

The new batch reactor heat transfer  
and chemical properties calculator



Version 5 – Volume 2

# Delta T Reactor

**OPERATING & REFERENCE MANUAL**

**VOLUME 2**

**PHYSICAL PROPERTIES DATABASE**

**AND PROCESS CALCULATOR**

Version 5

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# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

IMPORTANT NOTICE.....	8
Software Licence .....	8
Warranties and Remedies.....	8
Constant Properties.....	9
Variable Properties.....	9
GENERAL FEATURES .....	11
System Requirements .....	11
Software Installation after Email Download.....	11
General Operation .....	11
Help Screens .....	11
Local Menu .....	11
Module Menu .....	11
Selection of Options .....	11
Data Entry.....	12
Screen Warnings .....	12
COMPOUND SELECTION.....	13
Category List.....	13
Compound List .....	13
Synonyms and Structural Formula .....	13
Searching for Compounds.....	14
PROPERTIES DATABASE .....	15
Constant Properties.....	15
Print Screen.....	15
Data References.....	15
Variable Properties .....	16
Saturated & Unsaturated Conditions.....	16
Temperature Input.....	16
Pressure Input .....	16
Calculation/Display of Properties .....	17
Data References.....	17
Mixtures and Liquids Categories .....	17
Range Properties.....	17
Data Entry Procedure .....	18
Calculation/Display of Properties .....	18
Graphical Display of Range Properties .....	18

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

USER-DEFINED MIXTURES .....	19
Category List Box .....	19
Compound List Box .....	19
Mixture List Box .....	19
Mixture Name Entry Text Box.....	19
Composition Entry Text Box .....	20
Component Edit.....	20
Calculate/Save .....	20
General .....	20
Liquid Selection .....	20
Reference Temperatures .....	21
Specific Volume .....	21
Specific Heat.....	21
Viscosity.....	21
Conductivity .....	21
Low and High Limit Temperatures .....	21
Calculate/Save .....	22
UNITS SELECTION .....	23
PHYSICAL PROPERTY CORRELATIONS .....	24
GENERAL.....	25
Critical Temperature .....	26
Critical Pressure .....	26
Critical Volume .....	26
Normal Boiling Points .....	26
Freezing Points.....	26
Joback Group Contribution Method.....	27
Tyn & Calus Relation.....	27
LIQUID SPECIFIC VOLUME.....	28
Hankinson-Brobst-Thompson Equation .....	28
Rackett Equation .....	29
Liquid Expansivity.....	29
The Effect of Pressure on Liquid Specific Volume .....	30
LIQUID SPECIFIC HEAT .....	31
Rowlinson-Bondi Method.....	31
Missenard Method .....	31
The Effect of Pressure on Liquid Specific Heat.....	32
LIQUID VISCOSITY .....	33
Method of Van Velzen .....	33
Method of Morris.....	33
Method of Letsou and Stiel.....	34
Method of Przedziecki & Sridhar .....	35
Interpolation and Extrapolation.....	36

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

The Effect of Pressure on Liquid Viscosity .....	36
LIQUID THERMAL CONDUCTIVITY .....	37
Method of Latini et al .....	37
Method of Sato-Riedel .....	37
The Effect of Pressure on Liquid Conductivity .....	38
LIQUID SURFACE TENSION .....	39
Method of Brock and Bird .....	39
Method of Hakim et al .....	39
VAPOUR PRESSURE .....	40
Published Correlations .....	40
Gomez-Thodos Vapour Pressure Equation .....	41
Gomez-Thodos Vapour Pressure Equations .....	42
Lee-Kesler Vapour Pressure Equation .....	42
Interpolation and Extrapolation .....	43
Database Vapour Viscosity Values .....	43
The Methods of Lucas .....	43
Low-Pressure Equation .....	44
Low-Pressure Equation .....	45
High-Pressure Equation .....	46
Database Vapour Conductivity Values .....	47
Ely and Hanley Method .....	47
VAPOUR CONDUCTIVITY .....	48
Ely and Hanley Method .....	48
IDEAL GAS THERMODYNAMIC PROPERTIES .....	49
Method of Joback .....	49
Low-temperature values of $C_{p0}$ .....	49
Derived Ideal Gas Properties .....	50
THE EQUATIONS OF STATE .....	51
General .....	51
The Lee-Kesler Equation of State .....	52
The Lee-Kesler Equation of State .....	53
The Wu & Stiel Equation of State .....	53
The Wu and Stiel Equation of State .....	54
Calculation of Saturation Values .....	55
Enthalpy and Entropy Scales .....	56

