A Course in . . .

APPLIED BIFURCATION THEORY

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Bifurcation theory deals with the solution of nonlinear equations and is useful to chemical engineers studying nonlinear phenomena. Most of the traditional courses on applied mathematics offered by chemical engineering departments cover only linear analysis. While linear analysis is necessary, since it is the foundation of all nonlinear techniques, it does not prepare students to deal with the nonlinear problems that will be encountered later in research. This is especially true for students working on stability problems in fluid flow, heat and mass transfer, catalysis, reaction engineering, control, and separations.

For many years we have sent our University of Houston students to the mathematics department for courses on differential equations and dynamical systems, bifurcation theory, nonlinear dynamics, singularity theory, and group theory. We found, however, that many of these courses were too specialized, were abstract, and had a narrow focus (from an engineer's point of view). Typically, a student had to take three or four of these courses to grasp a few useful nonlinear techniques.

To address these problems, in 1989 the author designed a new course on applied bifurcation theory as a sequel to the two-semester applied mathematics course taught by Professor Neal R. Amundson. The course was well-received by the students and was repeated in the Spring of 1991, and with some minor changes and updating is scheduled to be taught in the Spring of 1994 and regularly thereafter.

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COURSE DESCRIPTION

Introduction to Applied Bifurcation Theory

The main goal of the course is to expose chemical engineering graduate students to some important nonlinear techniques and concepts. Table 1 gives an outline of the material that is covered in a fourteen-week semester. Although the course is for 3 credits, 28 two-hour lectures are necessary to cover the topics listed in Table 1.

The course is organized into six topics and two introductory lectures. The introductory lectures give a brief history of bifurcation theory, examples from various disciplines, and the usefulness and limitations of bifurcation theory. Several chemical engineering examples covering fluid flow, heat and mass transfer, catalysis and reaction engineering, separations, control and multi-phase transport are selected as model problems and are used throughout the course to illustrate various concepts. All the examples are deterministic models and vary from the following simple (but non-trivial) two ordinary differential equation models

$$\frac{dx}{dt} = -\frac{x}{Da} + (1-x)\exp\left\{\frac{\theta}{1+\theta/\gamma}\right\} \tag{1a}$$

$$Le\frac{d\theta}{dt} = -\frac{\theta}{Da} + B(1-x)\exp\left\{\frac{\theta}{1+\theta/\gamma}\right\} - \alpha(\theta-\theta_c) \tag{1b}$$

describing the dynamic behavior of a CSTR in which a first order exothermic reaction occurs to the following, somewhat complicated, model involving a set of six partial differential equations in three spatial coordinates and time

$$\nabla\cdot\mathbf{v} = 0; \quad \nabla\Pi = -\mathbf{v} - \frac{Ra}{Pe_h} y\mathbf{e}_z \tag{2a}$$

$$\frac{\partial y}{\partial \tau} + \mathbf{v}\cdot\nabla y = \frac{1}{Pe_h}\nabla^2 y + \beta\, Da\exp\left(\frac{\gamma y}{1+y}\right)c \tag{2b}$$

$$\sigma\frac{\partial c}{\partial \tau} + \mathbf{v}\cdot\nabla c = \frac{1}{Pe_m}\nabla^2 c - Da\exp\left(\frac{\gamma y}{1+y}\right)c \quad (0 < z, r < 1, 0 < \theta < 2\pi) \tag{2c}$$

boundary conditions:

at the wall
$$\mathbf{v}\cdot\mathbf{e}_n = 0, \quad \nabla y\cdot\mathbf{e}_n = 0, \quad \nabla c\cdot\mathbf{e}_n = 0 \tag{2d}$$

at the inlet (z=0)
$$y = 0; \quad c = 1; \quad v_z = 1 \tag{2e}$$

at the exit (z=1)
$$\frac{\partial y}{\partial z} = 0; \quad \frac{\partial c}{\partial z} = 0; \quad \Pi = \Pi_1 \tag{2f}$$

describing flow maldistributions and hot spots in a down-flow cylindrical packed bed reactor. After a brief discussion of model formulation and the origins of various nonlinearities, we discuss the advantages of using the function space formalism. It is shown that most of the models can be written in the abbreviated form

$$\mathbf{C}\frac{d\mathbf{u}}{dt} = \mathbf{F}(\mathbf{u}, \mathbf{p}) \tag{3}$$

where **p** is a vector of parameters, **C** is a capacitance matrix, and the vector of state variables **u** may be expressed in terms of the elements of a function space having certain properties, *e.g.,* satisfying differentiability conditions and the appropriate boundary conditions. The function spaces of interest are usually Banach or Hilbert spaces. The capacitance matrix **C**, the parameters vector **p**, and the nonlinear operator **F** on the function space **Y** are identified for some selected examples. Some of these include cases in which **C** is not invertible (differential-algebraic systems). For example, for Eqs. (1),

