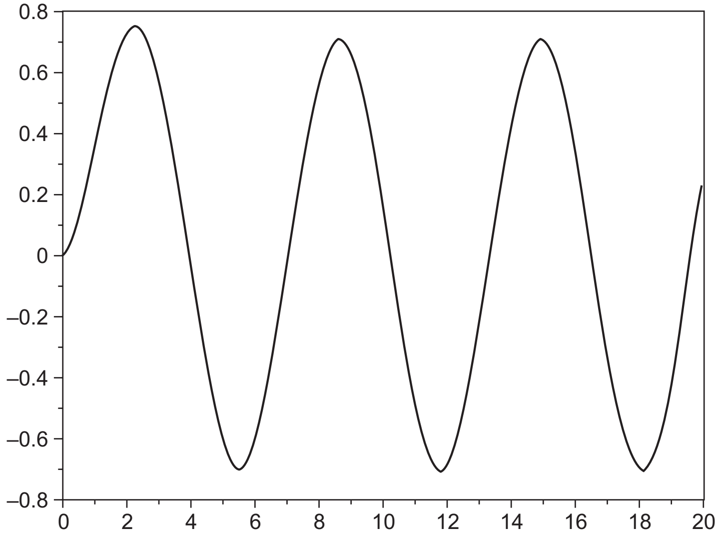
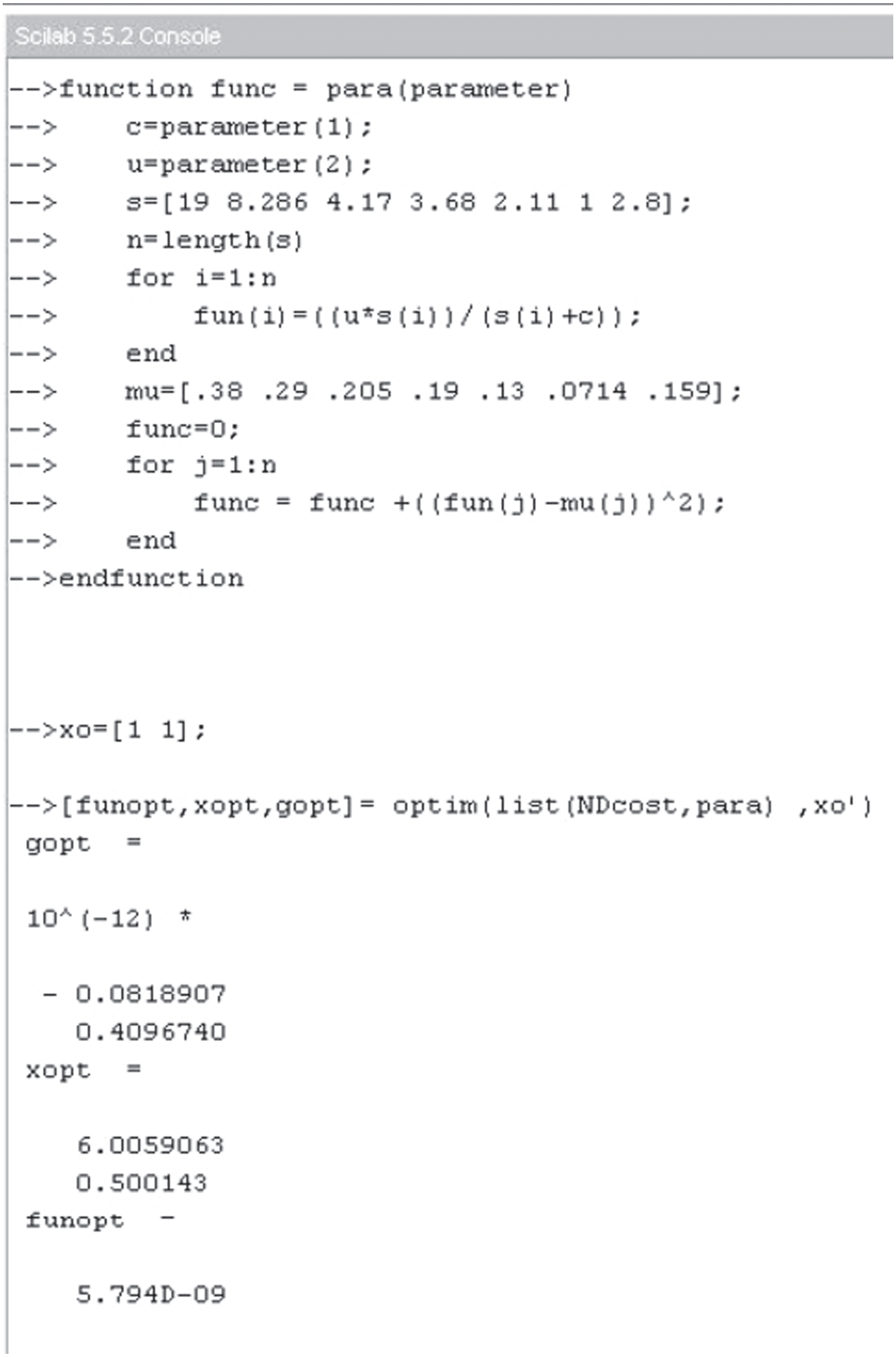


Fig. 10.6 Output for problem 10.21 using Scilab

Problem 10.22

$$\mu = \mu_m S/(C+S)$$

Given the experimental data of S versus μ obtain the values for C and μ_m



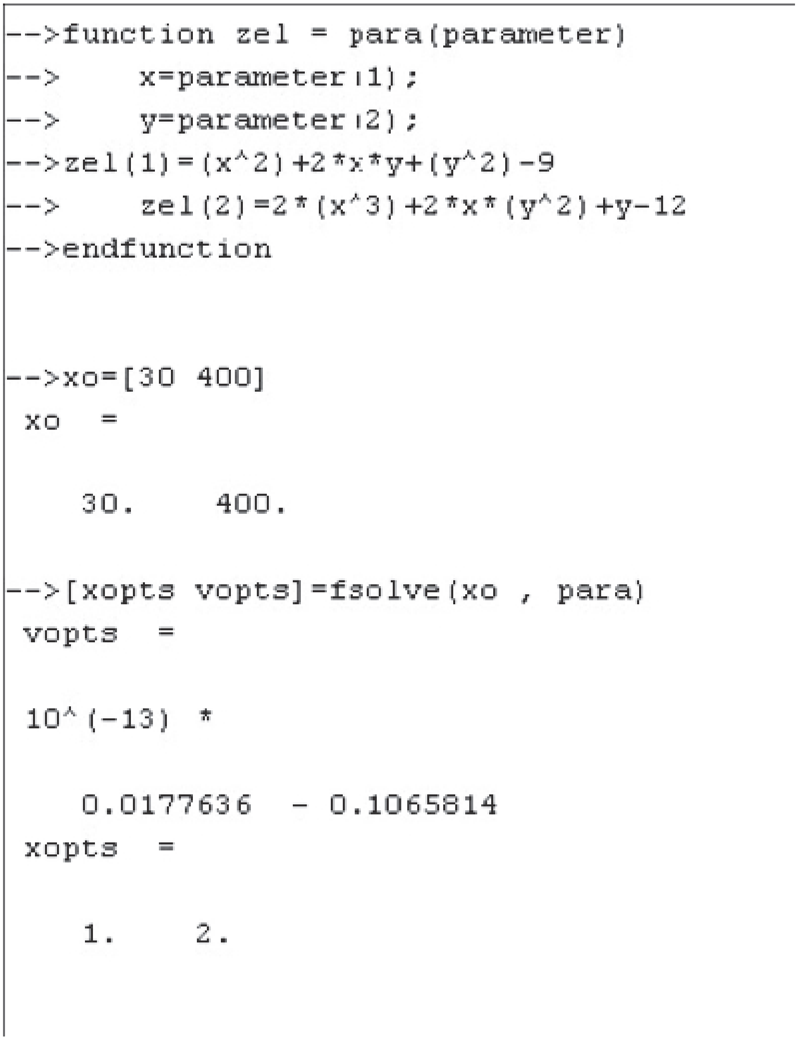
```
-->function func = para(parameter)
-->    c=parameter(1);
-->    u=parameter(2);
-->    s=[19 8.286 4.17 3.68 2.11 1 2.8];
-->    n=length(s)
-->    for i=1:n
-->        fun(i)=((u*s(i))/(s(i)+c));
-->    end
-->    mu=[.38 .29 .205 .19 .13 .0714 .159];
-->    func=0;
-->    for j=1:n
-->        func = func +((fun(j)-mu(j))^2);
-->    end
-->endfunction




-->xo=[1 1];

-->[funopt,xopt,gopt]= optim(list(NDcost,para) ,xo')
 gopt  =

 10^(-12)  *

  - 0.0818907
    0.4096740
 xopt  =

    6.0059063
    0.500143
 funopt  -

    5.794D-09
```