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

PROPERTIES OF MIXTURES.....	57
Scope of Correlations .....	57
Mixture Critical Properties .....	58
Critical Temperature .....	58
Critical Volume .....	58
Mixture Critical Properties .....	59
Critical Pressure .....	59
Acentric Factor .....	59
Mixture Liquid Specific Volume .....	60
Mixture Liquid Viscosity .....	61
Mixture Liquid Conductivity.....	61
Mixture Surface Tension.....	61
Vapour Pressure.....	62
THERMODYNAMIC AND TRANSPORT PROPERTIES OF MIXTURES .....	63
Vapour Viscosity .....	63
Vapour Conductivity .....	63
Ideal-Gas Mixture Properties.....	63
REFERENCES .....	65
PROCESS CALCULATOR.....	68
Introduction .....	68
Input Screen .....	68
Output Screen .....	68
Calculation Structure .....	69
Stage 1: Initial Conditions.....	69
Stage 2: After Isentropic change from Stage 1 .....	69
Stage 3: Non-Isentropic change from Stage 1 .....	70
LIST OF COMPOUNDS .....	71
Formula-Order List of Names.....	71
Alphabetical List of Compound Names and Synonyms .....	87
Contents .....	114

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

USER-DEFINED COMPOUNDS (Delta T Props2).....	115
General .....	115
Installation of Delta T Props2 .....	115
Outline Procedure.....	116
Constant Properties.....	116
Outline Procedure.....	116
Vapor and Liquid Properties.....	116
Other Vapor and Liquid Properties.....	117
Calculate Function.....	117
Graphics Display .....	117
Save Data Function .....	117
Compound Selection .....	118
Compound Selection List.....	118
Compound Naming.....	118
Compound Data Saving & Recall.....	118
Clearing Compound Data .....	118
Constant Properties.....	119
Specification of Methods .....	119
Note on Accuracy .....	119
Low-Pressure Vapor Specific Heat .....	120
Specification of Methods .....	120
Vapor Pressure.....	123
Specification of Methods .....	123
Critical Point.....	125
Liquid Specific Volume .....	125
Specification of Methods .....	125
Liquid Viscosity.....	127
Specification of Methods .....	127
Van Velzen Group Contribution Estimation Method.....	129
Liquid Conductivity .....	130
Specification of Methods .....	130
Liquid Specific Heat.....	132
Specification of Methods .....	132
Special Specific Heat Function.....	133
Liquid Specific Heat.....	134
Missenard Group Contribution Method .....	134
Liquid Surface Tension.....	134
Specification of Methods .....	135
Gas Viscosity.....	136
Specification of Methods .....	136
Calculate Function.....	137
Graphics Display .....	137
Save Data Function.....	137
Gas Thermal Conductivity .....	138
Specification of Methods .....	138

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

Gas Thermal Conductivity .....	139
Calculate Function .....	139
Graphics Display .....	139
Save Data Function .....	139
Sample Calculation.....	140
Compound Name .....	140
Constant Properties.....	140
Sample Calculation.....	141
Low-Pressure Vapor Specific Heat .....	141
Vapor Pressure.....	141
Liquid Specific Volume .....	142
Liquid Viscosity .....	142
Liquid Conductivity .....	142
Liquid Specific Heat.....	143
Liquid Surface Tension.....	144
Comparison of Results .....	144