$$\mathbf{C} = \begin{pmatrix} 1 & 0 \\ 0 & \mathrm{Le} \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} x(t) \\ \theta(t) \end{pmatrix}, \quad Y = \ {}^{2}, \quad \mathbf{p}^t = (\mathrm{Le}, \gamma, B, \mathrm{Da}, \alpha, \theta_c) \tag{4a}$$

and

$$\mathbf{F}(\mathbf{u}, \mathbf{p}) = \begin{pmatrix} -\dfrac{x}{\mathrm{Da}} + (1-x)\exp\left\{\dfrac{\theta}{1+\theta/\gamma}\right\} \\ -\dfrac{\theta}{\mathrm{Da}} + B(1-x)\exp\left\{\dfrac{\theta}{1+\theta/\gamma}\right\} - \alpha(\theta-\theta_c) \end{pmatrix} \tag{4b}$$

while for Eqs. (2)

$$\mathbf{C} = \begin{pmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \sigma \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} \mathbf{v}(z,r,\theta,t) \\ \Pi(z,r,\theta,t) \\ c(z,r,\theta,t) \\ y(z,r,\theta,t) \end{pmatrix}, \quad \mathbf{p}^t = (\mathrm{Ra}, \mathrm{Pe_h}, \mathrm{Pe_m}, \gamma, \beta, \mathrm{Da}, \sigma, \Pi_1, \alpha) \tag{5a}$$

$$\mathbf{F}(\mathbf{u}, \mathbf{p}) = \begin{pmatrix} \nabla\cdot\mathbf{v} \\ -\nabla\Pi - \mathbf{v} - \dfrac{\mathrm{Ra}}{\mathrm{Pe_h}} y\,\mathbf{e}_z \\ -\mathbf{v}\cdot\nabla y + \dfrac{1}{\mathrm{Pe_h}}\nabla^2 y + \beta\,\mathrm{Da}\exp\left(\dfrac{\gamma y}{1+y}\right)c \\ -\mathbf{v}\cdot\nabla c + \dfrac{1}{\mathrm{Pe_m}}\nabla^2 c - \mathrm{Da}\exp\left(\dfrac{\gamma y}{1+y}\right)c \end{pmatrix} \tag{5b}$$

TABLE 1
Course Outline for Applied Bifurcation Theory

Introduction
1. Definition and examples from different disciplines
2. Behavior of nonlinear systems; uses and limitations of bifurcation theory

Nonlinear Functional Analysis
1. Operators on Banach spaces; Fréchet derivatives
2. Contraction mapping theorem; iterative methods for nonlinear operator equations; uniqueness criteria
3. Implicit function theorem; necessary and sufficient conditions for bifurcation; determination of stationary stability boundary (Bifurcation Set)

Steady-State Bifurcation Theory
1. Liapunov-Schmidt reduction; elementary catastrophe theory
2. Singularity theory with a distinguished variable; classification of bifurcation diagrams; construction of phase diagrams
3. Effects of discrete symmetry (Z_2, D_3)
4. Shooting technique with sensitivity functions; determination of singular points of two-point boundary value problems; singular points of elliptic PDEs
5. Effects of symmetry on boundary value problems (Z_2, O(2))
   Branching equations with symmetries

Dynamical Systems
1. Invariant manifolds; Hartman-Grobman theorem; stable and center manifold theorems, applications
2. Amplitude equations; codimension 1, 2, 3 singularities
3. Poincaré-Birkhoff normal form; local codimention 1, 2 bifurcations
4. Floquet theory; degenerate Hopf bifurcations
5. Bifurcation theory for maps; normal forms of codimension one bifurcations ;attractors and basins of attraction
6. Poincaré maps; averaging method; Melnikov theory
7. Characterization of attractors ; attractor dimensions, K-entropy, L-exponents; analysis of experimental data
8. Poincaré-Bendixson theory; degree and index theory; group theory and normal forms; Hamiltonian chaos; fractals

Nonlinear Partial Differential Equations
1. Linear stability analysis of coupled PDEs
2. Center-manifold reduction of coupled PDEs; amplitude equations
3. Mode interactions; bifurcation with symmetry
4. Bifurcation in large systems (continuous spectrum); Landau and Ginzberg-Landau equations; phase and amplitude turbulence
5. Energy stability and Liapunov functions
6. Bifurcation theory for delay-differential, integral, and integro-differential equations

Nonlinear Wave Phenomena
1. Review of basic concepts; physical examples
2. Analysis of traveling waves and pulses

Computational Methods in Bifurcation Theory
1. Arc length continuation technique; continuation of steady-state and periodic branhces
2. Review of software on nonlinear dynamics and chaos

and **Y** is the space of 6-tuples of continuous functions in the variables (z,r,θ) satisfying the appropriate differentiability conditions and homogeneous boundary conditions.

