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Chapter 1

SIMULATION AND MATHEMATICAL MODELLING

1.1 WHAT IS SIMULATION?

Simulation in various forms is common in the environment in which all people live. Examples of simulation are:

(a) historical plays;
(b) games;
(c) flight training;
(d) hydraulic modelling; and
(e) materials testing.

One common feature of all this simulation is the ability to re-create or create a set of circumstances without actually creating the full surroundings. Actors staging a play with good stage settings can make one feel as though one is in the mountains of Norway while sitting in a comfortable seat in a warm theatre. This simulation permits one to appreciate why, without actually being there. There is no need to re-create the whole of that world—only a relevant part of it.

When people play games, it is to simulate a set of circumstances which may not exist. One may be a financier in Monopoly while still being a scientist. Senior officers play war games on tables with toy soldiers. The lessons learned and the theories developed can be checked in a larger simulation—manoeuvres. Both of these simulations are cheaper than a full-scale war, but the lessons may be the same. Pilots for the large commercial jet air-liners are trained partly on flight simulators, because, although costly to buy, the simulators are much cheaper to operate than the aircraft themselves. Hydraulic modelling and materials testing are both means of simulating without building and testing full-size prototypes, and are in common use.

Simulation, then, is a means of gaining relevant information on the characteristics of full-size prototypes without incurring the expense of building a full-size prototype to test. How many processing plants today fail immediately to produce to full capacity owing to 'teething troubles'? Occasionally plants are built which fail to produce the required product or fail to produce it in sufficient quality or quantity. It is to avoid such costly mistakes that simulation is used. In simulation many alterations and changes in processes can be made and the output of the plant checked, all before the design is finalised.

In mathematical modelling, simulation consists of a series of subprogramming modules, each of which attempts to re-create a segment of the prototype. It is usual to find that while insufficient information is available to provide an accurate simulation, it is immediately possible to determine where information is lacking and, therefore, accurately to define the experiments necessary to find that information. Even if experiments are not possible immediately, approximate solutions can define the nature of the interactions occurring and thus provide an insight into the final solution.

As in all engineering problems, the results obtained from the simulation are only as good as the assumptions on which they are based. Ignoring the limits of those assumptions will destroy the credibility of the mathematical model, and once that credibility is destroyed, the model is destined for the wastepaper-basket. That is an abrupt assertion, but it is a fact of life of which all intending modellers should be aware, as all too often mathematical science takes the place of engineering reality and the programs produce too many printed sheets of paper which can only be deciphered by the programmer and not the person who has to make decisions. Remember that in the field covered by this book the treatment plants are still designed on loading rates, overflow rates and three times the dry weather flow to produce tank sizes; if one's modelling works, the results will be based on other criteria such as substrate concentration and biological flocs and these results must be interpreted to the plant designers in a manner they can understand. The biological design, no matter how relevant and accurate, only represents about 10% of the design of the treatment plant; the other 90% consists of concrete, reinforcing, steel, pipes, layout, survey, earthworks, pumps, specifications, bills of quantity and tendering.

Simulation can be an important part of designing a treatment plant but it is only a part, and how important that part is depends on the ability of the modeller.

1.2 SYSTEMS APPROACH

In considering any simulation it is necessary to know what is required. The problem must be defined in order that an acceptable solution may be found. Part of that definition must be the extent of the problem, and this usually defines a system or collection of sub-units. One unit, such as an activated sludge tank, can be simulated, but one of the purposes of simulation is to optimise and ultimately control the process. It is possible to take an isolated unit such as an activated sludge tank and optimise its design to the exclusion of all other units. Should all the other units, in turn, be optimised and all the components in their optimised form connected together, then the plant is unlikely to achieve the desired result. The reason is simple: if the primary clarifier removes too much material, the input substrate concentration to the activated sludge tank may depart markedly from that required for optimum efficiency and the tank will not produce the treatment results desired. It therefore follows that none of the units has to, nor can it, work at its optimum. Rather, each unit should work within a range either side of the optimum but such that, when all units are connected together, the whole system produces a result, which should lie within the desired range. It is this result which then may be optimised as a system. In optimising a system alternatives are considered and differing layouts may be involved, but it is the system which counts—not the components.

1.3 MATHEMATICAL MODELLING

Why mathematical model? What advantages are there for the effort expended? The advantage lies in the fact that the processes involved are dynamic—that is, they are not constant with time. In the sanitary engineering field the input flow to a treatment plant is not constant: it varies its quantity with time and its composition with time. Furthermore, these variations are not the same from day to day or week to week, and, in addition, flow quantities usually increase with time. If one moves from London to the Midlands to the north-east (Newcastle), all these values and their periodicities will be different. It is the same in the United States: the flow and characteristics will be different as between New York, Miami, Chicago and Los Angeles.

