"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 $N = N_{species} - N_{elements}$. 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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