Next, an overview of bifurcation theory, and its potential uses and limitations, are reviewed by a discussion of the following frequently asked questions about nonlinear models: 1) Given a nonlinear model of a physical system, what are the different types of behaviors that are possible (for different choices of the parameters vector **p**)? 2) What are the regions in the parameter space in which the behavior of a model may be described by a lower dimensional simplified model containing fewer parameters and/or a lower dimensional state space? What is the simplified form of the model? 3) How does one construct *phase diagrams* in the parameter space which classify the **p** space into regions, in each of which a different type of behavior exists? 4) How do the predicted features of a model change when it is subjected to small perturbations (or equivalently, is the model structurally stable)?

Theoretical, experimental, and computational results are presented for some model systems to illustrate each of the above four important concepts in some detail. For example, the idea of constructing a phase diagram of a mathematical model or a physical system is illustrated by using experimental results for Taylor-Couette flow[1] and theoretical results for the steady-state behavior of a CSTR.[2] It is also noted that phase diagrams for many of the model problems (including the two above) are not available.

The limitations of bifurcation theory are also discussed by emphasizing that its most important results are only local in nature and have to be supplemented by global techniques or numerical simulations (often guided by the local theory) for a comprehensive analysis of the mathematical model or physical system under consideration.

Main Topics of Applied Bifurcation Theory

We now give a brief description of the six main topics covered in the course. Before doing this, it should be pointed out that each of these topics (and most of the single lectures outlined here) is broad, has considerable literature, and finds enough applications in chemical engineering to justify a full semester course! As stated earlier, however, the purpose of this general course is to present the most important concepts and techniques in a unified manner. Due to space limitations, we must omit many details here. A longer version of this article containing details, equations, and commentary is available from the author.

Nonlinear Functional Analysis • The course starts with nonlinear functional analysis which introduces the notation and forms the basis for all later topics. First, the concept of completeness and convergence in normed linear (Banach) spaces is reviewed in a non-abstract manner. This is followed by the definition of a *Fréchet derivative* (or local linearization) of a nonlinear operator, chain rule, partial and higher-order Fréchet derivatives, and Taylor's theorem in function spaces. The model problems are used for illustration with formulas such as

$$D_{\mathbf{u}}\mathbf{F}(\mathbf{u}_o.\mathbf{p})\bullet\mathbf{v}=\frac{\partial}{\partial s}[\mathbf{F}(\mathbf{u}_o+s\mathbf{v},\mathbf{p})]\Big|_{s=0} \tag{6a}$$

$$D^2_{\mathbf{uu}}\mathbf{F}(\mathbf{u}_o,\mathbf{p})\bullet(\mathbf{v},\mathbf{w})=\frac{\partial}{\partial s_1}\frac{\partial}{\partial s_2}[\mathbf{F}(\mathbf{u}_o+s_1\mathbf{v}+s_2\mathbf{w},\mathbf{p})]\Bigg|_{s_1=s_2=0} \tag{6b}$$

for determining the Fréchet derivatives of the nonlinear operators (such as those in Eqs. 4b and 5b). Next, the concept of a nonlinear operator being a contraction is introduced and the contraction mapping theorem is stated. This theorem is used to present a proof of the implicit function theorem. The usefulness of these two main theorems of nonlinear functional analysis is shown by discussing various applications. For example, the contraction mapping theorem is used to derive convergence criteria for the iterative method

$$\mathbf{u}_{n+1}=\mathbf{N}(\mathbf{u}_n) \tag{7a}$$

as well as uniqueness criteria for the nonlinear equation

$$\mathbf{u}=\mathbf{N}(\mathbf{u}) \tag{7b}$$

where **N** is a nonlinear operator on some Banach space **Y**. Specific examples dealing with algebraic equations (lumped models of reactors with single and multiple reactions, discretized models of convection), two-point boundary value problems (diffusion-reaction and diffusion-convection-reaction models in one spatial dimension), and elliptic partial differential equations (diffusion-reaction models in 2/3 dimensions) are discussed. The implicit function theorem is supplemented by stating sufficient conditions for bifurcation and the form of the bifurcating solution in terms of the eigenfunctions of the linearized operator. Application of the implicit function theorem is illustrated by deriving the stationary stability boundaries for various physical systems such as the CSTR with single and multiple reactions, classical Rayleigh-Bénard and Lapwood convection problems, and the Brusselator model for stationary patterns.