Problem 10.23

Problem solving by fsolve

$$x^2 + 2\,x\,y + y = 9$$

$$2xy^2 + 2x^3 + y = 2$$



```
-->function zel = para(parameter)
-->     x=parameter(1);
-->     y=parameter(2);
-->zel(1)=(x^2)+2*x*y+(y^2)-9
-->     zel(2)=2*(x^3)+2*x*(y^2)+y-12
-->endfunction



-->xo=[30 400]
 xo  =


    30.    400.

-->[xopts vopts]=fsolve(xo , para)
 vopts  =

 10^(-13)  *

    0.0177636  - 0.1065814
 xopts  =

    1.    2.
```

Review Problems

1. Write a matlab program to find the roots of the nonlinear algebraic equation: exp(x)-x^2-2x=0 for two different initial guess values.
2. Write a matlab program to solve the following simultaneous nonlinear algebraic equations: x^2y^2-2x-5$y^{0.5}$+6=0; x^4-6y^2x+5=0

3. Convert the nonlinear algebraic equation in Q(1) into an initial value ODE by method of Parameter Differentiation (MPD) and solve the resulting ODE by a suitable matlab routine.
4. Convert the nonlinear algebraic equations in Q(2) into a set of initial value ODEs by method of Parameter Differentiation (MPD) and solve the resulting ODEs by a suitable matlab routine.
5. Write a matlab program to solve the following initial value ODEs: $x'=x^2y+y+t$; $y'=2x-y^2-t$; with the initial conditions at t=0, x=0 & y=1.results are required from t=0 to t=5.0 at every t=0.5 (tprint).
6. Convert the following equations into a set of first order ODEs:

   $y'''+ty''+ty'-2y = t$; given the initial conditions $y(0) = 0$, $y'(0) = 1$, $y''(0) = 0$.
7. By using the shooting method, convert the BVP ODE into a set of IVP ODEs: $y''+3y^2 y'+ y\exp(-2x)=x^2$

   $-y'(x=0)+y(x=0)=1$; $y'(x=1)=2$ and write a matlab program to solve the resulting IVP ODEs (i) by using only ODE23 routine and (ii) using both ODE23 and fsolve routines.
8. Convert the BVP ODEs in Q(7) by a set of nonlinear algebraic equations by using the finite difference scheme. Use the number of internal grids as N = 5 Write a matlab program using the fsolve routine to solve the resulting nonlinear algebra equations.
9. Using the matlab routine pdepe, solve the equation:

   $\partial c/\partial t = (1/P)\partial^2 c/\partial x^2 - \exp(-x)\, \partial c/\partial x - [(k_1 c)/(1+k_2 c)]$

   BCs: at x=0: $\partial c/\partial x = P(c(x=0) -1)$; at x=1: $\partial c/\partial x = 0$; **ICs**: $c(0,x)=0$.

   $P=3$; $k_1=1$; $k_2 = 0.5$
10. Using the finite difference scheme method, convert the following PDE into a system of IVP ODES. Use the number of internal grids N=5.

    $$\partial^2 c/\partial y^2 + 1 = \partial^2 c/\partial x^2;$$

    at (y,0): $\partial c/\partial x = 0$; $c(1,x)=0$; $c(0,x)=0$; $c(y,0)=y^2$.

    Solve the resulting IVP ODEs by ODE45 routines

11

Model Based Control

In this chapter, a review is given on the basic principles of designing Proportional (P), Proportional and Integral (PI), and Proportional-Integral-derivative (PID) controllers. The methods are reviewed to obtain the linear model for the design of controllers. An introduction is given in designing PI controllers for unstable systems.

11.1 NEED FOR CONTROL SYSTEMS

In the design course, the method of designing, say, a distillation column is studied. Once the column is designed in order to maintain the specified concentration of the top product, we need to design control system to take care of any disturbance entering the system (for example, in the feed composition). The top composition is to be regulated by manipulating the reflux flow. This can be done automatically by a feedback control system. In case of systems which are open loop unstable (for example, a bioreactor or a CSTR), the system can be operated only under closed loop control (i.e., by feedback control system).

11.2 FEEDBACK CONTROL SYSTEMS

A typical block diagram of a feedback control system is shown in Fig. 11.1. The output of the process (y) is measured and its value is compared with the set point (y_r) to generate the error signal (e). Here d is the disturbance variable. The controller acts upon the error signal to generate a corrective action (x). The controller output and error signal can be related by the following way(s):

(i) the controller output is proportional to the error,

$$x = k_c e \tag{11.1}$$

where k_c is proportionality constant. The control action depends on the present error.

(ii) The controller output is proportional to the integral of the error, i.e.,

$$u = k_I(\int e\, dt) \tag{11.2}$$

the integration is from time 0 to t. The action is in some sense related to past errors.

(iii) The controller output is proportional to the derivative of the error. i.e.,

$$x = k_D\left(\frac{de}{dt}\right) \tag{11.3}$$

The action is in some sense related to future error.

In general, the controller output can be related to the linear combination of all the three actions:

$$x = k_c\left[e + \left(\frac{1}{\tau_I}\right)\int edt + \tau_D\frac{de}{dt}\right] \tag{11.4}$$

This action is called Proportional-integral-Derivative (PID) control action. K_c, τ_I and τ_D are called proportional gain, integral time and derivative time respectively. The integral action eliminates the steady state error and the derivative action imparts stability. The derivative action is sensitive to the noise in the measurement and hence the filtered signal is used for taking the derivative.