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## **IMPORTANT NOTICE**

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# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## INTRODUCTION

Delta T Reactor Physical Properties Database and Process Calculator (referred to simply as Delta T Props in this manual) provides the user with the thermodynamic and transport properties of liquids and vapors over wide ranges of temperature and pressure. The database contains 586 common chemicals for which the full range of properties is available in both the liquid and vapor phases. In addition over 60 common aqueous solutions and heat transfer fluids are contained in the database: properties are available for these in the liquid phase. The properties available are as follows:

### Constant Properties

- Compound Name
- Compound Formula
- Structural Formula
- Compound Synonyms
- Critical Temperature
- Critical Pressure
- Critical Volume
- Boiling Point
- Melting point
- Critical Compressibility
- Molecular Weight
- Acentric Factor
- Dipole Moment
- Enthalpy of Formation
- Gibbs Energy of Formation

### Variable Properties

- Vapour Pressure
- Specific Volume
- Expansivity
- Compressibility
- Specific Heat ( $C_p$ )
- Specific Heat ( $C_v$ )
- Enthalpy
- Internal Energy
- Latent Heat of Vaporisation
- Entropy
- Viscosity
- Conductivity
- Prandtl Number
- Surface Tension

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## INTRODUCTION (Cont./...)

These properties are generally available from the melting point to the critical point for liquids and from the melting point to 1300 K (1027 C, 1880 F) or the critical temperature (whichever is the greater) for vapours. The pressure range is from near-zero to twenty times the critical pressure. Saturated or unsaturated conditions may be chosen.

Certain variable properties may be ranged over temperature or pressure:

- Specific Volume
- Specific Heat ( $c_p$ )
- Enthalpy
- Entropy
- Viscosity
- Conductivity

Delta T Props provides other powerful facilities:

The user may define and store mixtures of components drawn from the database and compute their properties in a similar fashion to single components. The details are given in Section 5.

The user can define a liquid by specifying its properties at two reference temperatures. This is described in Section 6.

Metric and US units may be selected in any combination.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## GENERAL FEATURES

### System Requirements

The software requires the following operating configuration:

VGA or better monitor  
MS Windows compatible printer recommended  
MS Windows 95 or later

### Software Installation after Email Download

If the software has been downloaded from email, simply run the executable file. The program and data files will automatically unzip and install from this file.

If Delta T Props2 has been purchased, then the Delta T Props2 files must also be installed to the same directory as Delta T Props.

### General Operation

This section sets out some general notes on how to get around the program and to make fluid property calculations.

### Help Screens

In each module of Delta T Props accessing the Help Menu gives assistance in understanding module functionality, data entry and option selection.

### Local Menu

The Local Menu allows access to options such as Calculate, Graphical Display and Data References.

### Module Menu

The Module Menu enables movement between the various program main modules.

### Selection of Options

Screen options are selected from List Boxes (simple or drop-down).

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Data Entry

When a numerical entry is made, the entry is completed by pressing (enter) or by shifting focus to another screen control.

## Screen Warnings

Entry of out-of-range data (e.g. temperature too high or too low) results in a warning message being printed to the message box and rejection of the entered data.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## COMPOUND SELECTION

### Category List

The available categories of compounds are displayed in the left list box. These categories are:

- Alkanes
- Alkenes/Alkynes
- Halogenated Organics
- Ethers
- Ketones/Aldehydes
- Acids/Anhydrides
- Alcohols/Phenols
- Esters
- Benzene Derivatives
- Heterocycles/Polycycles
- Organic Nitrogen Compounds
- Organic Sulfur Compounds
- Inorganic Compounds
- Aqueous Solutions/Heat Transfer Liquids
- User-Defined Liquids
- User-Defined Mixtures
- User-Defined Compounds (Delta T Props2)

The current category will be shown highlighted on the screen. Clicking on a required category selects that category. When a category name is selected the compound list is automatically loaded and partially displayed.

