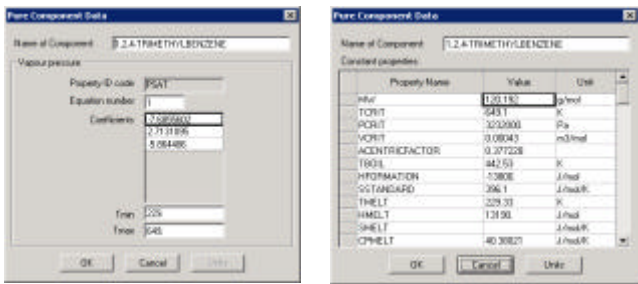




## User supplied data

Multiflash includes a variety of models and a 246 pure component databank that can be extended by licensing the more than 1900 component DIPPR™ databank. Even so circumstances may still arise where users wish to model systems that contain pure components not available from either data source. Multiflash allows users to add their own components. However, the assumption is that, for temperature dependent properties, the user has correlation coefficients for that property for an equation coded in Multiflash.



When this is not the case then a certain amount of data preparation is required. To help the user do this we have taken advantage of the facility to call Multiflash functions from Excel to set up spreadsheets to allow fitting of experimental or predicted pure component properties to acceptable equations. Other spreadsheets can be used to generate model interaction coefficient (BIPs) from binary vapour-liquid equilibrium data.

### Data preparation

Multiflash can be used to model phase equilibrium, volumetric, thermal and transport properties. Phase equilibrium, thermal and volumetric properties can be modelled by a single model or different models can be chosen for each. The transport properties are each modelled differently.

#### Model choice

Before collecting and fitting pure component data it is useful to consider which model/models will best describe the overall system as different models require different input data.

In general equations of state (EOS) require a minimum of critical temperature, critical pressure, acentric factor and ideal gas heat capacity. The advanced forms of the cubic EOS also need the saturated vapour pressure and the liquid density. The PSRK EOS need the components to be broken down into UNIFAC group structures. EOS can be used over wide ranges of temperature and pressure, including the subcritical

and supercritical regions. Usually cubic EOS are applied to light gas and hydrocarbon mixtures typical of oil and gas applications but use of a non-standard mixing rule, such as in the RKSA(Infochem) model, can extend their use to more non-ideal polar systems. Cubic EOS may not model liquid density accurately, although the Peneloux density correction in the advanced forms improves this. An alternative model, such as ideal solution, that derives the liquid density from the databank correlation may be preferable for volume.

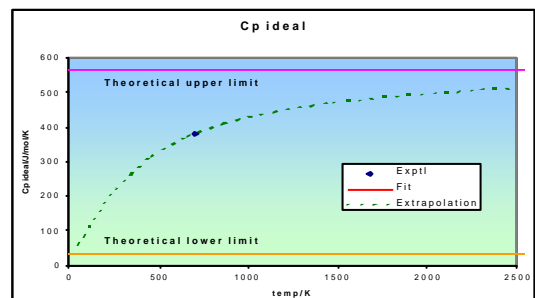
Activity coefficient models require more input data, including the vapour pressure, liquid density, Cp ideal and enthalpy of vaporisation. The activity liquid phase model, the gas phase model, Cp ideal and enthalpy of vaporisation are used to derive the liquid heat capacity and hence enthalpy rather than using a liquid Cp correlation directly. Activity models are used to describe highly non-ideal polar mixtures found in the chemical or petrochemical industries. They should only be used at low or moderate pressures and require BIPs for accurate results.

The transport property models in Multiflash are generally only applicable to oil and gas components. For mixtures of other components transport properties should be derived from the pure component correlations and mixing rules.

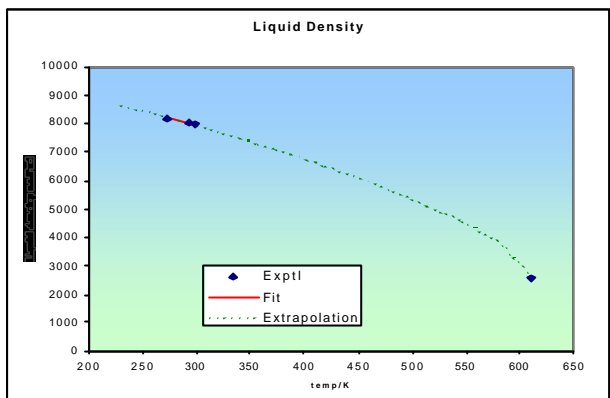
#### Pure component data fitting

Infochem does not currently offer any data prediction; data to be fitted should be experimental or derived from external prediction programs. The amount of experimental data available will vary between properties and components. Maximum value can be derived by a careful choice of correlation equation and supplementary information.