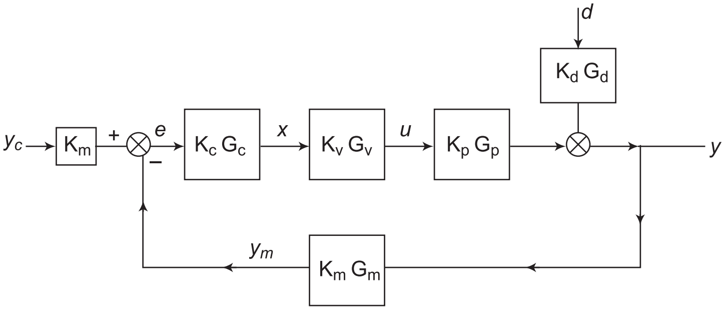


Fig. 11.1 Block diagram of a feedback control system

The design of a controller consists of the following two steps:

(a) Selection of the mode of the controller: say proportional or integral or derivative controller or their combination PI, PD and PID.

(b) Specification of the value of the parameters associated with the selected controller mode (k_c, τ_I and τ_D values).

The above two steps are to be carried out in order to meet the specification of the closed loop system in the time domain as:

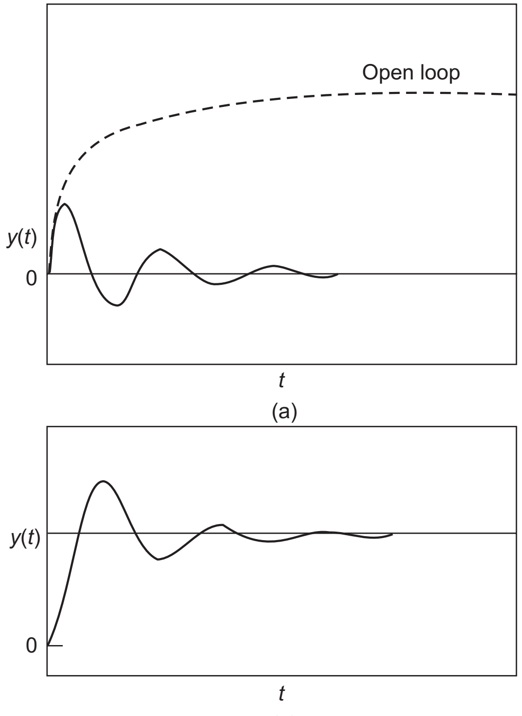
overshoot, decay ratio, settling time, rise time, etc.

(or)

in the frequency domain as gain margin, phase margin and bandwidth.

If the selected controller mode and the settings values do not give the desired closed loop system response with the given specifications, then the value of the controller settings is to be changed and/or the controller mode is changed. The performance of the closed loop system is usually evaluated for (i) regulatory problem-controlling the output at the desired level in the face of disturbances entering the process and (ii) servo problem-the ability of the output tracking the given set point change.

A typical time response of a closed loop system is shown in Fig. 11.2. The controller designed based on the nominal operating point should be able to give satisfactory responses even when there is a change in the process condition. The desired performance of the control system should be achieved within the given constraints on the manipulated variable.



(a)

(b)

Fig. 11.2 Typical response of a closed loop system [(a) for a load change (regulatory problem), (b) for a set point change (servo problem)

11.3 TRANSFER FUNCTION MODELS

To design a controller, we need to know the knowledge of the system in terms of the transfer function model. Transfer function is defined as the change in the output to that of the change in the input in the Laplace domain, i.e.,

$$k_P G_P = \frac{\Delta y(s)}{\Delta u(s)} \tag{11.5}$$

where k_P is the steady state gain and the input variable and output variable are in Laplace domain. The relation between the small change in the output variable to that of the small change in the input variable is given (for a first order system) in time domain as a linear differential equation with a constant coefficient:

$$\tau\left(\frac{dy}{dt}\right) + y = k_P\ u(t) \tag{11.6}$$

Similarly, for a second order model, we have

$$\tau^2 \frac{d^2 y}{dt^2} + (2\tau\xi)\frac{dy}{dt} + y = k_P\, u(t) \tag{11.7}$$

However, for systems with higher order dynamics we approximate the model by a first order plus time delay system:

$$\tau \frac{dy}{dt} + y = k_P\, u(t - L) \tag{11.8}$$

In Laplace domain this equation becomes

$$\frac{\Delta y(s)}{\Delta u(s)} = k_P \frac{\exp(-Ls)}{(\tau s + 1)} \tag{11.9}$$

It is known as first order plus time delay (FOPTD) model.

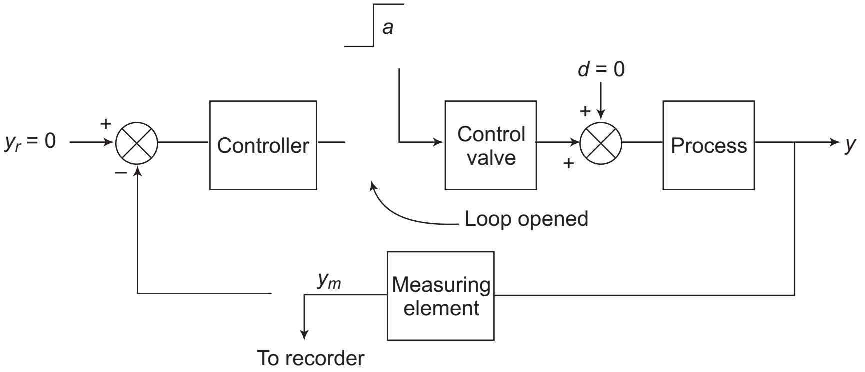


Fig. 11.3 Block diagram of an open loop system for obtaining the process reaction curve

The transfer function relates the Laplace transform of the deviation of the output to that of the deviation in input variable. The transfer function model can also be obtained by linearization of the mathematical model equations of the system around the nominal operating condition followed by taking the Laplace transformation of the resulting linear equations. Many of the processes can be adequately described by the first order plus delay transfer function model. The transfer function model can also be obtained by experimentally by the process reaction method. The method consists of giving a step change in the input (5% of the nominal value) and observing the change in the output variable (refer to Fig. 11.3 for the block diagram and Fig. 11.4 for the reaction curve). The ratio of the change in the final steady state value of the output to that of the input change gives the steady state gain (k_{pvm}) of the process. The time constant and the time delay are obtained from the following equations (Sundaresan and Krishnaswamy, 1977):

$$L = 1.3\, t_1 - 0.29\, t_2 \tag{11.10}$$

$$\tau = 0.67(t_2 - t_1) \tag{11.11}$$

where t_1 and t_2 are the time to reach respectively 35% and 85% of the final value in the output.

Example 11.1

The response of a system is obtained as (for a step change of input 0.5):

Time	0	0.5	1.0	1.5	2	2.5	3	4	5	6	7	9	11	13
y	0	0.028	0.144	0.34	0.56	0.80	1	1.36	1.58	1.71	1.84	1.94	1.98	2

Identify a suitable first order plus rime delay model.

From the given data, the steady-state gain is calculated as:

$$K_P = \frac{2}{0.5} = 4 \tag{11.12}$$

The fractional response (y/y_∞) is shown in Fig. 11.4. The times (t_1 and t_2) required to reach 0.35 and 0.85 fractional responses are noted as 2.35 and 5.7. Using the equations, Eqs. (11.10) and (11.11), we get

$$\tau_d = 1.3\, t_1 - 0.29\, t_2 = 1.40 \tag{11.13}$$

and

$$\tau = 0.67\,(t_2 - t_1) = 2.25 \tag{11.14}$$

Thus, the identified transfer function model is given by $4\exp(-1.4s)/(2.25s + 1)$. The step response (for a step change of 0.5) of the identified model is compared with the actual data in Fig. 11.4.

