

Data and Databanks

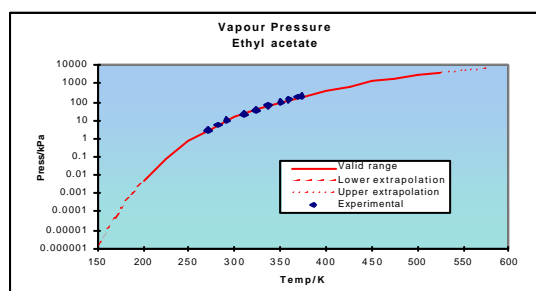
Infochem's MULTIFLASH package has a well defined interface to physical property databanks so that it may be used with any appropriate source of data. Infochem's proprietary databank is Infodata but we are a distributor for the DIPPR™ databank, produced by the American Institute of Chemical Engineers. In principle the user can, of course, interface to any specified data format or enter data directly.

In addition some properties may be calculated within Multiflash based on other stored physical constants or information supplied by the user. Examples would be modeling transport properties for Infodata hydrocarbon components using industry standard models or generating the properties of petroleum fractions using limited user-supplied information such as molecular weight or boiling point.

Infodata

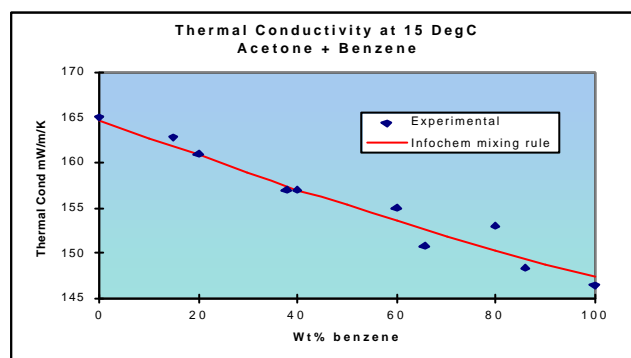
Infodata currently contains data on around 246 components, mainly, although not exclusively, light gases and hydrocarbons. It is especially suitable for use in the oil and gas industry and for this reason also includes components such as methanol, glycols, a "salt component" and sodium, potassium, calcium, chloride and bromide ions which are typically used as hydrate inhibitors.

Pure component properties are stored either as single value constants or as functions of temperature. In many cases both thermal and transport properties are derived from the models, see our *Models and Methods* leaflet. If you wish to derive properties directly from the databank Multiflash functions are available in Excel to allow you to do this. In the Windows version the Ideal model will allow direct retrieval of transport properties and liquid density.



Extrapolation routines are included in Multiflash so that pure component properties behave sensibly beyond the temperature limits of the correlation.

Data for mixtures are usually derived from the models but transport properties of mixtures can be calculated from pure component data using the mixing rule option.



The stored physical properties for any component can be displayed using one of the Multiflash menu options. Non-temperature dependent properties are shown as fixed values in the chosen units; stored temperature dependent properties are shown in the form of the coefficients of the correlating equation. Users may overwrite stored values for the duration of their calculation or save them to a file for future use, but must be aware of the effect changes may have on other properties.

DIPPR

DIPPR™ contains data on 39 properties for over 1900 components of industrial relevance. The database was prepared for the Design Institute for Physical Property Data, a cooperative project sponsored by over 40 major chemical manufacturers and related companies under the auspices of the American Institute of Chemical Engineers.

The properties covered include 26 property constants and thirteen properties which are functions of temperature. The data were carefully selected and can be supported by references to the sources of measured or predicted data that were used in the selection process, as well as an estimate of the accuracy.

Lists of Components

Components lists for all the above databanks can be supplied on request. Multiflash includes facilities to search the databanks by component name or formula or to look for substrings of either. It is also possible to display all synonyms listed for any component for unambiguous identification.

List of Properties

The following is a list of the properties available in Infodata and DIPPR.