Some lecture material on nonlinear functional analysis is taken from references 3 through 5 and 'translated' by the author into the engineer's language.

Steady-State Bifurcation Theory • The second topic of the course, steady-state bifurcation theory, is introduced by discussing the idea of reducing the dimensionality of a problem, also known as the elimination of passive modes (engineering), or the slaving principle (physics), or the Liapunov-

Schmidt reduction (mathematics). This is followed by a discussion of the branching equations and their Taylor expansions for finite dimensional problems and then is extended to infinite dimensional problems (Fredholm operators of index zero). For example, for the case of a single state variable bifurcation problem (characterized by dim ker $\mathbf{D_u F}(\mathbf{u}_o,\mathbf{p}) = 1$), the branching equation is shown to be

$$g(x,\mathbf{p}) = \langle \mathbf{v}_1, \mathbf{F}(x\mathbf{y}_1 + \mathbf{W}(x\mathbf{y}_1,\mathbf{p}),\mathbf{p})\rangle \tag{8a}$$

where x is a scalar state variable (projection of the solution onto ker $\mathbf{L}^*$), and $\mathbf{y}_1,\mathbf{v}_1$ are the eigenfunctions corresponding to the zero eigenvalue of $\mathbf{L} = \mathbf{D_u F}(\mathbf{u}_o,\mathbf{p})$ and $\mathbf{L}^*$ (adjoint operator), respectively. The function $\mathbf{W}(x\mathbf{y}_1,\mathbf{p})$ containing the slave variables (modes) is defined by the implicit equation

$$(\mathbf{I}-\mathbf{E})\mathbf{F}(x\mathbf{y}_1 + \mathbf{W}(x\mathbf{y}_1,\mathbf{p}),\mathbf{p}) = 0 \tag{8b}$$

where $\mathbf{E}$ is the projection operator onto the range of $\mathbf{L}$. Next, the main ideas of elementary catastrophe theory, such as *determinacy, transversality,* and *unfolding* are discussed, and Thom's classification and unfolding theorem is stated. The geometry of the elementary catastrophes (fold, cusp, swallowtail, butterfly, wigwam, and star) with the normal form

$$G(x,\varepsilon) = x^k - \sum_{i=0}^{k-2} \varepsilon_{i+1} x^i \qquad (k = 2,3,4,5,6,7) \tag{9}$$

and their bifurcation sets in the ε-space is discussed along with applications to lumped models of reactors and equations of state in classical thermodynamics.

The next lecture introduces singularity theory with a distinguished variable. First, the distinction between elementary catastrophe theory and singularity theory with a distinguished parameter is explained. For example, it is noted that the behavior of most physical systems is observed by measuring their response as a function of a distinguished physical parameter or variable (such as residence time, inlet temperature, etc.). In order to determine the different types of responses (bifurcation diagrams), it is necessary to rewrite the branching equation as

$$g(x,\lambda,\mathbf{p}^*) = 0 \tag{10}$$

where λ is the distinguished physical parameter and $\mathbf{p}^*$ is the vector of other parameters that are independent of λ. Next, the concepts of *contact equivalence, unfolding,* and *normal form* are discussed, along with a list of defining and nondegeneracy conditions for singularities up to codimension three. The different types of bifurcation diagrams that exist next to singularities of codimension one (hysteresis, isola, and double limit), codimension two (pitchfork), and codimension three (winged cusp) are reviewed. This is followed by a discussion of the method of constructing phase diagrams that divide the parameter space into regions with different types of bifurcation diagrams. The appearance and disappearance of solutions at the boundaries of the state variables and/or parameters is also discussed. The usefulness of the theory is illustrated by application to lumped models of chemical reactors.

The third lecture on steady-state bifurcation theory introduces the effects of symmetry. The occurrence of discrete symmetry is illustrated by giving physical examples with reflectional or Z_2 symmetry (two coupled identical cells and discretized models of convection) and permutational or D_3 symmetry (three coupled identical cells). Next, some important concepts of finite group theory such as *subgroup, group isomorphism, orthogonal representation,* and *irreducible representation* are discussed. The importance of these concepts is illustrated by discussing the invariance properties of kernel and range of $\mathbf{L}$ under the action of the group and the structure of the branching equations in the presence of these symmetries. This is followed by a statement of Thom's classification theorem for singularities with Z_2 symmetry and the geometry of the elementary catastrophes with this symmetry. The dihedral symmetry (D_3) is discussed, using the example of three coupled cells (simplest example where symmetry forces repeated eigenvalues).