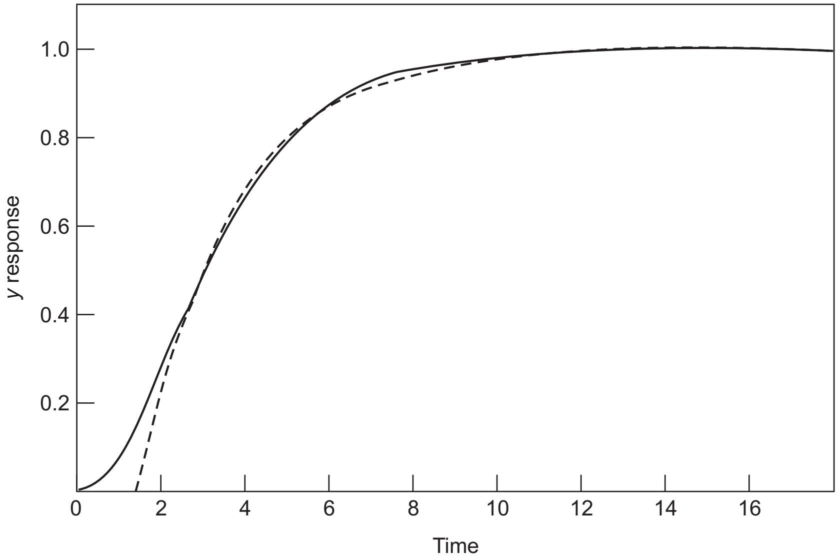


Fig. 11.4 Response comparison of the delay plus first order model with that of the actual system (–system response, --- first order plus time delay model)

11.4 STABILITY OF CLOSED LOOP SYSTEM

Given the transfer function model and the Δinput(s), we can get the value of Δoutput(s). For convenience, we use the notation $y(s)$ instead of $\Delta y(s)$. Similarly, we use the corresponding notations for all the other variables also.

From Fig. 11.1, we get:

$$y(s) = k_P G_P\, u(s) + k_d\, G_d\, d(s) \tag{11.15}$$

We have $$u(s) = k_c G_c\, x(s);\ x(s) = k_v\, G_v\, e(s);\ e(s) = k_m\, y_r(s) - k_m\, G_m\, y(s) \tag{11.16}$$

Hence, we get $$\frac{y(s)}{u(s)} = \frac{k_m k_c k_p k_v G_v G_P G_c}{[1 + \mathrm{KG}]} \tag{11.17}$$

where $$G = G_m G_v G_P G_c \tag{11.18}$$

$$K = k_m\, k_c k_P k_v \tag{11.19}$$

Similarly $$\frac{y(s)}{d(s)} = \frac{k_d G_d}{(1 + \mathrm{KG})} \tag{11.20}$$

KG is known as the open loop transfer function. Let us consider the servo problem. Let us give a unit step change in the set point y_r. That is

$$y_r(s) = \frac{1}{s} \tag{11.21}$$

Hence $$y(s) = \left(\frac{1}{s}\right)\frac{k_m k_c k_P k_v G_v G_P G_c}{[1 + \mathrm{KG}]} \tag{11.22}$$

Using the partial fraction method, we can invert this function to get the expression for $y(t)$ and then substituting $t = \infty$ in the resulting expression, we get the steady state value for $y(t)$ to check whether $y(t)$ reaches the desired value of 1 at the steady state condition. Instead of inverting the Laplace transform we can get $y(t \to \infty)$ by using the final value theorem:

$$y(t = \infty) = \mathrm{Limit}_{(s \to 0)}\, [s\, y(s)] \tag{11.23}$$

Thus multiplying the right side of Eq. (11.22) by s and apply the limit $s = 0$. Usually, $G_P\ (s = 0) = 1$ and so far the limits of G_v and G_m. Using the final value theorem we get:

$$y(t = \infty) = \frac{k_m k_c k_v k_P}{(1 + k_m k_c k_v k_P)} \tag{11.24}$$

In Eq. (11.24) if $k_m k_c k_v k_P$ is much greater than 1, then $y(t = \infty) = 1$. Since $k_m k_v k_P$ is given, we can select k_c such way that $k_m k_c k_v k_P >> 1$. In other words, the larger the value of k_c, the better the result of achieving $y = y_r$ at steady state condition. Let us see for given $k_P G_P,\ k_m G_m$, $k_V G_V$, is there any limit on k_c?

It is important to note that the final value theorem is valid only under the condition that all the roots of 1 + KG(s) = 0, lie in the left side of s-plane (for details, refer to any text book on Laplace Transform). That is, no real part of the roots of (1 + KG = 0) should be positive.

Let us consider a proportional controller, i.e., $k_c G_c = k_c$. As k_c is increased from a small value, the roots of 1 + KG = 0 are moving in the left side of s-plane. After a particular value of k_c, (known as $k_{c,\max}$) we find suddenly the roots start crossing the imaginary axis (of s-plane) and moving towards to right side of s-plane. This value of k_c gives at-least two roots lie in the imaginary axis, that is $s = \pm j\omega_c$.

Then the denominator of $1 + \mathrm{KG}(j\omega_c) = 0$ (11.25)

where ω_c is called the cross over frequency.

$$G(j\omega_c) = G_v(j\omega_c)G_P(j\omega_c)G_m(j\omega_c) \tag{11.26}$$

$$kG(j\omega_c) = -1 \tag{11.27}$$

[the above equation can be written as

$$\text{A}\exp(j\phi) = -1 \tag{11.28a}$$

$$= \exp(-\pi) \tag{11.28b}$$

Hence, $$A = 1 \text{ and } \phi = -\pi \tag{11.29}$$

Consider any simple system $1/(\tau s + 1)$. we can substitute $s = j\omega$ and rearrange the term as $(a + jb)$; where the amplitude is given by

$1/(a^2 + b^2)^{0.5}$ and phase angle is given by $\tan^{-1}(-b/a)$. $a = 1$; $b = \tau\omega$ Similarly for the system with the transfer function as $1/s$, we get the amplitude as $1/\omega$ and phase angle $= -\pi/2$. Similarly for system, $\exp(-Ls)$ we get amplitude = 1 and the phase angle is given by $\phi = -\tau_D w$. If we have a system $\exp(-Ls)/s(\tau s + 1)$, the amplitude is calculated as A_1, A_2 and A_3 as $1/\omega$; $1/(1 + \tau^2\omega^2)^{0.5}$, 1 and the phase angle is given respectively by $-\tan(\tau\omega)$, $-\pi/2$, $-L\omega$. The overall phase angle is given by the addition of all the individual phase angles (for denominator term) $= -\tan^{-1}(\tau\omega) - 0.5\pi - L\omega$.

