APPLICATIONS OF MOLECULAR SIMULATION IN THE OIL AND GAS INDUSTRY: Monte Carlo Methods (IFP Publications)

Philippe Ungerer, Bernard Tavitian, Anne Boutin

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Molecular simulation is an emerging technology for determining the properties of many systems that are of interest to the oil and gas industry, and more generally to the chemical industry. Based on a universally accepted theoretical background, molecular simulation accounts for the precise structure of molecules in evaluating their interactions. Taking advantage of the availability of powerful computers at moderate cost, molecular simulation is now providing reliable predictions in many cases where classical methods (such as equations of state or group contribution methods) have limited prediction capabilities. This is particularly useful for designing processes involving toxic components, extreme pressure conditions, or adsorption selectivity in microporous adsorbents. Molecular simulation moreover provides a detailed understanding of system behaviour. As illustrated by their award from the American Institute of Chemical Engineers for the best overall performance at the Fluid Simulation Challenge 2004, the authors are recognized experts in Monte Carlo simulation techniques, which they use to address equilibrium properties. This book presents these techniques in sufficient detail for readers to understand how simulation works, and describes many applications for industrially relevant problems. The book is primarily dedicated to chemical engineers who are not yet conversant with molecular simulation techniques. In addition, specialists in molecular simulation will be interested in the large scope of applications presented (including fluid properties, fluid phase equilibria, adsorption in zeolites, etc.).Contents: 1. Introduction. 2. Basics of Molecular Simulation. 3. Fluid Phase Equilibria and Fluid Properties. 4. Adsorption. 5. Conclusion and Perspectives. Appendix

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