### Compound List

On the right is a list box giving the list of compound formulas and names belonging to the currently selected category. Clicking on a compound name causes that compound to be selected.

### Synonyms and Structural Formula

Directly beneath the partial list of compounds are given synonyms and the structural formula for the currently selected compound.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## COMPOUND SELECTION (Cont./..)

### Searching for Compounds

As explained above, the compounds are displayed in category groups. Within each category, the compounds are stored in formula order. If the user knows which category the compound of interest belongs to and how many carbon atoms in the chemical formula, then it is easy to locate the compound quickly.

If, on the other hand, only the name or a fragment of the name is known, it will be more convenient to use the Search facility available. The user simply enters the name fragment in the Search text box and clicks on the Search command button. The search facility will locate in turn every compound in the database in which the string is found either in the compound's primary name or in its synonyms. The String Search facility is easy to use and prompts and warnings are displayed on the screen.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES DATABASE

### Constant Properties

This module displays the constant properties of the currently selected compound. These properties are:

- Critical Temperature
- Critical Pressure
- Critical Volume
- Critical Compressibility
- Normal Boiling Point
- Normal Melting Point
- Molecular Weight
- Acentric Factor
- Dipole Moment
- Enthalpy of Formation
- Gibbs Energy of Formation
- High and Low Limit Temperatures

Section 8 sets out definitions and details of the sources for this data.

### Print Screen

Selecting this option from the Local Menu sends the data displayed on the screen to the printer.

### Data References

Selecting this option from the Local Menu displays the source or estimation method of the property data shown on the screen for the currently selected compound. The user should also consult Section 8 where more details are given on the sources and estimation methods.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES DATABASE (Cont./...)

### Variable Properties

This module calculates the properties of the currently selected compound for specified values of temperature and pressure.

The following are the displayed properties:

- Phase/Conditions
- Vapour Pressure
- Specific Volume, Expansivity & Compressibility (liquid and vapour)
- Specific Heats ( $C_p$  and  $C_v$ ) (liquid and vapour)
- Enthalpy, Entropy & Internal Energy (liquid and vapour)
- Latent Heat (saturated vapour)
- Viscosity & Conductivity (liquid and vapour)
- Prandtl Number (liquid and vapour)
- Surface Tension (liquid)

### Saturated & Unsaturated Conditions

The saturation conditions should first be set between saturated and unsaturated conditions by clicking on the list box. For saturated input, either the temperature or the pressure may be specified by the user. For unsaturated input, both the temperature and pressure should be entered.

### Temperature Input

Temperature is entered in the specified units followed by (enter). If the chosen conditions are saturated, the saturation pressure corresponding to the entered temperature is calculated at once and displayed. If the temperature entered is outside the ranges specified in the constant properties module, a warning will be displayed and the input rejected.

### Pressure Input

Pressure is entered in the specified units followed by (enter). If the chosen conditions are saturated, the saturation temperature corresponding to the entered pressure is calculated at once and displayed. If the pressure entered is outside the permitted range (see Section 8) then a warning will be displayed and the input rejected.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES DATABASE (Cont./...)

### Calculation/Display of Properties

To carry out the calculation, press the Calculate button. For saturated conditions the properties of both liquid and vapour phases are calculated and displayed. For unsaturated conditions, the phase is calculated and properties are displayed for that phase. If the property is not available, then "N/A" will be displayed. The calculated property values may be printed out by selecting the Print Screen option from the Local Menu.

### Data References

Details of the data sources and estimation methods used for the properties of the currently selected compound may be viewed by selecting the Data References option from the Local Menu. The user can also consult Section 8.

### Mixtures and Liquids Categories

The procedure for calculating and displaying the properties of a User-Defined Mixture is generally similar to that outlined above with the exception that saturated properties are not available.

The procedure for items selected from the Aqueous Solutions/Heat Transfer Liquids or User-Defined Liquids categories is simpler than set out above. Only the liquid state is available for these and only temperature is available as an input option. The properties displayed are a combination of constant and variable properties for the selected compound. Data references cannot be accessed directly on the screen.