The next lecture deals with the bifurcation analysis of two-point boundary value problems. First, it is shown that the Liapunov-Schmidt reduction for many nonlinear two-point boundary value problems (such as diffusion-reaction, convection-reaction, and diffusion-convection-reaction models in one spatial dimension) can easily be accomplished by using the shooting technique and sensitivity functions. The usefulness of this method is illustrated by deriving stability criteria (cusp locus) for the catalyst particle and the tubular autothermal reactor models. As the shooting technique is not applicable in higher dimensions, a procedure is presented for the determination of singular points of elliptic boundary value problems of the form

$$\mathbf{Lu} + \mathbf{N}(\mathbf{u},\mathbf{p}) = \mathbf{0} \quad \text{in } \Omega \quad (\mathbf{u} = \mathbf{0} \text{ on } \partial\Omega \text{ or } \nabla\mathbf{u}.\mathbf{n} = 0 \text{ on } \partial\Omega) \tag{11}$$

where $\mathbf{L}$ has discrete spectrum with M zero eigenvalues, and $\mathbf{N}(\mathbf{u},\mathbf{p})$ is quadratic or higher order in $\mathbf{u}$. This problem is also used to illustrate the equivalence of the two main approaches to bifurcation theory, namely the Liapunov-Schmidt reduction and the perturbation (multi-scale) approach of Iooss and Joseph[6] using the Fredholm Alternative. The physical examples we discuss include problems of diffusion-reaction and diffusion-convection-reaction in higher dimensions consisting of a single or a pair of nonlinear elliptic partial differential equations with either Dirichlet, Neumann, or Robin boundary conditions.

The last lecture on steady-state bifurcation theory deals with the presence of symmetries in boundary value problems. First, examples of problems with reflectional (Z_2) and rotational symmetry ($O(2)$) are given (reaction-diffusion equations in a disk, ring, or line with Dirichlet or Neumann boundary conditions, problems of flow in pipes as well as artificially imposed periodic boundary conditions on physical systems). The presence of hidden symmetries (in the boundary conditions) is also illustrated. Next, the derivation of branching equations in the presence of Z_2 symmetry with single and double zero eigenvalue and O(2) symmetry with single (repeated) and double (repeated) zero eigenvalue is discussed. The occurrence of these bifurcations and the local bifurcation picture is illustrated by application to the buckling of a rectangular plate and the Brusselator model of pattern formation on a line and on a circular disk.

The lecture material on steady state bifurcation theory is taken from references 6 through 19, the author's thesis,[2] research publications, and notes.

Dynamical Systems • The third major topic, for which more than a quarter of the course is devoted, is bifurcation theory for ordinary differential equations. It begins with a review of the concept of asymptotic stability, the properties of hyperbolic fixed points, and the invariance of the generalized eigenspaces of the linear system with constant coefficients ($d\mathbf{u}/dt = \mathbf{Lu}$). This is followed by the linearization theorem of Hartman and Grobman for the local behavior of the nonlinear system

$$\mathbf{C}\frac{d\mathbf{u}}{dt} = \mathbf{Lu}+\mathbf{N}(\mathbf{u},\mathbf{p}); \quad \mathbf{N}(\mathbf{0},\mathbf{p})=\mathbf{D_u N}(\mathbf{0},\mathbf{p})=0 \quad \mathbf{u}\in\mathbf{Y}\subseteq R^n \qquad (12)$$

and the stable manifold theorem for a fixed point. Next, the slaving principle is explained in terms of the time scales (eigenvalues) associated with the eigenmodes and the Center Manifold theorem is stated. The usefulness of the Center Manifold theorem as a rigorous perturbation technique (that includes the classical regular perturbation/multiple-scale techniques) is illustrated by considering a two-phase model of a packed bed and deriving conditions under which it could be reduced to a single phase (pseudohomogeneous) model and the resulting model to infinite order!

The second lecture focuses on the application of Center Manifold theorem to reduce the dimension of the bifurcation problem defined by Eq. (12). First, a general procedure for determining the amplitude equations when **L** has r eigenvalues on the imaginary axis is presented (the nonlinear functional analysis and the notation are helpful in doing this in a compact manner). Specific results for the case of single zero eigenvalue, two and three zero eigenvalues, a pair of imaginary eigenvalues, and zero plus a pair of imaginary eigenvalues is presented. (Students are encouraged to verify and extend some of these formulas using symbolic manipulation.) For example, when a trivial solution exists for all values of the parameters vector **p** and there is a single zero eigenvalue at $\mathbf{p}_o$, it is shown that the amplitude equation to cubic order is given by

$$\frac{da_1}{dt} = a_i\left(\sum_{i=1}^{M} A_i\lambda_i\right) + Ba_1^2 + Ca_1^3 \qquad (13)$$

where $\lambda_i = p_i - p_{i0}$ (i=1,...,M) are the components of the parameters vector and p_{i0} are the parameter values at which there is a simple zero eigenvalue. The coefficients A_i, B, and C can be expressed in terms of some inner products involving the eigenvectors and adjoint eigenvectors of the linearized problem and higher order Fréchet derivatives of the function $\mathbf{F}(\mathbf{u},\mathbf{p})$.