The amplitude is given by the product of the individual amplitude terms: $1/[1 + \tau^2\omega^2]^{0.5}$, $1/\omega$, 1. Table 11.1 gives the expression for phase angle and amplitude ratio for few transfer function models. For Eq. (11.25), the complex number theorem says that

$$\text{Modulus of (KG)} = 1 \tag{11.30}$$

and $$\text{angle of } [\text{KG}(j\omega_c)] = -\pi \tag{11.31}$$

Table 11.1 *Magnitude and phase angle for simple transfer function models*

Transfer function	Magnitude	Phase angle
$\frac{1}{(\tau s + 1)}$	$\frac{1}{(1 + \tau^2\omega^2)^{0.5}}$	$-\tan^{-1}(\tau\omega)$
$(\tau s + 1)$	$(1 + \tau^2\omega^2)^{0.5}$	$\tan^{-1}(\tau\omega)$
$\frac{1}{s}$	$\frac{1}{\omega}$	-0.5π
s	ω	0.5π
$\exp(-\text{L}s)$	1	$-\text{L}\omega$
$\frac{1}{(\tau s - 1)}$	$\frac{1}{(1 + \tau^2\omega^2)^{0.5}}$	$-\pi + \tan^{-1}(\tau\omega)$
$(\tau s - 1)$	$(1 + \tau^2\omega^2)^{0.5}$	$\pi - \tan^{-1}(\tau\omega)$

That is, given $G(s)$, we have to substitute $s = j\omega_c$ and find that the phase angle and then equate it to $-\pi$ in order to get ω_c. Equation (11.30) gives the value for $K_{\max}$ and hence the value of $k_{c,\max.}$ The phase angle criterion can be solved either analytically (if possible) otherwise numerically by Newton–Raphson's method.

11.5 DESIGN OF CONTROLLERS FOR STABLE SYSTEMS

Usually, we assume first a proportional controller, i.e., $G_c = 1$. Then, we have to solve the amplitude criterion and the phase angle criterion to find the value of $k_{c,\max=}$ and $\omega_{c.}$ Using these values, we can design PI/PID controllers by Ziegler–Nichols tuning method as:

PI*:* $k_{c,\mathrm{des}} = 0.45\ k_{c,\max}\ ;\ \tau_I = P_u/1.2$ where $P_u = 2\pi/\omega_c$. (11.32)

PID : $k_{c,\mathrm{des}} = 0.6\ k_{c,\max}\ ;\ \tau_I = P_u/2;\ \tau_D = P_u/8$ where $P_u = 2\pi/\omega_c$. (11.33)

Calculate the value of $k_{c,\max}$ and ω_c for the system:

$$G(s) = \frac{1}{(\tau s + 1)^N} \tag{11.34}$$

The phase angle criterion is given by

$$-N \tan^{-1}(\tau\omega) = -\pi \tag{11.35}$$

We get

$$\tau\omega_c = \tan\left(\frac{\pi}{N}\right) \tag{11.36}$$

The amplitude criterion gives:

$$\frac{K_{\max}}{[\tau^2\omega_c^2 + 1]^{0.5N}} = 1 \tag{11.37}$$

$$K_{\max} = [\tau^2\omega_c^{\ 2}+1]^{0.5N} \tag{11.38}$$

$$= \left[1 + \tan^2\left(\frac{\pi}{N}\right)\right]^{0.5N} \tag{11.39}$$

$$= \left[\sec\left(\frac{\pi}{N}\right)\right]^N \tag{11.40}$$

The above equation is valid from $N \geq 3$. The values of $k_{\max}$ for different values of N are given as:

N	1	2	3	4	5	7	9	13	∞
$K_{\max}$	∞	∞	8	4	2.885	2.075	1.75	1.467	1

From the values of $k_{\max}$, and $\omega_c = (1/\tau)\tan(\pi/\mathrm{N})$, we can design PI or PID controllers by Ziegler–Nichols method (refer to Eqs. 11.32 and 11.33).

Many of the systems can be modelled as a First order plus time delay system (FOPTD) system:

$$K_P G_P = k_P \frac{\exp(-Ls)}{(\tau s + 1)} \tag{11.41}$$

Let us calculate the value of k_{max} and ω_c for the system. The phase angle is written as:

$$-\tan^{-1}(\tau\phi_c) - L\omega_c = -\pi \tag{11.42}$$

i.e.,

$$\tan(\pi - L\omega_c) = \tau\omega_c \tag{11.43}$$

Let

$$p = (\pi - L\omega_c) \tag{11.44}$$

Equation (11.43) can be written as:

$$\frac{(\pi - p)}{\tan(p)} = \frac{L}{\tau} \tag{11.45a}$$

The above equation cannot be solved analytically for p for a given the value for the ratio L/τ.

However, approximate solution can be derived as follows: when $L/\tau >> 1$, we can set tan(p) small and hence p is set smaller. Hence, Eq. (11.45a) can be written as:

$$\tan(p) = \pi\,(\tau/L) \tag{11.45b}$$

And hence

$$k_{max} = [1 + \tan^2 p]^{0.5} \tag{11.46a}$$

$$= \left[1 + \left(\frac{\pi\tau}{L}\right)^2\right]^{0.5} \tag{11.46b}$$

Using Eq. (11.46b) in Eq. (11.44), we get

$$\omega_c \approx \left(\frac{\pi}{L}\right) \tag{11.47}$$

Similarly for $L/\tau << 1$, we can set tan(p) is larger and hence

$$p = \frac{\pi}{2}$$

Hence Eq. (11.45a) can be written as:

$$\frac{(\pi - p)}{\tan(p)} = \frac{L}{\tau} \tag{11.48}$$

The above equation can be written as:

$$\frac{0.5\pi}{\tan(p)} = \frac{L}{\tau} \tag{11.49a}$$

(or)

$$\tan(p) = 0.5\pi\left(\frac{\tau}{L}\right) \tag{11.49b}$$

Hence

$$k_{max} = \left[1 + \left(\frac{0.5\,\pi\tau}{L}\right)^2\right]^{0.5} \tag{11.50}$$

This can be further approximated (since $L/\tau << 1$)

$$K_{max} = 1.57\,\frac{\tau}{L} \tag{11.51}$$

The value of ω_c can be approximated

$$\omega_c = \frac{0.5\pi}{L} \tag{11.52}$$

By Ziegler–Nichols method, $\tau_I = p_u/2$ and $\tau_D = p_u/8$ where $p_u = (2\pi/\omega_c)$.

With above approximated solution for $\omega_c = 0.5\pi/\text{L}$, we get

$$\tau_I = 2\text{L and } \tau = 0.5\text{L}. \tag{11.53}$$

Magnitude criterion is given by

$$k_{\max} = \sec(p) \tag{11.54}$$

Table 11.2 gives the expressions for $k_{c,\max}k_p$ and ω_c for some of the transfer function models.

