E. Analysis of particulates
Physical; inorganic chemical; organic chemical
F. Odor in ambient air
G. Analysis for gaseous pollutants
Inorganic gases; organic gases
H. Legal and administrative aspects

Students specializing in air pollution are studying a problem and the approaches to its solution. Consequently, two potential dangers must be carefully watched and avoided: first, that the core program can become too broad and too qualitative. To overcome this danger, fundamentals are stressed whenever possible, for example in considering atmospheric photochemistry or atmospheric diffusion, and engineering design is introduced whenever passible, for example in gas cleaning. The second concern is that the problem and the approaches to its solution change very rapidly. To overcome this danger, the only answer is the use of the latest research and development publications in the field.

ChE classroom

PROCESS DYNAMICS, Without Control

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Process dynamics has traditionally been closely associated with the field of process control. Indeed it was a natural marriage. Control systems by their very nature modify the unsteady state response of a process. However, process dynamics need not be so restricted in application. Clearly such diverse problems as dynamic measurement of rheological properties, batch processing, molecular excitation and relaxation, periodic operation of processes and the onset of hydrodynamic instabilities all have a common foundation in process dynamics. Problems in stability, for example, arise not only in analysis of control systems, but also in thermodynamics, boiling heat transfer, reactor analysis and hydrodynamics, among others.

There is a need then for a common fundamental discipline concerned with unsteady state problem is engineering. Presentation of dynamic ideas may come in a rather natural context in control system analysis. It is the writer's experience that more difficulties arise when presented in other surroundings. Chemical engineers have been traditionally steeped in steady state concepts. From the period when analytical description of processes became feasible, continuous steady state operation was the ideal. Only recently has this accepted norm been challenged. Periodic operation of processes can prove to be optimum in some economic sense. So ingrained is the steady state concept though, it is often difficult to get across the idea that a process cycle is not necessarily a repeating sequence of different steady states. This could be remedied by proper exposure to the fundamental concepts of process dynamics.

THE NEED FOR A fundamental understanding of process dynamics, divorced from specific fields of application, increases each year. Engineers are being called on to contribute their techology to important social problems. Blind application of traditional chemical engineering techniques to problems in biomedical and environmental engineering, for example, might prove disastrous. It is perhaps clear that processes occurring in the human body vary continually with time. The steady state concept may be virtually nonexistent there. Application of steady state analysis to environmental problems may be more insidious. A large lake, for example, may respond to changes with a time constant on the order of months rather than minutes. Changes with time may be so slow that the natural temptation would be to assume that a quasi-steady state prevails. Serious errors may result in trying to use steady state models to describe observed data.

The basic ideas of process dynamics must be incorporated into any chemical engineer's education. It is the writer's opinion that process dynamics should be taught in a core of fundamentals. Process control is an application of these fundamentals, but only one of a variety of applications. To a certain degree process dynamics is to process control as transport phenomena is to diffusional operations.

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These ideas are continually being incorporated into a one semester graduate level course entitled Process Dynamics taught at the University of Rochester. The course has evolved over several years, first being taught by the writer on the informal basis in an industrial environment and then at The Johns Hopkins University. The intent is to present a unified treatment of the unsteady state behavior of processes. Emphasis is on the physical interpretation of the time responses as well as the mathematical methods of analysis. Applications, in the form of examples, are taken from a spectrum of areas.

Students taking the course have a variety of backgrounds. No previous exposure to process dynamics or process control is required and indeed some have had none. The course is normally offered in the Spring semester so all students are expected to have a degree of mathematical maturity. Background in linear algebra, Laplace transforms, and techniques for solution of partial differential equations is built on. In addition to first year and more advanced chemical engineers both mechanical and electrical engineeds have enrolled. Full and part time students are included.

No attempt is made to cover applications to process control with any breadth. There is perhaps a bias toward these problems, but no systematic treatment. Students interested in advanced control concepts are encouraged to take a course in advanced servomechanisms taught in the Electrical Engineering Department or optimal control theory taught in the Mathematics Department at Rochester. The course in Process Dynamics provides sufficient motivation and background material for either. At present no course on control of chemical processes is offered, although one is currently being planned.