In research inputs are controlled and usually stable with time, and a 'steady state solution' is obtained. We can use this solution to calibrate or obtain biological constants for the mathematical model, but the process we

TABLE 1.1 Fixed Integration Methods, Program Time to Run Complete Program

METHOD	*DELT*			
	1.	.1	.01	.001
RECT	2.716	2.785	3.212	6.483
TRAPZ	2.772	2.754	3.844	9.883
SIMP	2.751	2.996	3.731	13.216
ADAMS	2.892	2.964	3.199	7.457
RKSFX	2.864	3.054	4.426	18.883

are modelling is dynamic: it changes particularly with time and with temperature, but also with other parameters. For example, at plant start-up it can take weeks to build up the biological organisms before producing the required standard of effluent. Under these circumstances only a dynamic mathematical model can produce the answers required; it is the only one which will automatically follow varying inputs and produce answers relating to the actual time-dependent output values. The accuracy of the outputs obtained depends on:

(a) the complexity of the model;
(b) the accuracy of the calibration constants;
(c) the modelling time interval chosen; and
(d) the skill of the modeller.

Examples of the relative times of computation on an IBM 360, and the values of the results obtained from the calculation of a simple biological reactor are shown in Tables 1.1, 1.2 and 1.3.

Mathematical modelling is a good test of whether the process is understood. If the model can be written, then an assumption of the

TABLE 1.2 Relative Computation Times for Variable Interval Integration Methods

METHOD	*Initial DELT Value* (*Final value DELT* = 0.5)			
Variable interval	1.	.1	.01	.001
MILNE	2.455	2.372	2.434	2.327
RKS	2.397	2.339	2.496	2.540

TABLE 1.3 End Bacteria Concentration for Simple CSTR Program

METHOD	*Initial DELT Value* 1.	.1	.01	.001
Fixed interval				
All methods	104.74	110.51	113.11	113.07
Variable interval (final DELT value = 0.5)				
MILNE	112.45	112.45	112.96	113.42
RUNGE–KUTTA	104.74	110.51	113.15	113.46

processes involved can be made and evaluated. If the model works and calibrates against the actual prototype, then it is probable that the model is a representation of a way in which the process actually works. Of course it is assumed that no breaking of fundamental chemical or physical laws has been proposed in the model.

1.4 TYPES OF MATHEMATICAL MODEL

There are two basic ways of representing the processes involved in a dynamic situation. The two methods are:

(1) The output is related mathematically to the input and a mathematical relationship is established between the two. No understanding of the processes occurring is needed. The resultant formula is often called an empirical relationship.

(2) The processes involved in the workings of the model are mathematically expressed and these process mathematics are linked together to form the complete model. If the processes are not understood, it is extremely unlikely that a working model will result.

There are disadvantages in each type of modelling, both of which need large amounts of data to provide a comprehensive and accurate model.

The main disadvantages of the empirical approach are that the relationships are based on inadequate data and that there is no indication of the process involved. The problem can be defined by use of a simple illustration: if O_2 is bubbled through water at 20 °C, a condition of equilibrium concentration will be reached which can be expressed mathematically. Note, first, that the expression will only give one value—equilibrium concentration—and no values for the time–concentration curve before equilibrium is reached, and, second, that the expression will give no information on what happens if the temperature increases to 25 °C when the O_2 concentration decreases; the formula will not provide this information unless a series of experiments have been performed which include temperature also. If the process is also rate-dependent (that is, the rate at which O_2 is bubbled through the water), then the simple formula will not be of any assistance. The implications inherent in this empirical method are:

(a) The formula only represents a steady state equilibrium result.
(b) The formula can only cover those input variables covered by the data and gives no indication of other variables omitted.
(c) The result can vary with the amount of data available: more results could mean a different equation, as the equation derived is based on statistical analysis.
(d) The exact degree of coverage of the reaction is in some doubt, as, even with a good statistical correlation, $R^2 = 80\%$, there is still 20 % of the variation unexplained.

One biological experiment consisted of an examination of thin films developed on rocks, and for each change in environment took approximately 40 days to reach equilibrium. The variables involved were

(1) input concentration;
(2) rock size;
(3) temperature;
(4) length of flow;
(5) type of nutrient;
(6) shape of rock; and
(7) dosing rate.