The third topic of discussion is normal form theory, or equivalently, the transformation of the amplitude equations into their simplest form. First, it is shown that the calculation of the normal form of a set of amplitude equations involves near identity transformations and the solution of certain linear equations in polynomial vector spaces. Next, the normal forms (along with their universal unfoldings) are presented for some codimension one bifurcations (saddle-node and Hopf) and codimension two bifurcations (Takens-Bogdanov, zero, and a pair of imaginary eigenvalues and two pairs of imaginary eigenvalues) followed by a discussion of the local bifurcation behavior next to these singularities and the construction of phase diagrams in the unfolding parameter space. The application of the center manifold and normal form theories is illustrated using lumped models of chemical reactors (CSTR with single and multiple reactions) and discretized models of convection (Lorenz model and the five equation models of thermohaline and binary convection).

The fourth topic of discussion is Floquet theory and degenerate Hopf bifurcations. First, the general theory of linear systems with periodic coefficients, the method of calculation of the monodromy matrix, and the Floquet multipliers are reviewed. Next, the main theorem that gives the stability of the periodic solution in terms of the Floquet multipliers is stated. The two main degeneracies that may occur when Hopf's hypotheses break down are stated (coalescence of two Hopf points and the vanishing of the cubic coefficient in the normal form). The method of determining periodic solutions by analyzing the zeros of a nonlinear operator defined on the space of 2π-periodic functions is discussed. The Fitzhugh-Nagumo equations for nerve impulse, the Glycolytic model for oscillations, the Gray-Scott isothermal autocatalysis model, and the CSTR model are used for illustrating the construction of phase diagrams in the parameter space.

The next lecture is devoted to discrete dynamical systems. As in the case of continuous systems, the properties of hyperbolic fixed points and invariance of the generalized eigenspaces of the linear discrete system with constant coefficients ($\mathbf{u}_{k+1} = \mathbf{Au}_k$) are reviewed. This is followed by the stable and center manifold theorems for the local behavior of the nonlinear system

$$\mathbf{u}_{k+1} = \mathbf{F}(\mathbf{u}_k,\mathbf{p}) = \mathbf{Au}_k + \mathbf{N}(\mathbf{u}_k,\mathbf{p}); \quad \mathbf{N}(\mathbf{0},\mathbf{p}) = \mathbf{D_u N}(\mathbf{0},\mathbf{p}) = 0 \qquad (14)$$

The calculation of the amplitude equations and the normal forms for codimension one bifurcations (saddle-node, transcritical, pitchfork, period doubling, and Naimark-Sacker) are illustrated. The different types of attractors (fixed points, periodic attractors, invariant circles, and strange attractors) of discrete dynamical systems, the types of bifurcations that occur, the basins of attraction, and the fractal nature of the basin boundaries are illustrated using classical examples such as the logistic map, the delayed logistic map, the Hénon map, and the complex Newton iteration method for determining the fourth roots of unity.

The sixth lecture on dynamical systems is devoted to Poincaré maps, averaging methods, and Melnikov theory. First, the reduction of a continuous dynamical system to a discrete one through the Poincaré map and the method of construction of this map for three specific cases (near a periodic orbit, near a homoclinic orbit, and for a forced periodic system) as well as in the general case (using the method of Hénon) is illustrated. Next, the averaging theorem is used to obtain the Poincaré map for periodically forced dynamical systems using the forced Duffing equation as an example. At this stage, the dynamics of two-dimensional maps near homoclinic points is explained intuitively and the Melnikov method is presented for detecting the transverse homoclinic points. Chemical engineering examples discussed include periodically forced reactors and the dynamics of a gas bubble in a viscous liquid with periodic pressure variations.

The next lecture deals with the routes to chaos, definition and characterization of attractors, and the treatment of experimental data. First, the differences between the flows of conservative and dissipative dynamical systems is reviewed. Next, a strange attractor is defined and the three well-known routes to chaos are illustrated using the example of two coupled cells with the Brusselator kinetic scheme. Different methods for the analysis of experimentally (or numerically) generated time series are discussed. The calculation of attractor dimensions (using the method of Grassberger and Procaccia), Kolmogorov entropy, Liapunov exponents, and power spectra (using FFT) is illustrated with examples.

