Development of an Equation of State Incorporating Molecular Architecture

By Kai Langenbach

Shaker Verlag Aug 2013, 2013. Taschenbuch. Condition: Neu. Neuware - The thermodynamic modelling of pure substances and mixtures has undergone large changes since the emergence of physically based equations of state that allow the description of thermodynamic properties in terms of the free energy. Most of these equations of state focus on the energetic interactions between equal or different functional groups and do not include the molecular architecture of the compounds in question other than through adjustable parameters typically fit to experimental data. For example if an isomer of a substance with similar molecular weight, but differing structure, is to be described, the whole set of parameters needs to be readjusted with this kind of theory. However, Freed and co-workers developed the Lattice Cluster Theory in which the molecular topology of a mixture's constituents directly enters into its free energy. As this theory is quite unwieldy in its original formulation, a simplification for engineering purposes is mandatory. Usually this simplification is performed by reducing the number of components from the multi-component case to e.g. two components and expanding the resulting equation in a series of its natural variables. In this thesis, the theory's complexity is reduced without losing any thermodynamic...

Reviews

Thorough manual! Its this kind of excellent study. It is actually loaded with knowledge and wisdom You can expect to like how the writer compose this book.

-- ***Marlin Ratke***

This is an amazing pdf that I actually have actually study. It is among the most amazing pdf we have read through. Its been written in an remarkably basic way and is particularly simply following i finished reading this ebook where basically altered me, alter the way i really believe.

-- ***Ms. Izabella Walter***