If *only* three values of each variable are utilised, then there are 2187 different combinations. At 40 days for the experiment plus 5 days to restart again, it would take 98 415 days to carry out all the combinations possible using those seven variables. If only 300 days are used per year because of holidays, experiments finishing at weekends, sickness, etc., then it would take 328 man-years to obtain the necessary sets of data to be absolutely sure of the result. If after that time $R^2 = 90\%$ (a very good result), perhaps something had been forgotten (e.g. a trace metal); then all those results may have to be repeated because that trace element was not measured!

The method involving processes (2) has often produced faster solutions and is more akin to the scientific method, but depends on the inspiration and understanding of the scientist concerned. This method uses the results of several hundred years of accumulated knowledge of physical and chemical laws. The application of these laws plus the inspiration of the researcher accurately to describe the process allows the data period to be shortened, as the multivariable model can be tested without the completion of all the variations necessary for the empirical method. The results must agree closely with the results obtained by experiment. The conceptual model also has the inherent ability to predict the results during the stage prior to equilibrium and thus provide continuous results for varying parameters. One unusual feature is that the model can be calibrated by use of constant parameters to reach the equilibrium condition and still be used to predict varying conditions. A characteristic of the mathematical model is its dependence on all the values necessary to create the model. The absence of the information necessary to complete the model tends to show up immediately and finally. It is thus a good indicator of research needed to complete an understanding of the processes involved.

1.5 THE COMPLEXITY OF THE MODEL

Mathematical models can be very complex or very simple. The simple, short model will give only elementary answers and be of limited value; it can usually be written and made to work in a short period of time. The complex model can include many variables, including temperature, but as the degree of complexity increases, so does the amount of information which has to be available in order to get the model to give appropriate answers; a complex model requires a much longer time to write and an even longer time to check and debug. Some very complex models have been under development for years, and the extremely complex ones for river systems such as the Hudson/Long Island Sound and the Trent River System will never really be complete. Some dynamic models, such as those portraying the movement of air masses and weather on a global scale but yet defining weather patterns in each and every city on Earth, have been attempted but accurate results are not expected, even by the planners, for years because of the sheer amount of data required, not to mention the computing capacity and the programming required.

A balance must be found between the time available and the complexity of the answer desired. An engineer has to produce a definite answer within a given time period, and failure to produce this answer can be expensive for the client and troublesome for the engineer. One approach often used in these circumstances is to develop a simple model first, examine the results to determine where answers are not as they should be and concentrate programming effort into a more complex model of that area.

1.6 ACCURACY OF THE CALIBRATION CONSTANTS

A dynamic or a steady state model is only as accurate as the values used to calibrate it. If the model is to match the subsequently measured values from the process, then the values used for its calculations must be appropriate and as accurate as possible. Since many of these values relate to biological processes, it is not always possible to be as accurate as desirable. One good reason for this is that values may have to be derived from pure cultures and not the heterogeneous cultures found in sewage treatment plants. These heterogeneous cultures produce lower values of growth rates under different conditions and the information will not always be available when required; it is a problem very familiar to those who have to produce answers. This lack of initial accuracy can be corrected in data derived from actual plants in operation, and it will be necessary to collect, analyse and update mathematical models to reflect these values.

Information on heterogeneous cultures and on the actual operation of plants is available in the literature, and so information is available for the production of the simpler mathematical models, but remember that temperature has a very large effect on biological reactions and should be carefully considered when the biological constants for a model are derived.

A simple, short, non-comprehensive list of biological values is given in Appendix 1. These values have been provided as a guide only, because the parameters are extremely temperature-dependent. One illustration of this dependence is the example of sewage stabilisation ponds, which take about 1 month to complete their biological activity in warm temperate zones, cease their activity almost completely in the winter of the northern, cold-temperature zones and take only 10 days to completion in the tropics. Partly for this reason and also to slow down the reactions, values much lower than those specified in the appendix have, in general, been used in this book. The reader is encouraged to be flexible in his approach to biological parameters.

1.7 MODELLING TIME INTERVAL

A balance must be achieved between the computing time involved and the time interval employed in the program. This decision will have a major effect on the value of the model and on the integration method employed and, hence, the accuracy.

A model on algal production based on photosynthesis must include both day and night and multiple calculations in each part of the day. An integration interval of 1 h would necessitate one of the most accurate integration methods such as the Runge–Kutta fourth-order with variable interval, whereas a decision to employ an integration interval of 0.01 min would only need a simple Euler (rectangular) method of integration. The use of the latter interval and Euler method would involve 6000 times as many calculations but would not take 6000 times as long to calculate as the Runge–Kutta method, because the latter may take 100 times as long to complete a calculation; the total time taken would therefore be only 60 times as long as that taken by the Runge–Kutta method. Under the integration step interval outlined the simple Euler method would almost certainly produce a more accurate result, but a different step interval will change the relative times and accuracy. The programmer must decide which method to use, and this decision will be based on the accuracy desired, the time interval specified and the computation time involved. In utilising a higher-level language such as CSMP the decision will not be governed by the complexity of programming the integration method, as the methods are already programmed in the compiler.

