

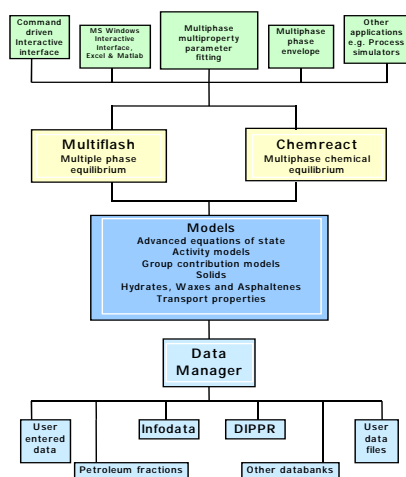
INFOCHEM

COMPUTER SERVICES LTD



Models and Methods

The Infochem Models module is a central element of the Multiflash program. It contains a wide range of models to support the complex multiphase systems 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 module is an advanced implementation of the thermodynamic models commonly used for process simulation. It has been designed to work efficiently when carrying out normal process calculations while offering the features needed for multiphase equilibrium calculations.

The software calculates the thermodynamic (including fugacity and activity coefficients) 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

The model library includes a range of models to handle a variety of different types of system. The program is both flexible and extendible and new models are easily incorporated. The models available fall into a few distinct categories.

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 their variants, which include fitting to pure component vapour pressure and Peneloux density correction (RKSA and PRA). 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 a variant of UNIFAC). Equations of state can be used over wide ranges of temperature and pressure, including the sub-critical and supercritical regions.

Non-cubic EOS include LKP and BWRS, which can produce improved prediction of thermal and volumetric properties, and CSM (a series of high accuracy equations for reference fluids). LKP and BWRS would normally be applied to non-polar or mildly polar mixtures such as hydrocarbons or light gases. CSM provides high accuracy data for pure light gases and low molecular weight hydrocarbons. Typical applications would be custody transfer or air separation.

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.

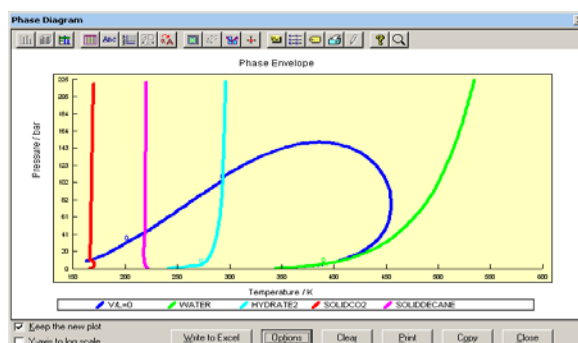
Solid models:

Multiflash also 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 or CO₂.

Transport Property models:

The transport properties of fluids (viscosity, thermal conductivity and surface tension) can be modelled by mixing pure component properties or for viscosity by the Pedersen, Lorentz-Bray-Clark or Twu models; for thermal conductivity by McLeod-Sugden; for surface tension by Chung-Lee-Starling.

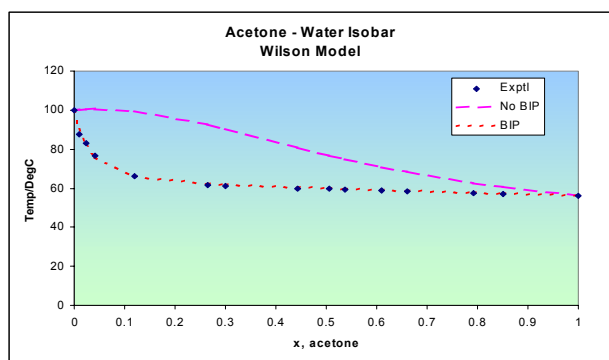
Fluid and solid models may be applied to the same stream to produce complex phase diagrams.



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, OILANDGAS, INFOBIPS and INFOLLBIPS. OILANDGAS supports the equation of state models and includes BIP correlations to generate values for light gas and hydrocarbon mixtures (including petroleum fractions) plus some polar components such as water and methanol. INFOBIPS and INFOLLBIPS mainly supply BIPs for the activity coefficient models, the VLE and LLE variants respectively, 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 else linear or quadratic functions of temperature. Their values can be viewed in Multiflash for Windows or via Excel functions and they can be supplemented or over-written by the user. Two BIP banks may be in force at any time. 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 use interaction parameters.

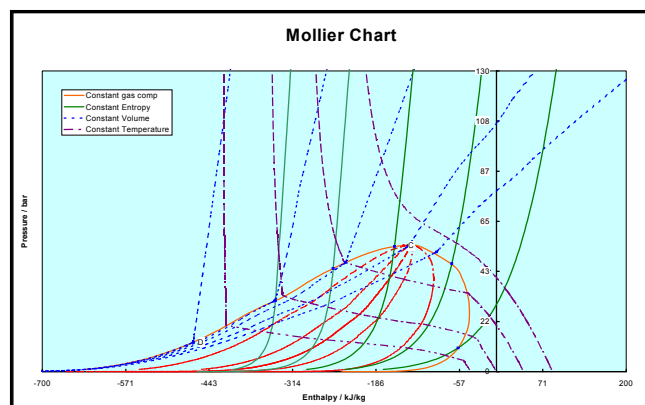


Flash calculations

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. Some flashes, T,P , dew and bubble points can also be calculated taking into account chemical equilibrium.

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 generate the starting values for the equilibrium calculation. 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 identify either the oil dew point, the water dew point or the first dew point that occurs. The program will also report the type of any phase (solid, hydrate, wax, asphaltene, liquid, gas) and whether the flash is stable or unstable (i.e. no solution).

Computational efficiency

Calculations 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 equations, the solution is found analytically in the most computationally efficient way; the method is numerically stable at extremes of temperature and pressure. For non-cubic equations, 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 but these derivatives with respect to pressure, temperature and mole numbers are implemented for all properties and all models. They may also be exploited (a) in process optimization, (b) in dynamic simulation or (c) in data regression.

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