### Range Properties

The purpose of this module is to select a property and to display its values for a temperature range or for a pressure range.

The properties that may be selected are:

- Specific Volume
- Specific Heat ( $C_p$ )
- Enthalpy
- Entropy
- Viscosity
- Conductivity

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES DATABASE (Cont./...)

### Data Entry Procedure

The procedure for data entry in this module consists of,

- Selecting the property
- Selecting range variable
- Entering range start
- Entering range end
- Entering the unranged (constant) variable

These selections are accessed by clicking on the appropriate list boxes.

Numerical values are keyed in followed by (enter). A screen warning will be issued upon entry of out-of-range values and the entered values rejected.

### Calculation/Display of Properties

When the required selections and data entries have been made, pressing the Calculate button causes the range of values of the selected property to be calculated and displayed along with phase state. If a property is not available or is not applicable then "N/A" will be displayed. The property range screen can be printed out at any time by selecting the Print Screen option from the Local Menu.

### Graphical Display of Range Properties

When the range values of the selected property have been calculated, selecting Graph Results from the Local Menu will display the results graphically on the screen. This option also allows hard copy from the printer. Note that this option is not available for two-phase results.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED MIXTURES

This module allows the user to define a mixture of up to 10 components selected from the database. Aqueous Solutions/Heat Transfer Liquids, User-Defined Liquids and other User-Defined Mixtures may not be selected as components of a mixture.

The mixture definition screen has the following main areas for selection or entry:

- Category List Box
- Compound List Box
- Mixture Name Entry Text Box
- Mixture List Box
- Component List Box
- Composition Entry Text Box
- Composition List Box

Within each area the options for selection and entry are as follows.

### Category List Box

A compound category is selected by clicking on the required category name in the Category List Box. When a category is selected, compounds belonging to that category are automatically displayed in the Compound List Box.

### Compound List Box

A compound within the current category is selected by clicking on the compound name in the Compound List Box. Selection of a compound places it in the first vacant slot in the Component List Box. Up to 10 components may be selected.

### Mixture List Box

The current mixture name is highlighted in the Mixture List Box. Clicking on a mixture name makes it the currently selected mixture; the information box displays the mixture name, location number and whether a valid mixture is defined for that location. The Components and Compositions can be retrieved and displayed by selecting the Retrieve Data option in the Local Menu.

### Mixture Name Entry Text Box

In the Mixture Name Entry Text Box, keying-in a mixture name followed by (enter) overwrites the current name.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED MIXTURES (Cont./...)

### Composition Entry Text Box

In the Composition Entry Text Box, the composition of the currently highlighted component in weight or mole percentage may be entered followed by (enter). The sum total of the compositions shown in the Composition List Box is automatically displayed on the screen. If a value greater than 100 or less than 0 is entered, a warning is issued and the input value is rejected. Entry of composition in mole% or weight% may be toggled via the local menu.

### Component Edit

During the process of defining a mixture it may be required to delete a component from the current component list. Pressing the backspace or escape keys or selecting the Delete Item from the Local Menu deletes the currently highlighted mixture component from the component list.

### Calculate/Save

When the mixture name, run number, components and composition have been defined, the mixture properties are calculated and saved by selecting the Calculate/Save option from the Local Menu. The defined mixture is now available for selection from the Compound Selection module.

Note that a previously-defined mixture can be recalled from disk, edited, changed, renamed, recalculated and saved.

### General

This module allows the user to define a liquid and store it in the database for future recall and calculation.

The user enters values of the following properties at two chosen reference temperatures: Specific Volume, Specific Heat, Viscosity and Conductivity. The user also enters the low and high limit temperatures for the defined liquid and enters an identifying name for the liquid.

### Liquid Selection

The currently selected user-defined liquid is shown highlighted in the Liquids List Box. A new selection can be made by clicking on the name of the required liquid. When a liquid is selected, the stored property data may be retrieved from disk via the Local Menu and displayed on the screen. If an unused location ("not in use") is selected the property values are cleared.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED MIXTURES (Cont./...)