The last lecture on dynamical systems is a survey of various topics such as the global theory (Poincaré-Bendixson) of dynamical systems in the plane, degree and index theory, use of group theory to calculate normal forms, Hamiltonian chaos, and fractals. The lecture material on dynamical systems is taken from references 20 through 31 and research articles in *Physica D*. Examples and applications are taken from the author's notes.

Nonlinear Partial Differential Equations • The fourth major topic of the course is bifurcation theory for nonlinear partial differential equations. This topic is introduced with the method of linearization of Eq. (3) around some base state ($\mathbf{u}_o$), the solution of the system of linear partial differential equations

$$\mathbf{C}\frac{d\mathbf{v}}{dt} = \mathbf{L}\mathbf{v} = D_{\mathbf{u}}F(\mathbf{u}_o)\mathbf{v} \qquad (15)$$

and the properties of the eigenvalue problem ($\mathbf{L}\mathbf{y}=\mu\mathbf{C}\mathbf{y}$) and the adjoint eigenvalue problem $\left(\mathbf{L}^{*}\mathbf{v}=\bar{\mu}\mathbf{C}^{*}\mathbf{v}\right)$. Next, the two main theorems stating the necessary and sufficient conditions for simple and Hopf bifurcations are presented. Applications of the theorems are illustrated by physical examples such as Taylor-Couette flow, Rayleigh-Benard convection (principles of exchange of stabilities), Lapwood convection, and pattern formation on a catalytic disk (stationary/oscillating patterns).

The second lecture deals with the application of center manifold theory to partial differential operators in finite domains (discrete spectrum). Center manifold reduction of a system of PDEs and the derivation of the amplitude equations for M eigenvalues on the imaginary axis are illustrated. (The unified notation is again helpful as the same formulas are applicable for finite as well as for infinite dimensional problems, the only difference being in the summations.) The reduction of the Navier-Stokes equations for pipe and plane Poiseuille flows to an infinite set of coupled quadratic ODEs and the computation of the coefficients of the linear and quadratic terms in the amplitude equations are illustrated. Once again, the usefulness of the center manifold theorem as a generalized perturbation technique is shown by discussing a classical chemical engineering problem (Taylor-Aris dispersion) from a new perspective. (This example was taken from the joint work of the author with Professor Chia Chang, University of Notre Dame.)

The third topic of discussion is mode interactions in the presence of symmetries. The derivation of amplitude equations in the presence of two zero eigenvalues with Z_2 symmetry and two zero eigenvalues (repeated) and a pair of imaginary eigenvalues (repeated) with O(2) symmetry is illustrated along with the local bifurcation diagrams. The physical examples discussed include the problems of flow maldistributions in packed beds, reaction driven convection in a rectangular box, and stationary and moving temperature patterns on a circular catalytic disk.

The fourth lecture is devoted to the case of continuous spectrum (bifurcation in large systems). Here, the multiple scale perturbation technique combined with the Fredholm Alternative is used to derive the Landau (or the nonlinear heat) equation

$$\frac{\partial U}{\partial t} = \nabla^2 U + aU - bU^3 \quad (\text{a,b real, U = real amplitude}) \qquad (16)$$

for the case of continuous spectrum crossing the imaginary axis at zero and the Ginzburg-Landau (or the Newell-Whitehead-Segal) equation

$$\frac{\partial U}{\partial t} = U + (1+i\alpha)\nabla^2 U - (1+i\beta)|U|^2 U; \quad \left(\alpha,\beta \text{ real}, U = \begin{matrix}\text{complex}\\ \text{amplitude}\end{matrix}\right) \qquad (17)$$

for the case of complex continuous spectrum crossing the imaginary axis. The spatio-temporal patterns predicted by these equations and the concepts of phase and amplitude turbulence are briefly discussed.

The fifth lecture on PDEs is devoted to global techniques such as Liapunov functions and energy stability theory. The classical Bénard problem is used to determine the stability boundary of the conduction state to finite perturbations (which coincides with the linear stability boundary). The example of through-flow in a porous medium is also used to illustrate the possibility of subcritical bifurcations predicted by energy stability theory. Finally, the construction of Liapunov functions is illustrated for some finite and infinite dimensional problems.

The last lecture is concerned with delay-differential, integral, and integro-differential equations (a topic that has applications in many areas of chemical engineering but is often ignored). The three examples include a system with time delay (Glass-Mackey model), a Fredholm integral equation of first kind with a symmetric kernel describing a diffusion-reaction problem, and an integro-differential equation describing the dynamics of a catalyst particle (with uniform internal temperature but non-uniform concentration gradients). These models show simple and Hopf bifurcations, period doubling, and chaotic behavior. For some of these cases, the local theory to compute the normal form is outlined.

