

EQUILIBRIA

Equilibria offers a comprehensive set of simulation tools to determine phase equilibria. Such simulations provide thermodynamic data, which assist materials research and process design in the chemicals and petrochemicals industries.

WHAT DOES EQUILIBRIA DO?

Equilibria incorporates the Gibbs Ensemble Monte Carlo method¹, a state-of-the-art technology to simulate chemical potential equilibrium between two phases. The Gibbs Ensemble method enables direct simulation of vapor-liquid and liquid-liquid phase coexistence properties of single components and binary and ternary mixtures from a single simulation. The methods implemented in Equilibria² allow phase coexistence to be determined even for chain molecules, and solubilities to be determined for organic molecules and polymers. Equilibria determines critical constants from the vapor-liquid equilibrium data, and provides a tool to determine the second virial coefficient of single components. Equilibria uses the carefully parameterized NERD^{2,3}, forcefield which provides accurate thermodynamic data, and allows the effect on phase coexistence of even small variations in molecular structure to be determined with confidence.

APPLYING EQUILIBRIA

Equilibria is an MS Modeling product and is operated from within the Materials Studio[®] software environment. Materials Studio provides a user interface that is easy to use and quick to learn, complying with Windows[®] standards.

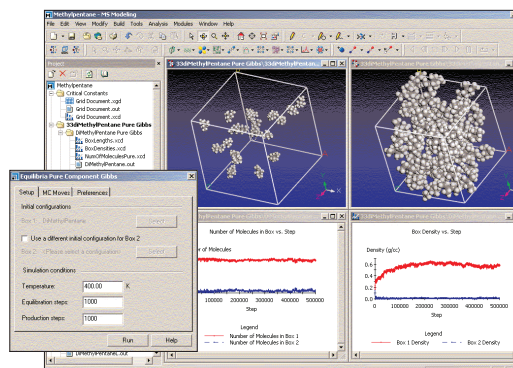


Figure 1: Equilibria, running within MS Modeling, brings one of today's most advanced atomistic simulation methods to your desktop.

Materials Visualizer, the core MS Modeling product, offers a wide range of model building and visualization tools. You can rapidly construct models of the systems that interest you, select Equilibria with a single mouse click, and then run an advanced simulation. A flexible client-server architecture means that calculations can be run on servers located elsewhere on your network. The results are then returned to your PC, where they may be displayed and analyzed. You can easily produce high quality graphics of molecular and materials structures. Structures, graphs, and other data can be instantly exchanged with other PC applications, helping you to share them with colleagues and analyze them using spreadsheets and other packages.

To use the Equilibria program, you begin with a periodic structure of the system you want to study. This can be constructed from the molecular structure of the component(s) by means of the Amorphous Cell module or using Crystal Builder components of the Materials Studio interface. You then set simulation parameters including the temperature and, in the case of mixtures, the pressure.

In order to determine phase coexistence, Equilibria performs a Gibbs Ensemble Monte Carlo simulation. Two periodic boxes are simulated (initially these may be identical, or may differ in composition and density), and during the simulation structure relaxation moves are performed using the Hybrid Monte Carlo method², molecules are exchanged between the boxes, and the box lengths are allowed to fluctuate.

The simulations thereby drive the boxes towards thermal, mechanical, and chemical equilibrium. The Critical Constants analysis in Equilibria lets you determine the phase diagram including the critical point from coexistence data.

To determine the Second Virial coefficient of a component, you simply require the molecular structure of the component.

FEATURES •

- Single Component Gibbs NVT ensemble to simulate vapor-liquid coexistence points for pure component systems at a given temperature.
- Mixture Gibbs NPT ensemble to simulate vapor-liquid or liquid-liquid coexistence points for binary and ternary systems at any given temperature and pressure.
- Expanded ensemble option to handle phase equilibrium simulations for long linear molecules.

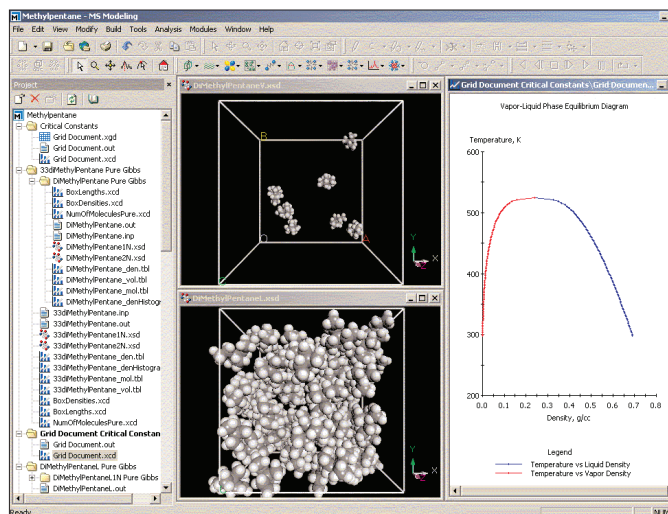


Figure 2: Molecular structure and vapour-liquid phase diagram of 3,3-dimethylpentane - an example of the type of branched hydrocarbons that can be modeled using Equilibria.

- Calculation of second virial coefficients of small molecules at any given temperature based on average interactions at a range of distances.
- Supported by the state-of-the-art NERD united atom forcefield. The current release includes parameters for all linear and branched saturated alkanes, α -alkenes, nitrogen, pentan-1-ol, hydrogen sulfide, diethyl sulfide and ethanethiol. The oxygen and sulfur parameters derived for this set can be applied to other homologues. Less extensive testing has been performed, although initial results (e.g., for longer alcohols) are encouraging³
- Critical constants calculation and phase diagram based on a supplied set of pure component coexistence points via the Ising scaling law⁴

To learn more about Materials Studio, go to accelrys.com/materials-studio

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