### Reference Temperatures

The reference temperatures are the temperatures for which the property values are entered. These must be less than or equal to 1300 K and must not be closer to each other than 1 K.

### Specific Volume

The software fits a straight line density function to the entered data to represent the specific volume over the temperature range. If identical values are entered at the two reference temperatures then the specific volume will be constant over the temperature range. This may not be of significance for specific volume but the derived values of expansion coefficient will be identically zero. If these values are subsequently used in Delta T-Reactor then calculated values of natural convection coefficients will be also be zero.

### Specific Heat

The software fits a straight line function to the entered data to represent the specific heat over the temperature range. If identical values are entered at the two reference temperatures, specific heat will be constant over the temperature range.

### Viscosity

The software fits a log viscosity versus inverse temperature function to the entered data. The values entered at the two reference temperatures may be the same, but if this is the case then the viscosity will be constant over the temperature range. This is normally a significant matter for viscosity.

### Conductivity

The software fits a straight line function to the entered data to represent the conductivity over the temperature range. If identical values are entered for conductivity, then conductivity will be constant over the temperature range.

### Low and High Limit Temperatures

These define the applicable temperature range of the calculated values. The same limitations that apply to the reference temperatures apply here too. In addition, the high limit temperature must be greater than the low limit temperature.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED MIXTURES (Cont./...)

### **Calculate/Save**

Once all data has been entered, selection of this option from the Local Menu calculates the fluid parameters and stores these for future recall and calculation. In addition the actual data entered by the user to define the liquid is also stored for future reference. Prior to saving, a check is carried out to determine if any of the properties have zero or negative values in the temperature range: if this occurs, a warning message is printed in the message box. In this case, the input data must be amended before it is accepted and stored.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## UNITS SELECTION

This useful module allows the user to select units individually for a range of quantities as follows:

Temperature:	deg K, deg C, deg R, deg F
Pressure:	Pa, Bar, psi (all absolute or gauge)
Specific Volume:	cum/kg, cc/g, cuft/lb
Viscosity:	Pa-s, cP, lb/ft.hr
Conductivity:	W/m.K, Cal/cm.s.C, Btu/ft.hr.F
Specific Heat:	J/kg.K, Cal/g.C, Btu/lb.F
Enthalpy:	J/kg, Cal/g, Btu/lb
Entropy:	J/kg.K, Cal/g.C, Btu/lb.F
Expansivity:	Per deg K, Per deg F
Surface Tension:	N/m, Dyne/cm, lbf/ft
Dipole Moment:	Debye, Coulomb-m

The options are selected by clicking on the drop-down list box and clicking on the required unit. The selected options can be saved to file for future reference by selecting the Save Selection option from the Local Menu.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PHYSICAL PROPERTY CORRELATIONS

General

Physical Constants

Liquid Specific Volume

Liquid Specific Heat

Liquid Viscosity

Liquid Thermal Conductivity

Liquid Surface Tension

Vapour Pressure

Vapour Viscosity

Vapour Thermal Conductivity

Ideal-Gas Thermodynamic Properties

Equations of State

Properties of Mixtures

Notation

References

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## GENERAL

This section sets out the data sources, correlations and estimation methods used in the Delta T Props database. In putting together the database, the methods and sources were selected in the following order of preference.

- Published experimental data
- Published correlations based on experimental data
- Specific category correlations
- General estimation methods

Madison Technical Software has followed the general recommendations in Reid and in Danner and Daubert as far as selection of specific category correlations and general estimation methods are concerned. In selecting specific compound data, a combination of sources has been used wherever possible. Important sources of specific compound data used by Delta T Props are:

- Reid et al
- Perry et al
- J Chem Eng Data
- Daubert & Danner
- ESDU publications
- API Technical Data Book - Petroleum Refining
- International Critical Tables
- CRC Handbook
- Vargaftik

In many cases, the compound property values are a combination of published data, published correlations and general estimation methods. Several properties in certain compound categories have been estimated or adjusted by Madison Technical Software. It has been our policy to adopt and maintain a critical approach to available data sources and correlation methods.

