TEACHING SIMULATION AND MODELLING AT ROYAL MILITARY COLLEGE*

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IN ITS PRESENT calendar, the Royal Military College of Canada offers to its fourth year fuels and materials engineering students a course in modelling and optimization. The course bears the number FME413B and CMF413B for the English and French versions respectively, and the calendar entry reads: "FME413B (CMF413B): Systems Analysis: Modelling and Optimization. Mathematical formulation and digital computer simulation of engineering problems are carried out and digital techniques are used to solve optimization problems. The emphasis is on writing the mathematical model from word statements and programming to predict the steady-state behaviour of various problems of contemporary and future significance to the Canadian Forces. A brief overview is given of major optimization techniques."

HISTORY

The course originated in the 1960's and it contained only the setting up of mathematical equations from problem statements. During the academic year 1974-75, the course was augmented to include process modelling and simulation techniques and in 1979 optimization was included with the introduction of the new Fuels and Materials Engineering program. It is now presented during the longer winter term (at three 45-minute lectures/week for sixteen weeks), which allows more time for computing projects than before.

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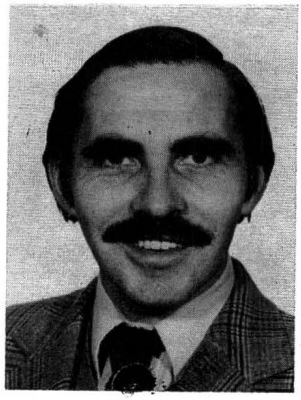

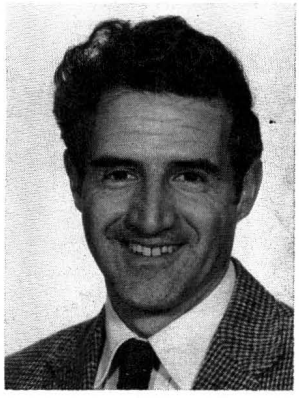

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Ron D. Weir is Professor of chemical engineering at The Royal Military College. His BSc was obtained in chemical engineering at The University of New Brunswick. He went to England as an Athlone Fellow to obtain his Diploma of the Imperial College of Science and Technology in London and PhD from the University of London, where he won the Lessing medal. He has also been a N.A.T.O. Fellow and National Research Council of Canada Fellow. Dr. Weir joined RMC from the NRC in 1968. In 1978-79, he was Senior Visitor in the Department of Inorganic Chemistry at the University of Oxford. Other courses currently taught by him are chemical and engineering thermodynamics, and fluid mechanics. His research involves orientational disorder in crystals via low temperature heat capacity measurements. **(R)**

PHILOSOPHY

The goal of the course is to assist students in writing differential equations to represent chemical processes and other natural phenomena, and to solve these problems on digital computers. Ultimately, the students are able to write mathematical models to represent specific chemical or physical processes, to solve the resulting equations in order to predict the behaviour of the system parameters according to the control and design variables and, finally, to use optimization techniques to obtain the values of decision variables that yield the best index of performance for the process. Only steady-state phenomena are studied due to lecture time constraints.

COURSE OUTLINE

Four main parts make up the course, *viz.*: I—Optimization, II—Simulation, III—Solution of differential equations, and IV—Mathematical Modelling. In addition, four projects are assigned, corresponding to the main parts of the course. A detailed plan of the course appears in Fig. 1.

FIGURE 1
Course Plan

FME 413B / CMF413B
SYSTEMS ANALYSIS: MODELLING AND OPTIMIZATION

PART I: OPTIMIZATION
- Introduction, principles, Lagrange multipliers
- Steepest Descent Techniques (Gauss', Newton's, Hestenes', Penalty Functions)
  (6 lectures, 1 quiz, 1 assignment, 1 project)

PART II: SIMULATION
- Possible approaches: Special-purpose programs; Building-block routines ("MECCANO" approach); General purpose programs for particular class of processes.
- "MECCANO" approach explained, with simple CSTR process taken as example
  (11 lectures, 1 quiz, 1 project)