Table 11.2 *Equation for k_{max} and ω_c for some of the transfer function models*

S. No	Process Model	$k_{c,mx}k_{pvm}$	ω_c
1	$\frac{1}{[(\tau_1 s+1)(\tau_2 s+1)(\tau_3 s+1)]}$	$(\tau_1+\tau_2+\tau_3)\left[\left(\frac{1}{\tau_1}\right)+\left(\frac{1}{\tau_2}\right)+\left(\frac{1}{\tau_3}\right)\right]-1$	$\left[\frac{(\tau_1+\tau_2+\tau_3)}{(\tau_1\tau_2\tau_3)}\right]^{0.5}$
2	$\frac{1}{(\tau s+1)^N}$	$\left[\sec\left(\frac{\pi}{N}\right)\right]^N$	$\left(\frac{1}{\tau}\right)\tan\left(\frac{\pi}{N}\right)$
3	$\left(\frac{1}{s}\right)\exp(-Ls)$	$\frac{0.5\pi}{L}$	$\frac{0.5\pi}{L}$
4	$\frac{\exp(-Ls)}{(\tau s+1)}$	$\left[1+\left(\frac{\pi\tau}{L}\right)^2\right]^{0.5}$ for $\frac{L}{\tau}<1$	$\frac{\pi}{L}$
		$\left[1+\left(\frac{0.5\,\pi\tau}{L}\right)^2\right]^{0.5}$ for $\frac{L}{\tau}>1$	$\frac{0.5\,\pi}{L}$
5	$\frac{1}{[s(\tau_e^2 s^2+2\tau_e\zeta s+1)}$	$\frac{2\zeta}{\tau_e}$	$\frac{1}{\tau_e}$
6	$\frac{1}{[s(\tau_1 s+1)(\tau_2 s+1)]}$	$\left(\frac{1}{\tau_1}\right)+\left(\frac{1}{\tau_2}\right)$	$\frac{1}{(\tau_1\tau_2)^{0.5}}$

$k_{pvm} = k_p k_v k_m$

11.6 DESIGN OF PI/PID CONTROLLERS FOR UNSTABLE SYSTEMS

Many real systems exhibit multiple steady states (i.e., for a given value of input variables there may be more than one value of the output variable) due to certain nonlinearity of the systems. Some of the steady states may be unstable. It may be necessary to operate the system at the unstable steady state for economical or safety reasons. Open loop instability means that the system will move away from the steady state for a small perturbation of the system (operating conditions/variables). Linearization of the mathematical model of such nonlinear systems around the unstable operating point will give a transfer function model which has at-least one pole in the right of s-plane (RHP). The response of such transfer function models for a small perturbation be ever increasing, but in case of nonlinear systems, the perturbation will cause the system to move to other but a stable steady state. The time delay is introduced in the transfer function description of such systems due to the measurement delay or by the approximation of higher order dynamics of the system in to the lower order transfer function plus time delay system. In this section, method of designing PI/PID controllers for unstable systems without time delay are first reviewed.

Let us consider a simple unstable first order system:

$$kpG_p = \frac{k_P}{(\tau s - 1)} \tag{11.55}$$

The characteristic equation (1 + KG = 0) of the closed loop system with a simple proportional controller is given by

$$1 + \frac{k_P k_c}{(\tau s - 1)} = 0 \tag{11.56}$$

gives
$$s = \frac{(1 - k_c k_P)}{\tau} \tag{11.57}$$

To make the closed loop system stable (i.e., to make the root of the closed loop system to lie in the left half s-plane) we must have $k_c k_{pvm} < 1$. Hence $k_{c,\min} = 1/k_{pvm}$. That is, k_c can be any value greater than $k_{c,\min}$, If $k_{c,\text{des}}$ value is lower than the minimum value, then the closed loop system cannot be stabilized.

Let us consider a second order system with one pole in the RHP (right half of s-plane)

$$K_p G_P = \frac{k_P}{[(\tau_1 s - 1)(\tau_1 s + 1)]} \tag{11.58}$$

The closed loop characteristic equation gives:

$$\tau_1 \tau_2 s^2 + (\tau_1 - \tau_2)\, s + (k_c k_p - 1) = 0 \tag{11.59}$$

The following conditions are to be satisfied for the system to be stable.

$$\tau_1 > \tau_2 \tag{11.60}$$

and
$$\mathrm{k_c} > \left(\frac{1}{k_p}\right) \tag{11.61}$$

For a system with $\tau_2 > \tau_1$, it can be checked that a derivative action may be required to stabilize the system.

Let us consider a third order system as follows:

$$\frac{K_p k_c}{[(\tau_1 s - 1)/(\tau_1 s + 1)/(\tau_3 s + 1)]} \tag{11.61}$$

With $\tau_1 = 10$, $\tau_2 = 1$ and $\tau_3 = 2$. The closed loop characteristic equation is given by:

$$20s^3 + 28s^2 + 7s + (k_c k_p - 1) = 0 \tag{11.62}$$

To stabilize the system, the following conditions are to be satisfied:

$$k_c k_p > 1 \tag{11.63}$$

and
$$k_{\max} k_p < 10.8 \tag{11.64}$$

That is,
$$k_{c,\min} = \frac{1}{k_p} \tag{11.65}$$

and
$$k_{c,\max} = \frac{10.8}{k_p} \tag{11.66}$$

That is, we have the conditional stability. The design value of the Proportional controller (which should be more than $k_{c,\min}$ and less than $k_{c,\max}$). The $k_{c,\text{des}}$ is given by the average value of these two min and max values of k_c.

$$K_{c,\text{des}} = (k_{c,\min} + k_{c,\text{mx}})/2 \tag{11.67}$$

The integral and derivative times can be obtained from $P_u/2$ and $P_u/8$ where P_u is to be calculated from $\omega_{c,\max}$ as $2\pi/\omega_{c,\max}$.

11.7 CONTROL OF UNSTABLE BIOREACTOR

The mass balance for biomass in a bioreactor can be rewritten as:

$$\frac{dX}{dt} = (\mu - D)\, X \tag{11.68}$$

Similarly for the substrate, we can write the mass balance as:

$$\frac{dS}{dt} = (S_f - S)D - \left(\frac{\mu X}{\gamma}\right) \tag{11.69}$$

where
$$\mu = \mu_{\max} \frac{S}{(K_m + S + K_1 S^2)} \tag{11.70}$$

D (= F/V) is called dilution rate. In Chemical reaction engineering, we call F/V as space time. The reactant concentration is termed in biochemical engineering as the substrate concentration. The stoichiometric coefficient in reaction engineering is called the yield factor, γ.

The model parameters are:

$$\gamma = 0.4\ \frac{g}{g};\ \mu_{\text{m}} = 0.53\ h^{-1};\ D = 0.3\ h^{-1};\ K_m = 0.12\ \frac{g}{l};\ K_1 = 0.4545\ \frac{l}{g};\ S_f = 4\ \frac{g}{l} \tag{11.71}$$

Here, X and S are the concentrations of the cell and substrate respectively. By making the terms dX/dt and dS/dt each zero, we get two nonlinear algebraic equations. Analytical solutions of the equations give three steady state solutions: ($X = 0$, $S = 4$), (0.9951, 1.5122) and (1.5301, 0.1746). It is desired to operate the system at unsteady state ($X = 0.9951$, $S = 1.5122$). On local linearization of the unsteady state nonlinear equations around the steady state (0.9951, 1.5122) gives the transfer function as:

$$\frac{X(s)}{D(s)} = -\frac{5.89}{(5.86s - 1)} \tag{11.72}$$

Consider a measurement delay of $L = 1$ hour. Hence, the transfer function model is given by

$$\frac{X(s)}{D(s)} = -\frac{5.89\exp(-s)}{(5.86s - 1)} \tag{11.73}$$

A PI controller can be designed (refer to the later section of the chapter) by synthesis method as $K_c = -0.7356$, $\tau_I = 5.452$. The closed loop response of the system with the control is evaluated on the nonlinear model equations. The response is shown in Fig. 11.5. Thus, the system is stabilized.