TABLE I PRESENTS an outline of the course content. It is divided into three major parts, the first being a rather brief introductory and motivational section. The remainder of the course is divided roughly into equal parts, treating problems described by ordinary differential equa-

Table I. Process Dynamics—Course Content

I. Motives and Methods of Process Dynamics
   A. Introduction
      Illustrative examples; dynamic versus static behavior
   B. Dynamic Process Models
      Lumped and distributed parameter systems
   C. Methods of Analysis
      Perturbation methods, linearization; linear algebra; Laplace transforms
II. Lumped Parameter Systems
   A. Input-Output Representation
      Transfer functions; time responses, short and long time expansions; frequency response; linear stability; Nyquist criterion
   B. State Space Representation
      Matrix exponential; eigenvalues, eigenvectors and response modes; modal control; optimal system responses
   C. Nonlinear Responses
      State plane response; perturbation methods; periodic processing; stability in the sense of Lyapunov, Lyapunov functions and system responses
III. Distributed Parameter Systems
   A. Linear Constant Coefficient Problems
      Wave and diffusion responses; simple time and frequency responses; Riemann representation, the method of characteristics; Laplace transform techniques, short and long time expansions; axial dispersion, Taylor diffusion; stability considerations; optimal responses
   B. Variable Coefficient and Nonlinear Problems
      Local linearization, relation to Riccati equations; some exact solutions; nonlinear problems, flow forcing problem, shockwaves; periodic processing, the parametric pump; application of modified lumped parameter methods of analysis.
   C. Approximation techniques
      Relation between lumped and distributed systems, discretization; method of moments; modal approximation; successive approximations; asympotic approximations.

tions and those arising from partial differential equation models. These are termed lumped and distributed parameter systems in control jargon.

As an introduction to the subject of process dynamics several diverse examples are discussed qualitatively. It is important to carefully distinguish between the true unsteady state and the quasi-steady and steady states. Only the first is a purely dynamic state in which there is a varying rate of accumulation of mass, energy or momentum. Then typical process models are considered as a basis for the general types of systems to be considered. Since all involve simply applications of conservation equations, models invariably are coupled systems of first order differential equations or first order (in time) partial differential equations.

Although an attempt is made to review or introduce mathematical tools in the context of the applications being considered, some introduction is given to the principal methods of analysis used throughout the course. The application of perturbation methods to general nonlinear equations is discussed to provide experience in obtaining linearized models to analyze. Care is taken to justify linearization not because real processes are linear but because only then can general analysis and interpretation be performed. Consequently most methods of analysis of nonlinear problems extend or build on the linear.

Treatment of lumped parameter systems is begun with a quick review of standard Laplace transform treatment of linear ordinary differential equations. Emphasis is placed on the physical, time domain, responses of these systems. Both long and short time expansions of transforms and their time responses are discussed. Transfer functions and their frequency response are treated only as they represent physical system models and their time response to sinusoidal disturbances. Typical example problems considered in this treatment might include the interpretation of complex viscosities obtained in rheological measurements or the choice of a forcing signal tending to amplify a system response the most.

More time is spent treating the same general N^{th} order system of linear lumped parameter equations from the state space point of view. General solutions are written in terms of the fundamental solution of the adjoint system of equations. The matrix exponential and the system eigenvalues, eigenvectors and response modes are interpreted physically. At each step full comparison is made between the same results obtained by general Laplace transform solutions and the state space solution. The problem of feedback control is introduced to illustrate that it is possible to tailor the dynamic response of systems to suit ones need. As a further example of the advantage of using the state space point of view the optimal control problem is considered. Elementary solutions to the variational problem are considered in examples.

Stability of linear systems is also treated from both the frequency response and state space points of view. Careful explanation of the feedback nature of the problem, either inherent or imposed, is included. From a general treatment of the analysis of roots of a characteristic equation the frequency domain methods are derived. In order to convey a physical feeling of the origin of the instability problem, example problems from a wide variety of areas are discussed. Both analysis of multiplicity of steady state solutions and of oscillatory storage and release of system "energy" are discussed physically and demonstrated mathematically.

The growth of a linearly unstable response to the point at which the linear model is no longer valid naturally introduces the analysis of nonlinear systems. The extensive work done on stirred tank reactor analysis can be used to illustrate the methods of classical nonlinear mechanics and the use of Lyapunov functions. Methods of analysis are developed as needed and compared with the limiting cases of linearized models. State plane dynamics and the geometric interpretation of stability in the sense of Lyapunov are rather easily presented after the linear canonical state space concept is grasped.

Although much of the material on lumped parameter systems is available in a variety of suggested textbook references, a conscious effort is made to use papers available in the literature for examples. It is felt that in this way the student is given a better feeling that these are indeed relevant problems of current research interest. In addition the point of view is made as broad as possible. Table II includes representative suggested references. Currently lecture notes are also distributed to the student to provide a unifying summary of the literature.