PART III: DIFFERENTIAL EQUATIONS
- Analytical: Review, Bessel Equations
- Numerical: Finite Difference method
  (7 lectures, $\approx$30 problems, 1 project)

PART IV: FORMULATION OF MATHEMATICAL EQUATIONS FROM WORD STATEMENTS
- Balance Equations: ACCUMULATION = INPUT-OUTPUT
- Illustration through several examples, such as
  - Multi-plates distillation column
  - Gas diffusion into a liquid with chemical reactions
  - Heat transfer through a cooling fin
  - Flow systems (Euler and Lagrange Methods)

(21 lectures, $\approx$10 assignments, 1 quiz, 1 project)

After the general principles of optimization are explained, the Lagrange multipliers technique is studied and applied to a few examples, with assignment.

The first part consists of a block of six lectures on several optimization techniques. After the general principles of optimization are explained, the Lagrange multipliers technique is studied and applied to a few examples, with assignment. Linear programming is mentioned, but this subject is not covered since several excellent routines exist in most computer systems and the application of the methods is limited.

The course goes into more detail on steepest descent techniques of the most robust kinds, such as Gauss', Newton's and Hestenes' methods. Examples for unconstrained problems are studied, and a method using penalty functions is explained for more realistic problems with constraints. The reason for the use of these search methods is that often chemical processes models cannot be expressed as simple analytical equations, and in these cases search methods are usually the only ones capable of solving these problems.

The philosophy is to provide some basic tools to perform mathematical optimization of chemical processes. Although this part does not follow any particular textbooks, several references are indicated, so that the students have a basis for understanding the best methods suitable for the practical problems they may encounter during their engineering career. The most important goal is achieved when the student is able to write a properly-defined mathematical optimization problem and to use an appropriate technique to solve it.

The second part of the course covers the simulation of the process itself. The students are told of three broad approaches to simulate physical and chemical processes. Since the course is of a very practical nature, staff insist on the most practical way to attack a simulation problem. Because many routines exist that simulate whole chemical processes or parts of them, the option of writing a special purpose computer program for a specific process is only mentioned, as is the option of operating an already complete program that simulates a given class of processes. The "building block" subroutines approach (or "MECCANO"

approach) is followed. The reason is that these subroutines (which simulate standard parts of chemical processes such as reactors, splitters, and flash separators) are often written in an optimal way that minimizes the memory space and the computer time. Therefore, the student is expected, through the use of an example, to make use of these standard subroutines in order to simulate a given chemical process. The example used is the continuously-stirred tank reactor (CSTR) process explained below (Fig. 2).

Part III consists primarily of a brief review of the solution of differential equations. This is done by means of lectures, handouts and assignments. Emphasis is put on the Bessel equations and their solutions. Simple numerical methods are investigated, including the Secant and the Newton-Raphson.

Finally, in the last part of the course techniques are described which allow mathematical models to be written from word descriptions of physical problems. The conservation principle is the basis. This enables the students to write balance equations for mass, energy, momentum, forces, electric charges, etc., applied to an elementary volume of the system under study. They are taught using a series of examples representing several classes of problems frequently encountered in chemical engineering. These sample problems viewed in class include a multiple-plate distillation column, gas diffusion into a liquid in which chemical reactions occur, and flow systems, among others. Flow systems are treated both by the Euler and the Lagrange methods. In the Euler method, the volume element on which the balance equations are applied is chosen as stationary, as opposed to the Lagrange method where this element moves with the fluid. To complement these examples, a series of ten to twelve assignment problems is given to the students.