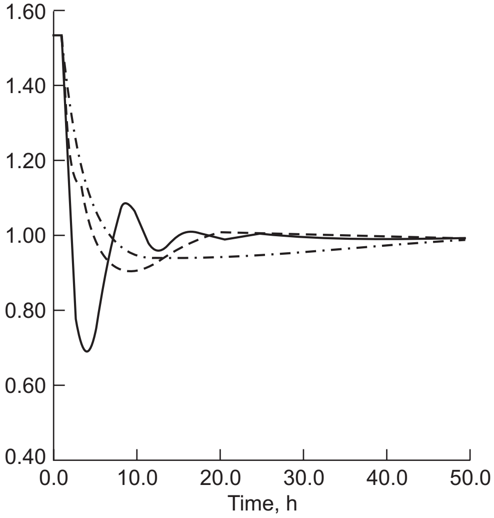


Fig. 11.5 Stabilization of the unstable steady-state at t = 0, X = 1.5301, S = 0.1746 [Solid: PI controller ($K_c = -0.7356$, $t_I = 5.452$) and dash: model reference present controller, $t_3 = 30$h, $\xi = 0.577$)]

11.8 CONTROLLER DESIGN BY SYNTHESIS METHOD

In the synthesis method for stable system, the closed loop transfer function model y/y_r is assumed to be a delay plus first order system with a unity gain. Using the process transfer function model, the controller transfer function can be derived. A simple feedback control system is shown in Fig. 11.6. The process transfer function and controller transfer function are given by G_p and G_c respectively. y is the output of the process, y_r is the set point and G_d is the load transfer function.

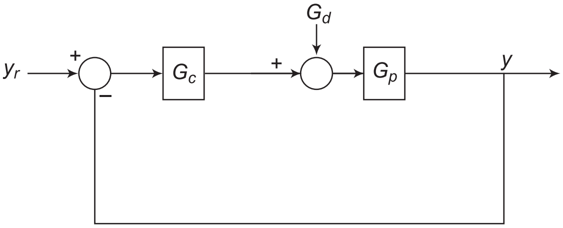


Fig. 11.6 Block diagram for simple feedback control system

First Order Plus Time Delay (FOPTD) systems

The FOPTD process transfer function model is given by

$$G_p = \frac{k_p}{\tau s + 1} e^{-Ls} \tag{11.74}$$

The closed loop transfer function (refer to Fig. 11.6) is assumed as

$$\frac{y}{y_r} = \frac{G_c G_p}{1 + G_c G_p} \tag{11.75}$$

From Eq. (11.75), G_c is given by

$$G_c = \frac{\dfrac{y}{y_r}}{1 - \dfrac{y}{y_r}} \frac{1}{G_p} \tag{11.76}$$

The desired closed loop response (y/y_r) is considered as first order response with time constant τ_c and time delay L is kept in the process because it is unavoidable.

$$\left(\frac{y}{y_r}\right)_{\text{desired}} = \frac{1}{\tau_c s + 1} e^{-Ls} \tag{11.77}$$

Substituting Eq. (11.75) in Eq. (11.76), the controller transfer function G_c is given by

$$G_c = \frac{1}{G_p} \frac{e^{-Ls}}{(\tau_c s + 1 - e^{-Ls})} \tag{11.78}$$

$$G_c = \frac{(\tau s + 1)}{k_p} \frac{1}{(\tau_c s + 1 - e^{-Ls})} \tag{11.79}$$

To derive PI settings first order Taylor series approximation of time delay $e^{-Ls} \approx 1 - Ls$ is used in Eq. (11.79). Then Eq. (11.79) can be written as

$$G_c = \frac{(\tau s + 1)}{k_p} \frac{1}{(\tau_c + L)s} \tag{11.80}$$

Equation (11.80) is a PI controller with

$$k_c = \frac{\tau}{k_p(\tau_c + L)} \tag{11.81}$$

and $$\tau_I = \tau \tag{11.82}$$

To derive PID settings first order Pade's approximation for time delay

$$e^{-Ls} = \frac{1-0.5Ls}{1+0.5Ls} \tag{11..83}$$

is used. Then Eq. (11.79) can be written as

$$G_c = \frac{(\tau s+1)}{k_p}\frac{(1+0.5Ls)}{[0.5L\tau_c{}^2 + (\tau_c + 0.5L)s]} \tag{11.84}$$

Equation (11.84) is rearranged as

$$G_c = \frac{(\tau+0.5L)}{(\tau_c+0.5L)k_p}\left(1+\frac{1}{(\tau+0.5L)s}+\frac{0.5L\tau}{\tau+0.5L}s\right)\frac{1}{\left(\frac{0.5L\tau_c}{\tau_c+0.5L}s+1\right)} \tag{11.85}$$

Equation (11.85) is a PID controller with a first order lag filter. $G_c = k_c\left(1+\frac{1}{\tau_I s}+\tau_D s\right)\frac{1}{(\alpha s+1)}$

where $$k_c = \frac{(\tau+0.5L)}{(\tau_c+0.5L)k_p} \tag{11.86}$$

$$\tau_I = \tau + 0.5L \tag{11.87}$$

$$\tau_D = \frac{0.5L\tau}{\tau+0.5L} \tag{11.88}$$

$$\alpha = \frac{0.5L\tau_c}{\tau_c+0.5L} \tag{11.89}$$

Controller design for Unstable FOPTD system

The process transfer function is given by

$$G_P = \frac{k_p}{\tau s-1}e^{-Ls} \tag{11.90}$$

The closed loop transfer function is assumed as

$$\frac{y}{y_r} = \frac{(1+\eta s)e^{-Ls}}{(\tau_1 s+1)(\tau_2 s+1)} \tag{11.91}$$

The values of η, τ_1, and τ_2 are specified as follows:

Substituting Eq. (11.91) and Eq. (11. 90) in Eq, (11.76), the following equation for the controller is obtained.

$$G_C = \frac{(\tau s-1)(\eta s+1)}{(k_p[(\tau_1 s+1)(\tau_2 s+1)-(\eta s+1)e^{-Ls}])} \tag{11.92}$$

The approximation for $e^{-Ls} = 1 - Ls$ is used in the denominator of Eq. (11.92). Then, to simplify the resulting expression for the denominator, the following assumption is made:

$$\tau = -\frac{\tau_1 \tau_2 + L}{(\tau_1 + \tau_2 + L - \eta)} \tag{11.93}$$

Then, Eq. (11.92) becomes

$$G_C = k_C \left(1 + \frac{1}{\tau_I s}\right) \tag{11.94}$$

where

$$k_C = \frac{1}{k_p(\eta - [\tau_1 + \tau_2 + L])} \tag{11.95}$$

$$\tau_I = \eta \tag{11.96}$$

From Eq. (11.93), the expression for η is obtained as

$$\eta = \frac{(\tau_1 \tau_2 + [\tau_1 + \tau_2 + L]\tau)}{\tau - L} \tag{11.97}$$

For the desired closed loop transfer function, the values of τ_1 and τ_2 are to be specified. The value of η is obtained from Eq. (11.97).