Constant properties

Molecular Weight
Critical Temperature
Critical Pressure
Critical Volume
Critical Compressibility Factor
Melting Point
Triple Point Temperature
Triple Point Pressure
Normal Boiling Point (at 1 atm)
Liquid Molar Volume at 298.15K
Standard Ideal Gas Enthalpy of Formation at 298.15K
Standard Ideal Gas Gibbs Energy of Formation at 298.15K
Standard Ideal Gas Entropy at 298.15K
Enthalpy of Fusion at Melting Point
Standard Net Enthalpy of Combustion at 298.15K
Acentric Factor
Radius of Gyration
Solubility Parameter at 298.15K
Dipole Moment
van der Waals Volume (UNIQAC r)
van der Waals Area (UNIQAC q)
Refractive Index
Flash Point
Lower Flammability Limit
Upper Flammability Limit
Autoignition Temperature

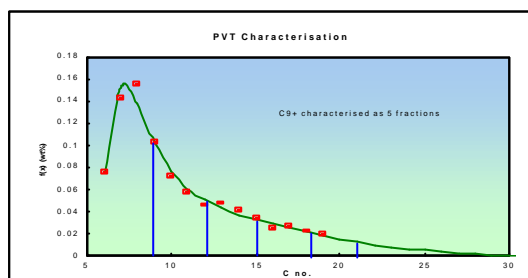
Both databanks also contain the UNIFAC group structures, where applicable. These are used to generate the binary interaction parameters (BIPs) for use with UNIFAC and PSRK to predict vapour-liquid and liquid-liquid equilibrium.

Temperature dependent properties

Liquid density
Vapour Pressure
Enthalpy of vaporization
Solid Heat Capacity
Liquid Heat Capacity
Ideal Gas Heat Capacity
Second Virial Coefficient
Liquid Viscosity
Vapour Viscosity
Liquid Thermal Conductivity
Vapour Thermal Conductivity
Surface tension

Petroleum fractions

Condensates and oils are multi-component mixtures broadly made up of alkanes, cycloalkanes and aromatics. The lighter constituents are well defined individual components. The heavier (C6+) fractions are each made up of a mixture of different components and are described in terms of their average physical properties. The properties of such pseudo-components are generated from a sub-set of physical properties for any fraction with Multiflash calculating the remaining properties. The minimum sub-sets are MW , MW and $Spgravity$, MW and T_b , T_b and $Spgravity$ or T_c , P_c and $?$. The sub-set data and the amount of each fraction are supplied by the user.



Or you can use the PVT Analysis facility to enter directly the compositional analysis provided by PVT laboratories. These analyses, either for gas and liquid or recombined fluid, allocate compositions for individual carbon number cuts. Multiflash fits a function to this compositional analysis and then splits or groups the heavy end into the number of fractions specified by the user. The amount of each fraction is determined by the PVT Analysis and its properties are calculated based on tables of average MW and specific gravity of the cuts. Some properties of petroleum fractions can be then modified in order to match known properties of the whole fluid, such as dew and bubble points, density and viscosity. An additional facility enables you to characterise the fluid from either TBP or ASTM D86 distillation data.

High Accuracy Equations of State

The CSM model is based on a collection of very accurate equations of state for a number of reference fluids. It provides accurate values of thermodynamic properties for a number of reference fluids. These include argon, iso-butane, n-butane, CO, CO₂, ethane, ethylene, fluorine, H₂S, hydrogen, methane, nitrogen, octane, oxygen, n-pentane, propane, water, xenon, helium, hexane, heptane, octane, ammonia, neon, propylene, R123, R152a, R124, R125, R134a, R22, R32, R11, R113, R114, R115, R116, R12, R13, R14, R23, R143a, R245fa and RC318. The reference equation of state used for water is the IAPWS-95 scientific formulation. This and the CO₂ equation are available as separate options. Typical applications for CSM are custody transfer and calculations in the power industry including fuel cells.

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