THE SUPER PROJECTS

A substantial part of the course is taken up by the four computer projects, since they are seen as the best way for students to acquire these modelling and optimization techniques. These projects are: 1) Steepest descent techniques, 2) simulation of the CSTR, 3) numerical solution of a system of differential equations, and 4) optimization of the CSTR. Project 1 requires the use of some steepest descent techniques to solve simple optimization problems, namely by writing computer programs in FORTRAN to implement optimization

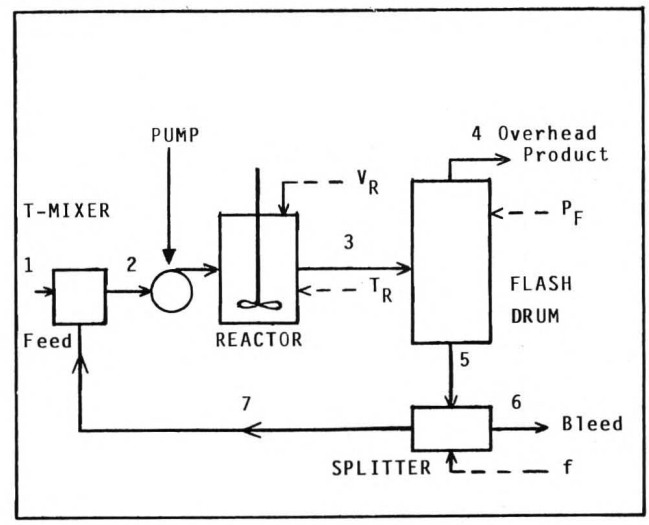

FIGURE 2. Hypothetical chemical process involving CSTR and flash separator.

algorithms such as Gauss', Newton's and Hestenes' methods. Unconstrained problems are first studied, and in the last exercise of the project, students are asked to use penalty functions to solve a simple constrained problem. In addition to analyzing the problems, the students compare the various methods in terms of convergence speed and computer effort. Although this seems quite simple, it represents a major effort by the students since most of them have limited computer experience and need more practice.

The goal of Project 3 is the application of numerical methods to a practical problem of solving a system of differential equations. The students must derive the numerical equations based on a finite difference method and solve on the computer the resulting algebraic equations. Also, they are required to carry out several runs with different numbers of mesh points in such a way that they can see how to control the error associated with this numerical technique. A simple graph is required from which the order of the method can be determined, and in their report the students discuss the method and outline ways to improve it. The problem used is simple heat transfer in nuclear engineering, and it consists of calculating the temperature distribution in a fuel element plate made of uranium metal protected by a sheath. The mesh spacing in each region is kept constant in order to keep the numerical equations fairly simple. Since the computer used (PDP-11) was capable of only modest performance, it was decided not to use large number of mesh points for this exercise.

SIMULATION AND OPTIMIZATION OF THE CSTR

The heart of the course is the simulation and optimization of the Continuously-Stirred Tank Reactor (CSTR) process. A diagram appears in Fig. 2. This chemical process is composed of a "T-mixer," a "CSTR," a "flash separator" and a "splitter." In this process, a chemical component P is produced through a chemical reaction in the CSTR from a component A which is fed to the system in pure form. The chemical reaction is $A \rightarrow P$, but a secondary reaction occurs in which P forms an undesirable material G. The mixture of the three chemical components is then sent to the flash separator where pure product P is extracted. The residue is then sent back to the reactor in order to improve the yield. However, a fraction "f" of the recycled stream is bled off, for the component G would eventually clog the piping.

The mass and energy balance equations are derived in class, and the students are given the listings of the subroutines which solve these equations. Also in class, the nomenclature and the various arrays which contain pure components, equipment and stream parameters are covered. The students are shown how to make use of a special equipment unit (called the "convergence block") to perform the iterations needed by the presence of a feedback loop in the chemical process. The routine associated with the convergence block modifies the stream parameters values of stream #7 until these values become such that equilibrium occurs in the system, within tolerances fixed by the student.

Project 2 consists in writing the main FORTRAN program that calls the various subroutines (stored on a disk), in order to simulate this chemical process. In Project 4, the students maximize the yield of product P as a function of one design variable, V_R, (the CSTR volume), and four control variables: F (the feed rate of pure component A), T_R (the CSTR operation temperature), P_F (the flash separator pressure), and f (the bleed fraction).

Two approaches are possible for optimizing this system. The simplest is to run the program successively using different parameters and then chosing the set of decision variables that gives the best index of performance. This was done in past years, but since the technique is obvious and tedious it was not making the best use of the students' time. The students are now required to use the optimization method of their choice. Most selected a simple steepest descent algorithm which improved the current estimate by performing a line search for the optimum along the direction of the largest partial derivative (which was computed numerically).