BECAUSE OF THE importance of partial differential equation models in chemical engineering an attempt is made to spend nearly half a semester on distributed systems. The nature of distributed systems dictates that examples from research papers be used much more than general analysis. In contrast to lumped systems there are no adequate textbooks available with a systematic treatment of distributed parameter systems. The use of current research papers is not only advisable but necessary.

Table II. Representative References

I. Motives and Methods
A. Himmelblau and Bischoff, *Process Analysis and Simulation;* Bird, etal, *Transport Phenomena*
B. Collins, *Mathematical Methods for Physicists and Engineers;* Amundson, *Mathematical Methods in Chemical Engineering.*

II. Lumped Parameter Eystems
A. Coughanowr and Koppel, *Process Systems Analysis and Control;* Campbell, *Process Dynamics;* Aris, *Introduction to the Analysis of Chemical Reactors.*
B. DeRusso etal, *State Variables for Engineers;* Rosenbrock, CEP 58, No. 9, 43, (1962); Lapidus and Luus, *Optimal Control of Engineering Process*
C. G. Davis, *Introduction to Nonlinear Differential and Integral Equations;* Minorsky, *Nonlinear Oscil-tions;* Douglas and Rippin, *Chem. Eng. Sci.* **21**, 305, (1966); Horn and Lin, *I/EC Proc. Des. and Dev.* 66, 21, (1967); Lasalle and Lefschetz, *Stability by Liapunov's Direct Method;* Berger and Perlmutter, *AIChE J.* 10, 233 (1964); Gurel and Lapidus, *I/EC* **61**, No. 3, 30, (1969)

III. Distributed Parameter Systems
A. Gould, *Chemical Process Control;* Koppel, Introduction to Control Theory; Courant and Hilbert, *Methods of Mathematical Physics,* vol. II, Chap. V., Taylor, *Proc. Roy, Soc.* A219, 186, (1953); Hsu and Gilbert, *AIChE J.* 8, 593, (1962); Yang, *J. Heat* Trans. **86**, 133, (1964); Carslaw and Jaeger, *Conduction of Heat in Solids*
B. Bilous and Amundson, *AICHE J.* 2, 117 (1956); Crider and Foss *AIChE J.* **14**, 77 (1968); Stermole and Larson, *I/EC Fund.* **2**, 62 (1963); Koppel, *I/EC Fund.* **1**, 131 (1962); Hart and McClure, *J. Chem. Phy.* **32**, 1501, (1959); Orcutt and Lamb, Proc. 1st IFAC Congress, vol. 4, p. 274; Wilhelm etal, *I/ES Fund.* 7, 337, (1968)
C. Rosenbrock, and Storey, *Numerical Computation for Chemical Engineers;* Paynter and Takahashi, *Trans. ASME* 78, 749 (1956); Gould, *Chemical* Process Control; Schone, Proc. 3rd IFAC Congress, p. 10, b. 1.

Dynamic distributed parameter systems are classified naturally as either hyperbolic or parabolic. Flow problems are most frequently simplified to the extent that they belong in the former class. After first looking at some simple examples of transformed solutions to distributed systems, the striking contrasts with lumped parameter results are drawn. Complex transcendental transforms, infinite series time responses, and delays are the rule rather than being nonexistent.

It is felt that a useful introduction to the types of linear responses expected from hyperbolic systems can be gained using the time domain Riemann representatives for the solution. The Rieto the adoint system of equations and serves the same function as the matrix exponential in the standard state space analysis. The analogous interpretation of the Lagrange multipliers or adjoint variables of the calculus of variations problem ties these three subjects together neatly.

Fig. 1 illustrates the utility of the Riemann representation as applied to the simple counterflow double pipe heat exchanger. The solution at any position and time $M(\zeta, \tau)$ is written as a linear functional of the initial and boundary conditions given between the points P and Q, connected with M by the characteristic lines PM and QP. The natural appearance of delays and their relation to domains of dependence and influence can be readily interpreted graphically and physically. From this, appearance of reflected waves can be easily explained. Since the responses tc all hyperbolic systems can be interpreted in terms of system waves, this conceptual aid has a great deal of utility.

Once the expected wave behavior is understood thoroughly, it is a much more straightforward task to obtain and interpret solutions for hyperbolic systems both in the time and frequency domains. Recurring resonance phenomena in frequency responses of these systems is easily explained. Methods of expanding and inverting transforms of hyperbolic systems can be tailored to the physical interpretation. Short time (high frequency) solutions emphasize the wave behavior; long time (Heaviside expansion) solutions emphasize approach to steady state and stability. Interpretation of time delays is straightforward once they are expected. The effect of time delays on stability can be readily explained on physical grounds.