To design a PID controller, first order Pade's approximation for the time delay is used, i.e.

$$e^{-Ls} = \frac{1 - 0.5Ls}{1 + 0.5Ls}$$

Hence, the expression for G_c from Eq. (11.92) is given by

$$G_C = \frac{(\tau s - 1)(\eta s + 1)(1 + 0.5Ls)}{k_P q_1} \tag{11.98}$$

where

$$q_1 = \frac{c}{a}s^2 + \frac{b_1}{a}s + 1 \tag{11.99}$$

with

$$a = \tau_1 + \tau_2 + L - \eta \tag{11.100}$$

$$b_1 = \tau_1 \tau_2 + 0.5L(\tau_1 + \tau_2) + 0.5L\eta \tag{11.101}$$

$$c = 0.5L\tau_1 \tau_2 \tag{11.102}$$

The expression for q_1 can be further simplified as

$$q_1 = (1 - \tau s)(1 + \alpha s) \tag{11.103}$$

Hence, the expression for the controller [Eq. (11.98)] is simplified as a PID controller in series with a first order filter:

$$G_C = k_C \left(1 + \frac{1}{\tau_I s} + \tau_D s\right) \frac{1}{(\alpha s + 1)} \tag{11.104}$$

where

$$k_C = \frac{-(\eta + 0.5L)}{(k_P[\tau_1 + \tau_2 + L - \eta])} \tag{11.105}$$

$$\tau_I = 0.5L + \eta \tag{11.106}$$

$$\tau_D = \frac{0.5L\eta}{0.5L + \eta} \tag{11.107}$$

Equating Eqs. (11.99) and (11.103) along with the expressions for a, b_1 and c, the following equations for η and α are obtained as:

$$\eta = \frac{p_1 + 0.5Lp_2 + 0.5p_1\left(\frac{L}{\tau}\right) + (p_2 + L)\tau}{\tau - 0.5L} \tag{11.108}$$

with
$$p_1 = \tau_1\tau_2 \tag{11.109}$$

$$p_2 = \tau_1 + \tau_2 \tag{11.110}$$

$$\alpha = \frac{0.5L\tau_1\tau_2}{\tau(\eta - \{\tau_1 + \tau_2 + L\})} \tag{11.111}$$

The PID settings are obtained from Eq. (11.105), Eq. (11.106) and Eq. (11.107). For the specification of the desired closed loop transfer function, only the two time constants (τ_1 and τ_2) are to be specified. The value of η is calculated from Eq. (11.108). It is found that the value of the filter time constant α from Eq. (11.111) is negligible (less than 0.12τ). Hence, the controller is essentially a PID controller.

The assumption of $\tau_1 = \tau_2$ is made (The method has a single tuning parameter). By assuming various values for τ_1, the closed loop simulations are carried out in order to get a better robust response. The following equations are fitted for τ_1:

For PID:

$$\frac{\tau_1}{\tau} = 2.03\varepsilon^2 + 0.4958\varepsilon + 0.0326 \qquad \text{for } 0 \le \varepsilon \le 0.8$$

$$\frac{\tau_1}{\tau} = 4.5115\varepsilon^{5.661} \qquad \text{for } 0.8 < \varepsilon \le 1.0$$

For PI:

$$\frac{\tau_1}{\tau} = 0.025 + 1.75\varepsilon \qquad \text{for } \varepsilon \le 0.1$$

$$\frac{\tau_1}{\tau} = 2\varepsilon \qquad \text{for } 0.1 \le \varepsilon \le 0.5$$

$$\frac{\tau_1}{\tau} = 2\varepsilon + 5\varepsilon(\varepsilon - 0.5) \qquad \text{for } 0.5 \le \varepsilon \le 0.7$$

The PI and PID settings are calculated for various values of $\varepsilon\left(=\frac{L}{\tau}\right)$. The settings are fitted by the following equations.

For PID:

$$k_C k_P = 4282\varepsilon^2 - 1334.6\varepsilon + 101 \qquad \text{for } \varepsilon < 0.2$$

$$k_C k_P = 1.1161\varepsilon^{-0.9427} \qquad \text{for } 0.2 \le \varepsilon \le 1.0$$

$$\frac{\tau_I}{\tau} = 36.842\varepsilon^2 - 10.3\varepsilon + 0.8288 \qquad \text{for } 0 \le \varepsilon \le 0.8$$

$$\frac{\tau_I}{\tau} = 76.241\varepsilon^{6.77} \qquad \text{for } 0.8 < \varepsilon \le 1.0$$

$$\frac{\tau_D}{\tau} = 0.5\varepsilon \qquad \text{for } 0 \le \varepsilon \le 1.0$$

$$\frac{\alpha}{\tau} = 0.1233\varepsilon + 0.0033 \qquad \text{for } 0 \le \varepsilon \le 1$$

For PI:

$$k_C k_P = 49.535e^{-21.644\varepsilon} \qquad \text{for } \varepsilon < 0.1$$

$$k_C k_P = 0.8668\varepsilon^{-0.8288} \qquad \text{for } 0.1 \le \varepsilon \le 0.7$$

$$\frac{\tau_I}{\tau} = 0.1523e^{7.9425\varepsilon} \qquad \text{for } 0 \le \varepsilon \le 0.7$$

The following points are to be considered while selecting the closed loop transfer function.

1. The numerator of the closed loop transfer function consists of two parts. The first part comprises of the positive zeros of the process and the second part accounts for the negative zeros introduced by the controller (some researchers used one zero and some others used two zeros).
2. The order of the denominator is to be selected one or two orders more than numerator.
3. The closed loop time delay is considered at least equal to the open loop time delay
4. Depending on the approximation used for the time delay term (first order Pade or second order Pade), the mode of the controller (PI/PID/PID with first order lag filter/PID with second order lag filter/PID with first order lead lag filter/PID with second order lead lag filter) is obtained.

Review Problems

1. Using the derived equations, calculate the values of $k_{c,\max}$ and ω_c of the following systems:
    a) Delay plus first order system ($L = 1$; $\tau = 2$, $K_P = 3$)
    b) Delay plus first order system ($L = 1$, $\tau = 0.5$, $K_P = 2$)
    c) 3 first order system in series ($\tau_1 = 1$, $\tau_2 = 3$, $\tau_3 = 5$; $K_P = 2$)
    d) 8 (equal τ) first order plus system in series ($\tau = 1$, $K_P = 2.5$)
    e) Delay plus integrating system ($L = 1$; $K_P = 3$)
    f) Delay plus second order system with an integrator ($\tau_1 = 2$, $\tau_2 = 5$, $L = 2$, $K_P = 1$)
2. For Problem (1a) Design a PI controller by (i) open loop Ziegler–Nichols method (ii) closed loop Ziegler–Nichols method.
3. Design a PI controller for the system 2 exp($-s$)/s by (i) synthesis method and by (ii) ZN method.

4. Design a PI controller for the system 2 exp(–s)/(4s – 1) by synthesis method.
5. The response of a thermocouple for a step change in the temperature (initially at room temperature 27 degree C is kept suddenly in a hot water bath which is at 85° Cis as follows:

t, sec	0	1	2	4	6	8	10	≥ 12
y, $^{\circ}$C	27	27	66	72	80	84	86	88

Fit a first order plus time delay transfer function model.

6. Calculate the $K_{c,\min}$ and $K_{c,\max}$ of the unstable system 2/(5s – 1)(s + 1)(2s + 1).

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