ChE book reviews

Mathematical Methods of Chemical Engineering. Vol. 3. Process Modeling Estimation and Identification.
By J. H. Seinfeld and L. Lapidus.
Prentice-Hall, 545 pages.

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Any topic in applied mathematics which has attained reasonable maturity will have acquired a considerable primary and secondary literature into which the engineer must dig in his efforts to master its methods. But, if his first steps may seem simple, like those of the descent to Avernus, the task of really penetrating the subject and winning his way back again to the daylight is, as Virgil says, another story—'hoc opus, hic labor est'. Hence the peculiar value of reliable guides to that nether world of mathematical ideas that lies at the foundation of our profession and provides the basis for understanding of chemical processes. Lest it seem ambiguous to commend one's friends as guides to the underworld, I hasten to add that they are no flunkeys of the tourist industry but members of that select company of erudite guides of which Virgil himself is the best known. For this book will not yield much to the casual reader who thinks he can breeze through it with half his attention, but will be found invaluable by the serious student who wants to understand the modern theory of estimation and identification.

In stressing these, the second and third divisions of the book, I am not overlooking the early discussion of modeling and Laplace transform. A brief introductory chapter leads to a discussion of the types of equation that are of value in modeling chemical processes. The emphasis here is not on illustrating the details of actual derivations, but on the rationale of model building and the types of system that arise and their inter-relations. This is followed by an excellent survey of the Laplace transform which includes both the discrete z-transform and a treatment of the numerical inversion.

There are of course many books available on the Laplace transform and several on modeling, though the treatment here is admirably clear, but what makes this book uniquely valuable is the subsequent discussion of stochastic models, estimation theory and process identification. This covers

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the passage of matter. If open systems are considered, the energy flow associated with the flow of matter must be added to each energy definition, *i.e.* $dE = TdS - PdV + \Sigma\mu_i dn_i$, where μ_i is the chemical potential of species i and dn_i is the change in the number of moles of species i in the system. Note that E is related to extensive measures of the system. We can speak of molar entropy, molar volume, and number of moles in the extensive measures. The enthalpy change has one less extensive change in its definition, replacing the —PdV used in dE with VdP. Similarly, dA has one intensive change in its definition, while dG has two intensive changes, VdP and —SdT.

The intensive counterpart of $\Sigma\mu_i dn_i$ is $-\Sigma n_i d\mu_i$, and if we draw a second diamond for energy relations in which the intensive term $-\Sigma n_i d\mu_i$ is used, we replace the pointer terms, dE, dH, dA, dG, with new energy variables d(TS—PV), d(TS), d(—PV), and O (the last not being a definition). Gangi, Lamping, and Eubank elaborate on the relations involving this side of the diamond and have a copyrighted design, called a THERMODORM, to illustrate them. The definition of d(TS —PV) involves one intensive term; those of d(TS) and d(—PV) involve two.

Additional relations may be developed if heat capacities are related to entropy, if electromotive force is related to Gibbs free energy, or if equilibrium constants are related to Gibbs free energy. The reader is encouraged to elaborate these as an exercise. The frequent use of $\Delta H - T\Delta S$ in place of ΔG for processes ocurring at constant temperature and pressure may be understood in terms of the diamond. At constant T and P we have simply $dG = \Sigma\mu_i dn_i$, which is what d Hwould be at constant pressure if we subtracted out the TdS term.

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TEMPERATURE PREDICTION: Finger et. al.

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$A = A'(M)/K_s$
A' = pre-exponential kinetic constant
$B = E/R_g$
c = oxygen concentration, moles/liter
$D = \frac{AL^2}{cD}$
$D = \frac{AH\,X_o\,L^2}{k(T_m - T_o)}$
$D' = \ln D$
D = diffusivity of oxygen
E = activation energy
H = heat of reaction (per unit of 0_2 consumed)
k = thermal diffusivity
K_s = Michaelis constant
L = thickness of decomposing mass
(M) = concentration of microorganisms
N_i = molar flux of species i
R = rate of substrate decomposition
R_g = universal gas constant
T = temperature, °K
T_m = maximum anticipated temperature
T_o = minimum anticipated temperature
$T^* = T/(T_m - T_o)$
$T^*|_o$ = value of T^* at $y^* = 0$
μ = specific growth rate of microorganisms
μ_{max} = maximum specific growth rate of microorganisms
X = oxygen concentration, mole fraction
X_o = oxygen concentration in the atmosphere
$X^* = X/X_o$
$X^*|_o$ = value of X^* at $y^* = 0$
y = distance from center of the decomposing mass
$y^* = y/L$

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some areas of comparatively recent development and there is no other reference where a useful introduction can be found in one place. This demands an introduction to probability theory which is provided in chapter 4 where the concept of the random variable and its characterisation is carefully explained. Next comes a discussion of stochastic processes, their description and governing equations. Of particular value here is the explanation of the differences between the calculus of Ito and that of Stratonovich. The sixth chapter on the theory of residence time distributions discovers a habitat where the behavior of both deterministic and stochastic models can be observed.

The remainder of the book is devoted to parameter estimation and process identification, the former being the appropriate task when the structure of the model is fully known, the latter when it is unknown. In both cases there is a natural distinction between linearity and nonlinearity with a simpler set of methods for the linear. In the estimation problem, algebraic, differential equation and stochastic models are discussed, as are frequency domain, moment, gradient and search methods. There follows a valuable chapter on the design of experiments in the light of the estimation problem.

In introducing the subject of the realization of systems for which the structure of the model is unknown the dual concepts of controllability and observability are first explained and some specific algorithms are then developed. The final chapter is on process identification of nonlinear systems, a problem of peculiar difficulty which brings the student near to the frontier of the subject.

For anyone giving a course in methods of process analysis at a graduate level this book will provide a splendid text, while, for the student wanting to study the subject on his own, its organization and clarity make it equally useful. Altogether it is one of the best books in the Prentice-Hall Series in the Physical and Chemical Engineering Sciences.