Problems arising with parabolic partial differential equations are contrasted with hyperbolic, wave problems as well as lumped parameter problems. The t—z diagram of Fig. 1 can also be used to qualitatively interpret diffusion responses but with characteristics which are horizontal, corresponding to infinite wave velocities. The Riemann representation naturally reduces to the Green's function solution. No delays are encountered. For these problems also both short and long time solutions prove to be useful in interpreting the results. Typical example problems treated in parabolic systems illustrate that real systems, whether by virtue of Taylor diffusion, axial disperson or whatever means, never achieve the ideal limiting behavior of hyperbolic systems. A physical interpretation of the effect of superimposing a small amount of diffusion into a purely wave response is then given.

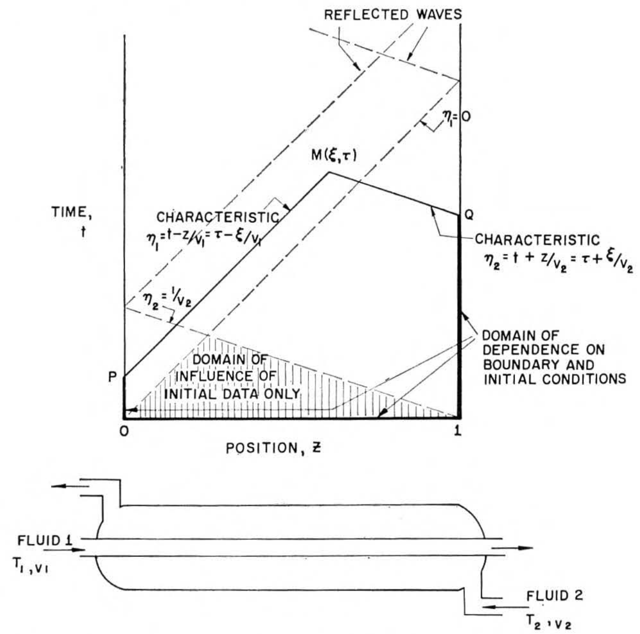

Fig. 1. Domains of dependence on initial and boundary data—double pipe heat exchanger.

The above problems all arise from linear constant coefficient distributed parameter models. Much can be said in general about variable coefficients and nonlinear problems. The former are treated by first transforming and making the change of variable to the corresponding Riccati equation. This illustrates the very real problem that although linear and transformable, distributed parameter systems do not always even yield transfer functions, let alone meaningful expressions for time responses. Several well known problems which can be solved are illustrated and discussed in terms of their peculiar characteristics. Strictly nonlinear or semilinear problems are treated in much less detail. Examples of solutions by the method of characteristics and perturbation techniques are discussed. The parametric pumping concept is a useful illustration.

In view of the general complexity of distributed parameter problems when solvable and the real possibility that some linear problems cannot be solved, approximation methods are given special emphasis here. Available techniques such as quantization, the method of moments, modal approximation, successive approximations and asymptotic approximations are all introduced. Typical sample problems are used to illustrate the low frequency applicability of the first three and the high frequency utility of the last two. The value of the approximations are judged in terms of their utility in frequency response, time response as well as the general physical interpretation of responses.

Rather than following one wag's assessment that, having lost control, one teaches process dynamics; it is useful to teach process dynamics, without control.

IN VIEW OF THE expressed intention of applying process dynamics to as broad a spectrum of applications as possible the course content is evolving gradually as better and more diverse illustrations become available. Problems given as assignments are chosen to reflect the breadth of application. To the extent possible students are permitted a wide degree of choice of examination problems and term paper topics so that special interests can be accommodated. One interested in control problems can specialize his applications just as one interested in reactor design and technology. Perhaps this breadth of interest is reflected by the following selected term paper titles: 'Noninteracting Control of Distillation Columns," "Analysis of the Filtration of a Puff of Cigarette Smoke," "Relation between Singular Perturbations and System Simplification," "Analysis of an Electro-hydraulic Valve," "Thermal Regulation in the Human Body," and "Physical Interpretation of the Oscillatory Stability Criterion in a Stirred Tank Reactor."

Process dynamics is a subject of infinite variety. Like transport phenomena it consists of a core of fundamentals applicable to diverse situations. Dynamics is not synonomous with control. "Processes" maybe interpreted as a piece of equipment in a plant, a single molecule, or the human body. The underlying principles of process dynamics are common to all applications. A combination of a unified treatment of these fundamentals and illustrative examples of applications in a range of fields is the intent of this course. Rather than following one wag's assessment that, having lost control, one teaches process dynamics; it is useful to teach process dynamics, without control.