The lecture material and examples on this topic are taken from References 10, 15, and 32 through 36, *Physica D,* and the author's research articles.

Nonlinear Waves • The fifth topic is nonlinear waves. Since the students are familiar with linear and hyperbolic (shock) waves covered in the applied mathematics course, some important concepts (such as phase velocity, group velocity, dispersion, and front steepening) are reviewed. Next, two chemical engineering examples (waves on a falling film and temperature waves on a catalytic wire or ribbon) are presented and some model wave equations, such as the long wave equation and the generalized Fisher's equation

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} + f(u, \mathbf{p}) \tag{18}$$

are derived. The rest of the discussion is concerned with the wave properties of Eq. (18) and the nonlinear partial differential equation

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \nu\frac{\partial^2 u}{\partial x^2} + \mu\frac{\partial^3 u}{\partial x^3} + \lambda\frac{\partial^4 u}{\partial x^4} = 0 \tag{19}$$

which includes as special cases some of the most widely studied equations, such as the Burger's equation ($\mu = 0$, $\lambda = 0$), the Korteweg-de Vries equation ($\nu = 0$, $\lambda = 0$), and the Kuramoto-Sivashinsky equation ($\mu = 0$). Substituting the traveling wave assumption

$$u(x,t) = h(z), \qquad z = x - ct \tag{20}$$

reduces Eq. (18) to a set of two ODEs (which can be analyzed by phase plane techniques) and Eq. (19) to a set of three ODEs which exhibit periodic, quasiperiodic, and chaotic solutions. The physical interpretation of these solutions as well as the variation of the wave speed with the parameters of the system are discussed.

The lecture material for this topic is taken from references 37 and 38, along with the author's notes.

Computational Methods • The last two lectures are devoted to computational methods in bifurcation theory. First, the arc length continuation technique as described by Kubicek and Marek[39] is presented. This is followed by a review of the software (such as DERPAR, AUTO2, etc.) for the continuation of steady-state and periodic branches. The recent software package KAOS of Kim and Guckenheimer is also reviewed and used by some students. It is also noted that there are very few algorithms available for computing bifurcation branches in the presence of symmetries. The lecture material for this topic is taken from references 39 and 40.

STUDENT PERFORMANCE

A set of fifty homework problems are given to the students after the introductory lectures and the students are asked to attempt five of them and submit a written report on one problem. More than half of these problems are open-ended and challenge the students (four of the problems later became topics of the students' PhD dissertations and led to several refereed publications).

A combined total of twenty-four students took the course for credit (and many others audited). In general, the students fell into two groups: those who were doing either experimental or theoretical research on nonlinear systems, and those who took the course to complete their graduate course requirements. The second group of students attempted straightforward homework problems such as computing the attractor dimensions or extending the Liapunov-Schmidt/Center Manifold calculations using symbolic manipulation. The first group of students attempted open-ended problems, but their solutions were incomplete (some were completed a few years later).

CONCLUSIONS

Linear analysis played a key role in the development of applied sciences during the nineteenth and first-half of the twentieth century. It is believed that nonlinear analysis combined with the power of the computer will play a similar role in the next century. The local nonlinear techniques of bifurcation theory extend the traditional linear analysis and are essential in the development of algorithms for computation. They also guide the search for solutions of nonlinear systems in multidimensional parameter spaces. The computer experiments play a complementary role and extend and validate the local theory as well as lead to new and unexpected results (such as the discovery of the soliton). It is the author's opinion that some analysis and computational experience with nonlinear systems should be part of a standard training program for all graduate chemical engineers.

ACKNOWLEDGMENTS

The author is indebted to Professors Martin Golubitsky and Giles Auchmuty of the mathematics department at the University of Houston, with whom he has had many discussions on singularity, bifurcation, and group theories. This article was written while the author was on sabbatical leave at the University of Minnesota.

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ChE *book review*

ELEMENTS OF CHEMICAL REACTION ENGINEERING:

2nd Edition

by *H. Scott Fogler*
Prentice Hall, Englewood Cliffs, NJ (1992)

Reviewed by
P. R. Westmoreland
University of Massachusetts

The second edition of this text already comes about as close to universal usage as a chemical engineering text can, including wide international use in addition to 108 schools (in a recent count) in the U.S. It is not as well suited for graduate study, but (as far as I am concerned) it is the best undergraduate reaction engineering text available, based on its content, structure, and wide variety of good problems.

This edition, like the first edition did, covers the necessary subject territory of reaction engineering within its fourteen chapters:

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