the earlier theoretical value of 0.0106 mol. Although this calculation is relatively coarse, it does indicate that the Fe_2O_3 goes completely to Fe_3O_4. In future work, the composition of the solid will be measured directly by x-ray diffraction.

Conclusions

- It is possible to use chemical looping with a solid fuel, such as coal, provided a gasification agent like CO_2 is introduced into the reactor. The gasification agent converts solid carbon to CO the gas phase, where it can be oxidized, together with any H_2 from reaction 3, by the solid oxygen carrier, for example Fe_2O_3.
- The heights and durations of the peaks for CO in Figures 1 to 3 indicate that gasification is probably the rate-limiting step. Consequently, the reaction of these sintered compacts of for example, Fe_2O_3, appears to be sufficiently rapid at 900°C to make the earlier cyclic process feasible and worthy of further investigation.

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Manuscript received Feb. 16, 2006, and revision received Jun. 2, 2006.

BOOK REVIEW

COSMO-RS, From Quantum Chemistry to Fluid Phase Thermodynamics and Drug Design

By Andreas Klamt, Elsevier Science, 2005, 246 pp., $165.00.

This book gives a comprehensive overview of the wide range of problems that can be addressed with the COSMO-RS method for predicting thermodynamic properties of pure and mixed fluids which are important in many areas, ranging from chemical engineering to drug design. It is a high-quality reference book written in a clear and self-consistent style by the creator of this novel approach for predicting vapor-liquid equilibria, based on *ab-initio* calculations of molecular interactions in a fluid mixture.

After an excellent and concise description of models used for describing solvation effects in quantum calculations in which he summarizes the equations used in a easy to read format, the author clearly underlines the advantages of COSMO model in which the surrounding medium is modeled as a conductor rather than as a dielectric in order to establish the initial boundary conditions. The assumption that the solvent is well modeled as a conductor simplifies the electrostatic computations, and corrections may be made *a posteriori* for dielectric behavior. By adopting a stepwise and methodological approach for explaining the physics of the COSMO theory, the author reveals the logical sequence of the choices he has done, as well as their implications.

Charge surfaces and charge distributions profiles of isolated molecules obtained through QM-COSMO calculations are used as quantitative molecular descriptors for characterization of their electrostatic behavior in different solvents. The author introduces then the concept of COSMO-RS/COSMO*therm* methodology for predicting several macroscopic properties for a wide variety of molecular mixtures simultaneously in a unified framework with few parameters from COSMO molecular surface polarity distributions, unlike group contribution methods which depend on large experimental databases or quantitative structure-property relationships (QSPR).

The specific problem of predicting vapor-liquid equilibria of fluids and fluid mixtures, based on theory and realistic models requires a combination of different computational approaches, going from the quantum electronic-structure theory of the isolated molecule to statistical physics description of fluid mixtures. In bridging this gap, this text provides what I believe to be an original, comprehensive, careful, meticulous, and clear development.

The book combines advances in fundamental scientific knowledge with novel computational technology for industrial applications in fluid phase thermodynamics and drug design. It will be helpful to both students and academic researchers and industrial experts in computational chemistry, theoretical chemistry, molecular simulation, physical chemistry and chemical engineering. The book will also particularly suit those researchers who use commercial "molecular modeling" software, by allowing them to understand more fully what they can and cannot do with such packages. I believe that Andreas Klamt's book will substantially contribute to the recognition of the fact that computational chemistry is serious science that promises new ways to tackle the problems of real-world applications.

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AIChE Journal, Vol. 52, 3328 (2006)

DOI 10.1002/aic.10906
Published online July 13, 2006 in Wiley InterScience (www.interscience.wiley.com).