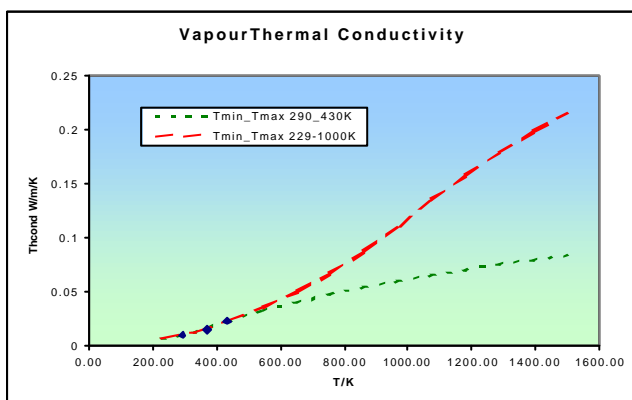
For instance, the Harmens correlation for ideal gas heat capacity has two coefficients that can be related to the theoretical upper and lower boundaries for Cp. This produces a well behaved correlation even with minimal input.



For other properties experimental data can be supplemented from known physical chemistry, e.g. the surface tension and enthalpy of vaporisation will be zero at the critical temperature or the value of the density at  $T_c$  will be  $1/V_c$ .



Multiflash includes extrapolation procedures if property correlations are used outside the values the user sets for the correlation limits. For most properties these will come into effect at a certain proportion of  $T_c$  or  $T_{melt}$  or  $T_{max}$  and  $T_{min}$  whichever is the most conservative. Especially for limited data sets and properties where the value at  $T_c$  is unknown it is worth checking the values set for the correlation limits and the behaviour of the property correlation when extrapolated.



When fitting pure component data:

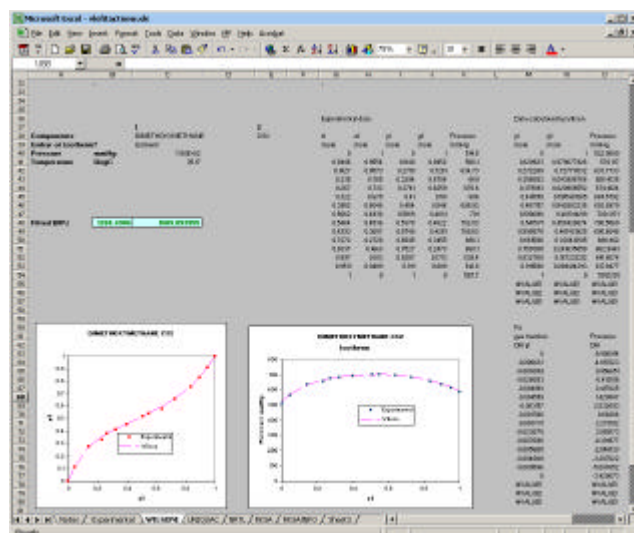
- Choose a correlation that has the correct limiting behaviour and/or represents the correct behaviour of the property with temperature
- Fix values for correlation coefficients where they have physical significance
- Consider adding known data points to supplement experimental data, such as  $1/V_c$  at  $T_c$  for liquid density
- Choose the correlation equation that gives the best fit with the least number of correlation coefficients
- Check extrapolation if calculation may be required outside correlation limits

## Phase equilibria

Predictions of phase behaviour are often significantly improved if BIPs ( $k_{ij}$ s) are available, particularly in the case of activity coefficient models. Multiflash includes three sources of BIPs, any two of which may be in force at any one time.

- OILANDGAS stores the correlated BIPs for hydrocarbons, light gases, water and hydrate inhibitors used with the cubic equations of state and LKP.
- INFOBIPS contains BIPs for BWRS, LKP and CSM for some systems and for the cubic EOS where these are not available in OILANDGAS, e.g. systems containing ammonia. It also includes BIPs for the activity coefficient models for systems containing water or an alcohol, ketone, aldehyde or ether as one component of the binary pair
- INFOLLBIPS stores BIPs for the LLE variants of the activity models for a selected number of systems

Stored BIPs may be supplemented or over-written. If values are not available from the literature then they can be generated by fitting to experimental VLE or LLE data using Excel.



The spreadsheet is designed to take a single set of experimental data and to fit this to your chosen model in linked worksheets. The data source for the pure component properties can either be Infodata or DIPPR or a file containing the properties of a user component. The fitted BIPs can be supplied in an input file or using the Tools/BIP option in Windows.

	PROPANE	BUTANE	PENTANE	HEXANE
PROPANE				
BUTANE	0			
PENTANE	0.0271965			
HEXANE	0.0308746	0.0270731		
HEPTANE	0.0254252	0.0006727	0.01587204	

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