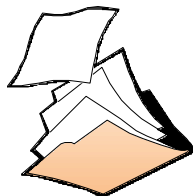


INFOCHEM

COMPUTER SERVICES LTD



Data and Databanks

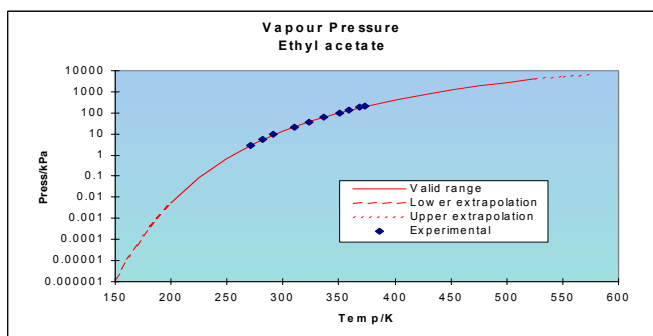
Infochem's MULTIFLASH package has a well defined interface to physical property databanks so that it may be used with any appropriate source of data. Infochem has two proprietary databanks, one for fluids (Infodata) and one for condensed components (Infocond), and we are a distributor for the DIPPR™ 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 of the former are the transport properties for Infodata components; typical of the latter are the properties of petroleum fractions.

Infodata

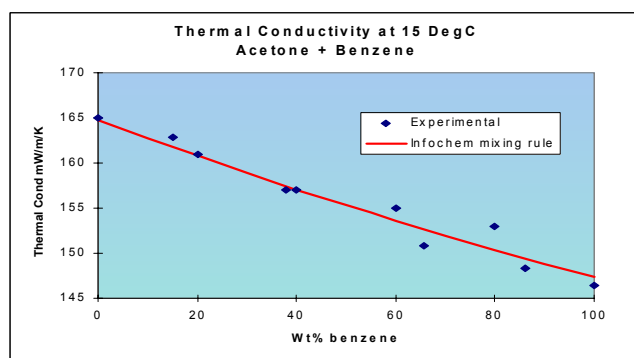
Infodata currently contains data on around 223 components, mainly, although not exclusively, light gases and hydrocarbons. It is especially suitable for use in the oil and gas industry and for this reason also includes components such as methanol, glycols a "salt component" and sodium, potassium, calcium and chloride ions which are typically used as hydrate inhibitors.

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.



Infocond

The Infocond databank includes about 140 solid compounds. The data are limited to molecular weight, normal melting point, normal boiling point, the enthalpy of formation in the condensed state at 298.15K, the standard entropy in the condensed state at 298.15K and the heat capacity in the condensed state as a function of temperature. It is intended for use with Infochem's chemical and phase equilibrium module.

DIPPR

DIPPR™ contains data on 39 properties for over 1800 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

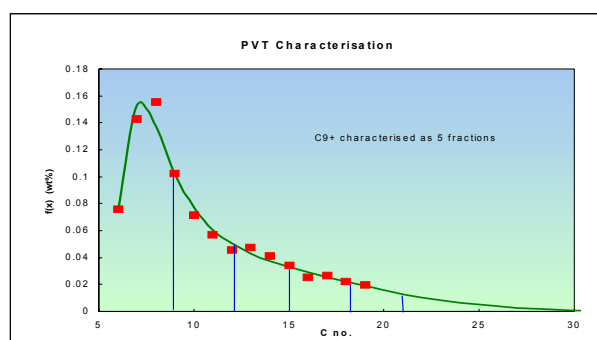
Both databanks also contain the UNIFAC group structures, where applicable. These are used to generate the binary interaction parameters (BIPs) for use with UNIFAC and PSRK to predict vapour-liquid and liquid-liquid equilibrium.

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 made up of a mixture of different components which are described in terms of their average physical properties. In Multiflash the properties of such pseudo-components can be defined in two ways. The user can define a set, or a minimum sub-set, of physical properties for any fraction and allow the software to calculate the remaining properties or define only the carbon number of the fraction, e.g. C10. The minimum sub-sets are *MW and Spgravity*, *MW and T_b* , *T_b and Spgravity* or *T_c , P_c and ω* . The amount of each fraction is supplied by the user.



Alternatively, you can use the PVT Analysis facility that allows you 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. Some properties of petroleum fractions can be altered in order to match known properties of the whole fluid, such as dew and bubble points, density and viscosity.

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 will provide accurate values of thermodynamic properties for a number of reference fluids. The current implementation includes 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, and RC318. The reference equation of state used for water is the IAPWS-95 scientific formulation. Typical applications for CSM are custody transfer and calculations in the power industry including fuel cells.

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