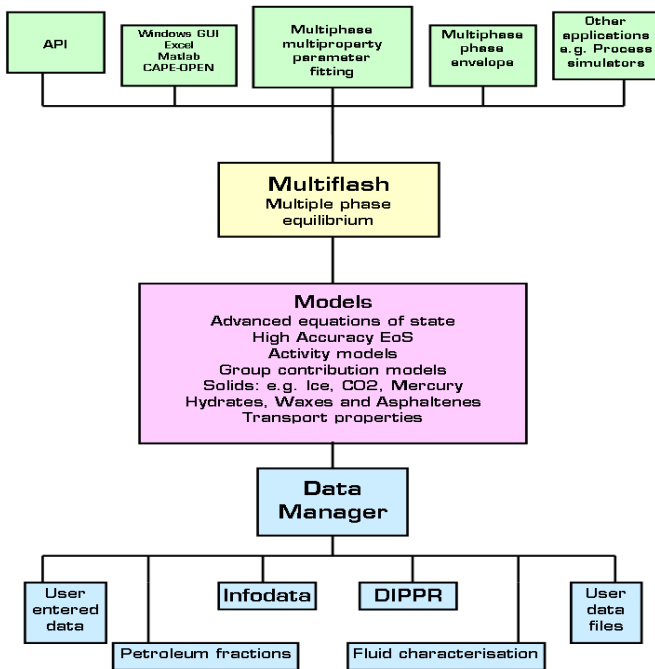


## Multiflash: Models and Methods

The Multiflash models library contains a wide range of models to support the complex multiphase systems that Multiflash is designed to handle. These systems include multiple liquid and solid phases, each of which may have differing properties and require modelling in different ways.



The models library provides an advanced implementation of the thermodynamic models commonly used for process simulation plus many specialised models. It has been designed to work efficiently when carrying out normal process calculations while offering the features needed for multi-phase equilibrium calculations.

The software calculates the thermodynamic and transport properties for a given phase at specified conditions. All thermodynamic properties may be calculated with the same model or else different models may be used for each property.

### Models available

There is a range of models to handle a variety of different types of mixtures. The software is both flexible and extendible and new models are easily incorporated.

### Equations of State (EOS)

Mostly used in the oil and gas industry this group includes the cubic equations of state, e.g. RKS and PR, and advanced variants (RKSA and PRA) that include the Peneloux density correction and parameters fitted to pure component vapour pressure. EOS based on RKSA with modifications to allow prediction of polar, particularly aqueous, phases are CPA (RKSA with an association term),

RKSAInfo (RKSA with an excess Gibbs energy mixing rule) and PSRK (RKSA with a mixing rule based on variants of UNIFAC or NRTL). Equations of state can be used over wide ranges of temperature and pressure, including the subcritical and supercritical regions.

Non-cubic EOS include LK, LKP and BWRS, which can produce improved prediction of thermal and volumetric properties, and CSMA (a series of high accuracy equations for reference fluids). CSMA provides high accuracy data for pure substances and non-polar or mildly polar mixtures such as hydrocarbons, air or other light gases. Typical applications would be custody transfer, acid gas injection or air separation.

The PC-SAFT equation is used primarily to model polymer solutions, although it can be applied to asphaltenes.

### Activity Coefficient models

These are typically used to describe highly non-ideal polar mixtures found in the chemical or petrochemical industries and include Ideal, Wilson, NRTL, UNIQUAC and UNIFAC. They should only be used at low or moderate pressures and require model interaction parameters for accurate results.

### Models for Solid Phases

Multiflash includes models for hydrates, waxes and asphaltenes plus a freeze-out model that can be applied to any component in the system such as ice, CO<sub>2</sub>, mercury or halide scales.

Fluid and solid models may be applied to the same stream to reproduce complex phase behaviour.



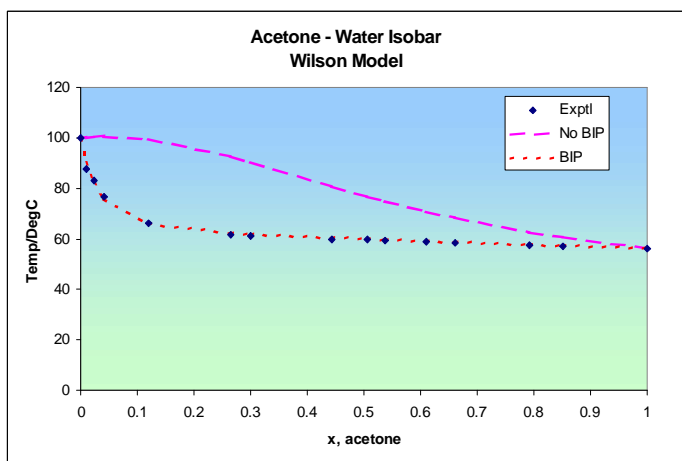
### Transport Property models

A range of models is available for the transport properties of fluids. The simplest approach is to use mixing rules. More advanced models include: for viscosity the Pedersen, Lorentz-Bray-Clark or Twu models; for thermal conductivity the SuperTRAPP or Chung-Lee-Starling models; for surface tension the Linear Gradient Theory or McLeod-Sugden models.

