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Book Review

Mathematical modeling and scale-up of liquid chromatography, by Tingyue Gu, Springer-Verlag, Berlin, Heidelberg, New York, London, Paris, 1995, ISBN 3-540-58884-1. XIV+125 pp., DM 98.00.

The author attempts to present the physics and modeling of nonlinear, nonideal chromatography in a hundred pages. The topic being vast, he succeeds only in explaining the main features of the general rate model of chromatography. The presentation of the model and the discussion of its properties are clear and comprehensive. The discussion of the procedures involved in the use of this model (including some elements of program code) will be useful. However, there are no comparisons between experimental profiles and the results of the numerical calculations performed with the general rate model, using a set of parameters which have been properly determined or estimated. This is quite surprising since there are good examples of such comparisons in the work of Beringer and N.-H.L. Wang, that the author cannot ignore. This work, although quite relevant, is not even quoted. The reader is left without a critical piece of information: what is the cost of this effort, its validity, its relevance?

Although the general rate model of chromatography is certainly the most rigorous one from the point of view of physical chemistry, it is also the most impractical to use and its rigor is rarely useful. Certainly, personal computers allow the calculation of reasonably accurate numerical solutions for such a model in a relatively short period. However, numerical values for the parameters of the model have to be introduced in order to allow numerical calculations to proceed and this is the difficult issue: the determination of the model parameters requires independent measurements whose complexity increases rapidly with the number of parameters required. Furthermore, identification of the parameters, which becomes lengthy and tedious even with fast personal computers, is unwise as has been often shown. The procedure is a circular argument whose validity cannot be checked. It affords values for parameters which cannot be used to obtain valid, trustworthy solutions in a range of experimental conditions differing from the sets of conditions used to acquire the solutions on which the identification is based. In modeling the behavior of industrial units, the simplest possible model must be used because it is the one which requires the least work to determine the parameters required. The ideal model requires only the isotherm parameters. This is already not a trivial task and many chemists balk from it. It may take a week in reasonably simple cases, several weeks in complex ones. The equilibrium-dispersive model requires also the classical HETP curve that any chromatographer can determine in a few hours. In addition to that, the lumped kinetic models require the mass transfer rate constant which can be determined by identification from the profiles of the steps used for isotherm determination by frontal analysis. The determination of the whole set of kinetic parameters requires a series of complex experiments and the use of more or less reliable correlations. The gain in accuracy is doubtful. The increase in cost is considerable.

This book will be useful to academics in chemical engineering who are looking for interesting problems for graduate level classes and to those who want to

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apply the general rate model to the solution of very difficult problems. It is too incomplete and too heavily biased toward complexity for its own sake to be useful to the separation chemists in industry.

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