

explanations do not have the complete agreement of the polymer science community or the majority of the membrane community.

Finally and perhaps most disappointing was the incomplete discussion of the processing involved in forming the so-called prism α membrane or other competitive gas separation membranes. Indeed, since both of the authors know the details of such processes intimately they could have offered a wealth of details on what is done and why it is done in the actual spinning, drying and post treatment of these membranes. I would have found this "how to" discussion more useful than the highly speculative explanations of the effects of the process on the substrate and skin morphology. I had expected that this book would be the "inside story" of how the membranes are really made with some treatment of the considerable art involved in formulating dopes and balancing the processing variables to arrive at the graded density morphology that characterizes the prism α structure. It does not do this.

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Fluctuational Effects in the Dynamics of Liquid Crystals

By E. I. Kats and V. V. Lebedev, Springer-Verlag, New York, 1994, 170 pp.

This is a highly specialized monograph dealing with the fluctuation dynamics of liquid crystalline systems about their equilibrium state. Although primarily a book written for theoretical physicists by theoretical physicists, it may have limited appeal to the chemical engineering community as well.

The authors focus very narrowly on the near-equilibrium dynamics of nematic, smectic, columnar and chiral liquid crystalline phases. They discuss these phases only very briefly; a much more detailed introduction to liquid crystals is contained in the recently revised text by de Gennes and Prost (*The Physics of Liquid Crystals*, 2nd ed., Oxford, New York, 1993). However, Kats and Lebedev take great care in setting up the governing fluctuating hydrodynamic equations, discussing both the derivation of the re-

versible terms arising from Poisson brackets and the irreversible terms involving transport coefficients. This presentation is somewhat more detailed than the corresponding material in de Gennes' and Prost's text, but is not as elegant as in the classic article by Martin et al. (*Physical Review A* 6, 2401, 1972).

After setting up the appropriate continuum description for each type of liquid crystal phase, the authors embark on a very careful analysis of fluctuation effects. In particular, they discuss the role of fluctuations in renormalizing the elastic constants and the linearized transport coefficients, such as the various viscosities that characterize liquid crystalline phases. A nice feature of the monograph is that all of these different phases are treated within the same theoretical framework. The formalism, however, is a bit heavy at times. The authors adopt the functional integral representation of stochastic dynamics due to de Dominicis and Janssen, but have a nonstandard way of dealing with the functional Jacobian that enters the theory and preserves causality. In my opinion, the use of Fermi fields and associated Grassmann algebra to represent the Jacobian is a bit of an overkill for the problem at hand.

I suspect that the technical details of this monograph may be inaccessible to many chemical engineers. In particular, there are probably very few engineers with a sufficient background in quantum field theory to fully appreciate the calculations outlined in this book. Nevertheless, the conclusions are potentially of importance to engineers: thermally excited fluctuations in liquid crystalline systems can lead to unusual linear elastic and dissipative properties. For example, if one is to understand why certain of the viscosity coefficients of smectics are larger than others, these fluctuation effects must be considered. On the other hand, engineers are often concerned with the processing of liquid crystalline materials under conditions where nonlinear rheological behavior is the norm. The text makes no attempt to address such far-from-equilibrium dynamical behavior.

Overall, I strongly recommend this monograph for that rare engineer who has a strong background in theoretical physics and who needs to understand in detail the linear response properties of liquid crystalline systems. Chemical engineers not in this category will probably

benefit more from the broad coverage in the text of de Gennes and Prost or from a rheology text that has some discussion of liquid crystalline systems, such as that of Larson (*Constitutive Equations for Polymer Melts and Solutions*, Butterworths, Stoneham, MA, 1988).

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Reduced Kinetic Mechanisms for Applications in Combustion Systems

Edited by N. Peters and B. Rogg, Springer-Verlag, New York, Lecture Notes in Physics, Monograph 15, 1993, 360 pp.

This monograph describes the status of a reaction-engineering approach developed almost solely by mechanical engineers: reducing large sets of elementary reactions into minimum sets of species and global combustion reactions. Almost no chemical engineers work in this specific area, even though many chemical engineers are active in combustion research (e.g., four sessions at the 1994 AIChE Annual Meeting). On the other hand, the approach is relevant to chemical processes from steam cracking to plasma processing to catalysis.

