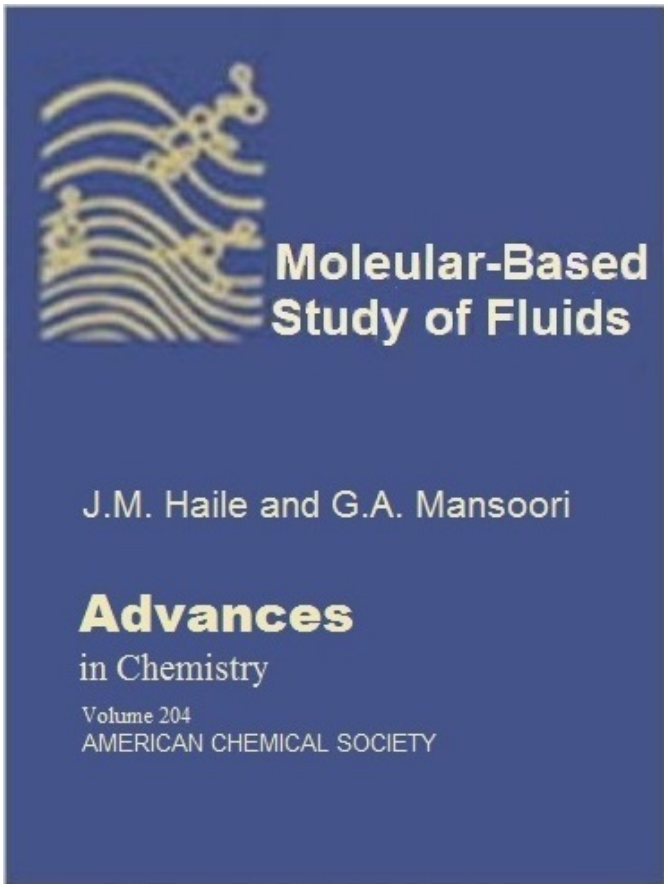
Molecular-Based Study of Fluids

Advances on Chemistry Series, Volume 204, ACS, Washington, D.C. 1983



Editor(s): J. M. Haile, G. A. Mansoori
Volume 204
Publication Date (Print): **June 01, 1983**

ISBN13: 9780841207202
eISBN: 9780841223868
DOI: 10.1021/ba-1983-0204

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PREFACE

THE MOLECULAR THEORY OF LIQUIDS AND DENSE GASES is currently in the midst of a healthy period of growth and expansion. Much of the activity in the area has been instigated by the wide-spread availability of high-speed digital computers coupled with significant advances in a number of experimental methods for measuring fluid properties and exploring fluid-phase behavior. The computer has not only provided the means for generating quantitative results for problems defying analytic solution, but it also has enabled direct simulation of molecular behavior in fluids via techniques known as Monte Carlo, molecular dynamics, and Brownian dynamics. Important experimental advances include high-flux nuclear reactors and pulsed-neutron sources for determining a variety of static and dynamic fluid properties; lasers for extracting information on dynamic relaxation processes; improved molecular beams for ascertaining details of intermolecular pair potential functions; and ellipsometry for probing fluid interfaces. These various computer simulation and experimental methods are providing molecular theorists, as never before, with a wealth of data to be digested, organized, interpreted, and made predictable.

Numerous theoretical tools have been developed in attempts to cope with the profusion of simulation and experimental data. The more successful theoretical developments include integral equations for molecular distribution functions, perturbation and variational theories, analytic expressions for the thermodynamic properties of the hard-sphere and Lennard–Jones fluids, and improved forms for intermolecular potential energy functions. The success of the molecular approach to the study of fluid behavior is indicated by the fact that many of these theoretical advances are replacing empiricisms in engineering design and process analysis computations. Furthermore, molecular-based corresponding states and conformal solution theories are now widely used by the engineering community.

Thus, the molecular-based study of fluids is a multidisciplinary endeavor that involves chemists, physicists, and engineers. This volume reflects the breadth of the endeavor as indicated by the variety of phenomena under investigation, the diversity of scientists and engineers involved in the research, and the internationally recognized importance of the problems to be solved. In this collection of papers, we have emphasized, with some exceptions, static properties at the expense of dynamic properties, because substantially more progress has been made in resolving difficulties in the theory of static properties. The only con-

straints we have placed on the authors are to insist that results take priority over methodology and that the papers present a juxtaposition of two from the following triad: theory, experiment, and computer simulation. We hope this collection of papers communicates to the research specialist, the curious nonspecialist, and the practicing engineer the recent progress made towards a more complete explanation of fluid-phase behavior.

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November 29, 1982