1.8 THE SKILL OF THE MODELLER

In engineering it is necessary to adopt a pragmatic approach to the problems encountered. In engineering and the applied sciences it is expected that all graduates can program a computer in a higher-level language such as ALGOL, BASIC or FORTRAN. This is not necessarily true in other disciplines, nor perhaps do they have as much need of the ability.

Languages such as ALGOL, BASIC or FORTRAN permit an ability to program which is independent of the way in which the computer works. These languages are mathematically akin and accept ordinary mathematical statements subject only to a few simple rules such as defining very clearly the calculation desired—for example, that

$$a/b * c = \frac{ac}{b}$$

and not

$$= \frac{a}{bc}$$

which should have been programmed as

$$a/(b*c)$$

These higher-level languages are aimed at reducing the necessary skills of the professional programmer down to a level such that programs can be written by people trained in other disciplines. There is still a degree of skill needed to deal with idiosyncrasies of any language, and this is achieved only with time, use and training. The use of higher-order languages therefore only has the effect of reducing the initial skill before programming can be commenced.

Skill cannot be eliminated completely, because even with simpler (higher-level) languages there still exist different ways of achieving the same result; here skill and experience will continue to play a major role in program development.

Chapter 2

COMPUTERS AND THE CSMP LANGUAGE

2.1 COMPUTERS

Much has been written and spoken about computers in the last two decades. Some of those who have voiced opinions seem to be afraid of a machine with human intelligence. If such a machine were available, it would simplify the programming; what is available, however, is something very different. Computer technology has advanced from

	radio valves	(first generation),
	discrete transistors	(second generation),
	integrated circuits	(third generation),
to	large-scale integration	(microcomputers).

Computers can talk to us using prerecorded sounds or in squawky machine-generated sounds; we can understand the computer talking to us. We can talk to a computer using our voice but as yet it does not understand us in our multiplicity of accents, dialects and languages, even though it can translate from some languages to others. The computer has just 'learned' to read writing by following a very detailed program. It still has not been credited with being able to 'think' in human terms; it may be possible to build a thinking machine when we fully understand how the human brain works, how it stores and retrieves information, but even so it can be anticipated that it will still be following a detailed program which some human has programmed and read into its memory store.

A computer may be a glorified 'number-cruncher' but nevertheless it is a 'moron', it does precisely what it is told to do and only what it is told to do. If a mistake is made in a program, it can only correct it if a correction subprogram covering that particular eventuality has already been inserted by the programmer. A programmer will wish it were otherwise, but, barring a hardware malfunction (rare), it will produce an answer determined exclusively by the program. If the program does not run, it is because something was left out; if it gets the wrong answer, the program was wrong. Kick the computer (if you can get near it) by all means. It may help your feelings, but it will not change your program and will not improve the accuracy of the answer—you will still have to correct your program if you want the right answer. Write your initial development of the program with the realisation that it will not work and arrange for sufficient calculated values to be printed out in order to determine where the program is in error. Every program should be calculated with a desk calculator to be certain that it is doing what it is supposed to be doing. You will be surprised at the number of mistakes which have crept into the final program. As a program is written, it should be documented—that is, an explanation should be written of the formulae steps and assumptions made in the process of writing. A month away from the program working on another program will result in the loss of the thought process involved if this documentation is not carried out initially.

2.2 MODERN COMPUTERS

Modern computers consist of three main types: big ones, little ones and micros. The big ones are firmly under the control of professional programmers and one is physically locked out. Most little ones are like the big ones but it is possible occasionally to touch, run, load, change discs and operate the printer oneself. The micros are the smallest, and one suitable for running the programs in this book in BASIC can be purchased for about £3500.

All computers have an operating system or resident monitor which controls the way in which the machine works. This monitor is part of the software and can be changed by overwriting it with a new program. This software is written by professional programmers and is virtually immune to anything that can be done using one of the higher-level languages. You are therefore advised 'If in doubt—try it'; 'If you don't know—try it'. If the machine 'crashes' (stops working) because of something you do in your program, then it is a fault in the software and not a fault of yours.

The operating system determines whether the computer works in batch, terminal or combined mode.

Effectively, to a user, the batch mode operation consists of a box where programs are put in and another box where the output comes out some hours later.