A survey of the technique and its applications is reported, growing out of a series of mechanism-reduction workshops beginning in 1987. Contributors started with a common 87-reaction set for gas-phase combustion of C_1 to C_3 hydrocarbons and methanol. (Note that "mechanism" is used in this context to mean the set of reactions, not a specific sequence of steps by which an overall reaction takes place.)

The book first describes this reaction set, the transport models, and laminar flame-speed data for comparisons. Then, it divides its cases by separately considering simple premixed flames and counterflow diffusion flames. For each flame type, mechanisms are reduced and calculations are analyzed for fuels of increasing complexity— H_2 , H_2/CO , CH_4 , C_2H_6 , C_2H_4 , C_2H_2 , C_3H_8 , and CH_3OH . NO_x chemistry is also considered briefly.

The methods are like those used in developing Lindemann, Langmuir-Hinshelwood-Hougen-Watson, Monod, or Michaelis-Menten rate expressions. A

"complete" set of elementary reactions is assembled. The species conservation equations can then be expressed as $L(x_i) = r_i$. Here, L is an operator combining accumulation, convection, and diffusion terms for the species i of mole fraction x_i , and r_i is the net rate of formation from all reactions involving this species. The number of linearly independent global reactions is initially $N = N_{\text{species}} - N_{\text{elements}}$. This number is further reduced by the number of species treated as being at steady state, and their concentrations are derived by setting $L(x_{i,ss}) = 0$.

Most of the method's difficulties come from this application of the pseudo-steady-state hypothesis. The steady-state expressions may easily be too nonlinear or too complex to be solved directly. Terms can be dropped if unimportant for a particular species, and equilibrium constants can be used to give some additional relations if "partial equilibrium" (dynamic equilibrium for a given reaction) can be established. Also, a species may remain acceptably at steady state but be high enough in mass fraction that the mass defect must be corrected.

Results are generally impressive. Predictions by the large set are closely reproduced with two to nine global reactions. Such reduced mechanisms make computational fluid mechanics with real chemistry feasible, just as power-law kinetics makes stability analysis of CSTRs manageable.

Reaction engineering is full of such useful approximations. For example, consider unimolecular reactions, first-order catalytic kinetics, perfectly stirred reactors, and plug-flow reactors.

Like these other approaches, however,

the global reactions can be misapplied. The reason that simple flames are explored is to try to establish conditions where the approximations hold. Also, reduced mechanisms rely crucially on the full sets being accurate, as the authors note. For several cases in the book, mistakes in the basis set of kinetics seem to be the obvious causes of misprediction.

Really large numbers of reactions, such as for burning gasoline or cracking naphthas, might make the procedure more troublesome than it is worth. Other approaches like structure-oriented lumping are very promising for such problems. Happily, though, many chemical processes convert relatively simple feeds. The book provides a helpful entry point for chemical engineers to understand this potentially useful approach.

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The Design of Drugs to Macromolecular Targets

Edited by C. R. Beddell

This book contains eight chapters which, in the words of the editor "... stand independently, but they are ordered to provide a logical progression from consideration of "The Role of Macromolecules in Drug Action" through the physicochemical principles ... to experimental studies ... " They are all focused strongly on the title subject of drug design or interaction of various molecules with active sites on enzymes,

proteins, and so on. Thus, for most chemical engineers this book would only be of general interest in seeing how this relatively well developed area could be applied to other types of catalytic sites in chemical processing. Of course, bioengineers possibly could find more specific applications.

After the first two general chapters, except for the final chapter which describes QSAR (quantitative structure activity relationships), the remaining chapters focus on specific examples of how molecular calculations and knowledge of structure can be utilized to gain exceptional basic understanding of the drug-active site interactions and what this means for drug action. Chapter 3 considers binding to hemoglobin, Chapter 4 is concerned mostly with the well studied dihydrofolate reductase and binding of anticancer drugs. Two other chapters cover specific case studies, and Chapter 6 focuses specifically on "Computer Modelling of Drug-DNA Intercalative Interactions."

In summary, this book provides several general and specific examples of utilizing quantitative molecular methods in the study of molecule-active site interactions (with copious references) and would be very useful for those in the area of drug design and other enzymatic systems. For more general chemical engineering it could provide interesting clues as to how these techniques might be useful in studying other types of active sites in chemical processing.

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