## Binary Interaction Parameters

Binary interaction parameters (BIPs) are model parameters that are adjusted so that predictions from a model reproduce as closely as possible the experimental data. Multiflash has three BIP databanks. The OILANDGAS correlations support the equation of state models and generate BIP values for light gas and hydrocarbon mixtures (including petroleum fractions) plus some polar components such as water, methanol and other inhibitors. The INFOBIPS and INFOLLBIPS databanks mainly supply BIPs for the VLE and LLE variants of activity coefficient models, although they do contain BIPs for some EOS for particular binaries e.g. refrigerant mixtures. Interaction parameters for UNIFAC and PSRK are generated from component group structure.

The BIPs may be constants or functions of temperature. Their values can be viewed in the Multiflash GUI or via Excel functions and they can be supplemented or overwritten by the user. If no BIP is found for a particular binary pair, and none is provided by the user, then the default value appropriate to the model is taken. To obtain accurate predictions from any activity coefficient model, except UNIFAC, you need to specify interaction parameters for all components.

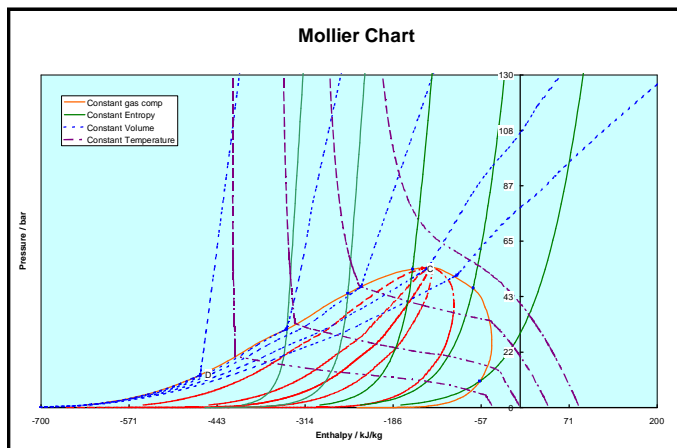


## Flash calculations

For any combination of phases, Multiflash can carry out the full range of flashes:  $(T,P)$ ,  $(H,P)$ ,  $(H,T)$ ,  $(S,P)$ ,  $(S,T)$ ,  $(S,H)$ ,  $(S,V)$ ,  $(V,P)$ ,  $(V,T)$ ,  $(U,P)$ ,  $(U,T)$ ,  $(U,V)$ ,  $(P, \text{phase fraction})$ , and  $(T, \text{phase fraction})$  with the full range of models. This allows you to choose the flash calculation most appropriate to your engineering application, for instance, an adiabatic flash across a valve, or an isentropic flash for a compressor or expander, and not only calculate the resulting temperature or pressure but also identify any new phases which might form. For example, if a drop in pressure results in a significant lowering of the temperature a hydrate may form or a trace element, such as mercury, may drop out. Multiflash also includes a tolerance calculation. This calculates the amount of a second stream that needs to be

added to the main stream in order to meet a fixed constraint such as the amount of inhibitor needed to suppress hydrate formation at given  $T$  and  $P$  or the amount of water required to saturate a gas.

The multiplicity of flash functions and the ability to solve for any value of mole, mass or volume fraction allows the user to build up complex phase diagrams, such as Mollier plots.



## Phase stability/Phase tracking

Multiflash can work out which phases are present at equilibrium and automatically generates the starting values for all calculations. The user only needs to select the phases of interest for any model. The program will also establish whether additional phases can form. The chosen phases are tracked automatically, enabling Multiflash to search for dew or bubble points of specific phases. For example, in oil/gas/water systems you can distinguish between the hydrocarbon dew point and the water dew point. The program will also report the type of any phase (solid, hydrate, wax, asphaltene, liquid, gas) and whether the system is stable or unstable (which means that more phases should form).

## Computational efficiency

Flashes are solved using a powerful 2-tier algorithm that is very efficient for dealing with straightforward problems but switches to advanced numerical methods to deal reliably with difficult cases. For cubic EOS, the volume is found analytically in the most computationally efficient way; the method is numerically stable at extremes of temperature and pressure. For non-cubic EOS, a rapidly converging second-order solution method is used that can also detect cases of unstable phases.

The second-order methods can converge particularly difficult problems such as equilibria near critical points. They require the use of analytical derivatives of the thermodynamic quantities concerned. These derivatives with respect to pressure, temperature and mole numbers are implemented for all properties and all models. They may also be exploited in process optimization, dynamic simulation or data regression.

Contact details:

13 Swan Court, 9 Tanner Street, London SE1 3LE, UK  
Tel: +44 (0)20 7357 0800 Fax: +44 (0)20 7407 3927

Email: [info@infochemuk.com](mailto:info@infochemuk.com)  
Website: [www.infochemuk.com](http://www.infochemuk.com)