DISCUSSION

The first aspect to be discussed is the topic arrangement in the course, which may seem reversed. A more logical order might be: mathimatical modelling, differential equations, simulation and optimization. However, if this order were followed, all computer work would be cramped into the last part of the semester. At RMC, the officer cadets have a solid block of ten hours a day of academic and military/sports activities, which leaves them only evenings and some weekends for computer work. Therefore, computer time must be spread out over the entire semester. Since the optimization part is self-contained, it provides a good topic in which to assign the first computer project and thereby refresh computer skills.

The philosophy is to provide some basic tools to perform mathematical optimization of chemical processes. Although this part does not follow any particular textbooks, severel references are indicated, so that the students have a basis for understanding the best methods suitable for the practical problems they may encounter during their engineering career.

In addition, since the mathematical modelling part of the course involves only non-computer assignments it is saved for the last part of the semester so that these assignments and the last project can be done simultaneously. As is now obvious, time is a critical factor. With only three formal lectures per week and the heavy work load on the students, there is insufficient time for good coverage of the material by all students, and some projects must be done in groups. One consequence of this is that only a few students become "experts"; the others adopt a passive attitude and probably derive only marginal benefit from the computer part of the course.

Another problem area comes from the dependence of this course on many other courses such as mathematics (calculus, differential equa-

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outlet is again monitored. Curve fitting techniques can then be used to obtain the time constants. At the University of Edinburgh step tests and pulse tests on various arrangements of stirred vessels were carried out by students as a laboratory project lasting for a week. In addition they were required to construct the conductivity-concentration calibration curve. This was again carried out with the aid of the microcomputer. The project proved to be a very effective tool for illustrating the principles of process dynamics in general and the dynamics of stirred vessels in particular. □

ACKNOWLEDGMENTS

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SIMULATION AND MODELLING

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tions), thermodynamics, heat, mass and momentum transfer, as well as computer programming. It is possible to exert some control on the background in many topic areas, but in some key subjects (such as programming) the background varies widely among the students. These students have usually followed the prerequisite courses at other military colleges before transferring to RMC for their final two years. It is therefore unavoidable that some precious time has to be spent in bringing all the students up to the same level.

One handicap is in the lack of good textbooks. Presently, Mickley, Sherwood and Reed [1] is used for the modelling part, and Daniels [2] is used as a reference for the optimization part. The need for more recent textbooks, especially in modelling, is obvious, and a search for them is always under way.

On the positive side, the small size of the classes (twenty students) is a real asset; the course can be more tutorial in nature and more time can be devoted to each individual. Assessment of the students can be performed more often, with three quizzes and a final 3-hour exam in addition to the assignments and projects. The performance of each student can be monitored closely and problems cured soon after they show up.

The course is considered as a dynamic process, where improvements are continuously sought and made. Currently, more simultation problems are needed in order to cover the spectrum of chemical processes and of systems suitable for simulation. It is necessary to expand the course to include economical models within the mathematical models of the processes. Finally, as RMC is about to acquire a new and more powerful computer, it is expected that the limitations imposed by our present computer will vanish and that more interesting simulation/optimization problems can be solved by the students in a more efficient manner.

CONCLUSIONS

The present simulation/optimization course taught at RMC is the result of rapid evolution over several years. Divided into four main parts (optimization, simulation, differential equations solutions and mathematical modelling), the course emphasizes the effective writing of differential equations in order to simulate chemical processes or physical systems and the solution of these mathematical equations either analytically or numerically.

Simulation of the systems in steady state allows the prediction of the properties of that system as a function of the value of the various control or design parameters, which can be optimized using suitable optimization techniques. This permits the effective design of chemical processes to meet the needs of industry or the armed forces particularly.

Although the course is satisfactory for the moment, the staff wishes to make further improvements. Better text books and a greater variety of simulation problems are needed. Hopefully this presentation will bring comments, criticisms and suggestions from readers with relevant experiences. □

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