The following sections set out details of the correlations and estimation methods used. In certain cases, the user is directed to the original references, particularly where the method is complex.

Data sources for Aqueous Solutions/Heat Transfer Liquids are published experimental data and correlations based on experimental data.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Critical Temperature

The great majority of values are believed to be experimental. Where values had to be estimated, the Joback method was used.

## Critical Pressure

Most of the values are experimental. In cases where experimental data were not available, the critical pressure was derived from the Joback method.

## Critical Volume

A majority of the values are experimental. A great majority of the remaining compounds for which experimental values were not available had accurate boiling-point volumes available from which critical volume estimates were derived using the Tyn and Calus correlation. For a few substances, estimates of the critical volume were derived from the Joback method.

## Normal Boiling Points

All values are believed to be experimental. In some cases, the values were slightly adjusted for vapour pressure.

## Freezing Points

Where possible, quoted freezing points are experimental. No accurate method of estimation of compound freezing point is available. In the absence of experimental data, a rough estimate was derived from the Joback method.

## Acentric Factors

The acentric factor is defined as

$$w = -\log_{10}(P_{vr} \text{ at } T_r = 0.7) - 1$$

In all cases the acentric factor was derived from the vapour pressure correlation ( see section 8.8)

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Joback Group Contribution Method

The Joback method is used to derive values of  $T_C$ ,  $P_C$ ,  $V_C$  and  $T_f$  where no experimental data or other predictive method was available.

$$T_C = T_b / (0.584 + 0.965 \text{ Sum}(D_t) - \text{Sum}(D_t)^2)$$

$$P_C = 1 / (0.113 + 0.0032 n_a - \text{Sum}(D_p))^2$$

$$V_C = 17.5 + \text{Sum}(D_v)$$

$$T_f = 122 + \text{Sum}(D_f)$$

where  $n_a$  is the number of atoms in the molecule and the D contributions are given by Joback and by Reid et al (1987). Error magnitudes for the Joback method are as follows:

Critical Temperature: average error about 1%

Critical Pressure: average error about 5%

Critical Volume: average error about 2%

Freezing Point: average error about 11%

## Tyn & Calus Relation

Tyn & Calus showed a close (< 3% error) relation between molar volume at normal boiling point and the critical molar volume of the form,

$$V_b = a V_C^n$$

$$a = 0.285$$

$$n = 1.048$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID SPECIFIC VOLUME

Liquid specific volume rises slowly and approximately linearly with rise in temperature to about  $T_r = 0.8$ . At higher temperatures, the values rise more rapidly to the critical point.

Experimental data or correlations derived from experimental data are available for most compounds.

### Hankinson-Brost-Thompson Equation

The saturated specific volume is given by,

$$V_S/V^* = V_r(0)(1 - w_{srk}V_r(1))$$

$$V_r(0) = \text{Sum}\{a_n(1 - T_r^n/3)\} \quad 0.25 < T_r < 0.95$$

$$V_r(1) = \text{Sum}\{b_n T_r^n / (T_r - 1.00001)\} \quad 0.25 < T_r < 1.0$$

$$a_0 = 1$$

$$a_1 = -1.52816$$

$$a_2 = 1.43907$$

$$a_3 = -0.81446$$

$$a_4 = 0.190454$$

$$b_0 = -0.296123$$

$$b_1 = 0.386914$$

$$b_2 = -0.0427258$$

$$b_3 = -0.0480645$$

$V^*$ ,  $w_{srk}$  and  $T_c$  are tabulated property constants. The user is referred to Hankinson, Thompson and to Reid et al (1987). Errors are typically about 1% with most being less than 2%.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID SPECIFIC VOLUME (Cont./...)

### Rackett Equation

If a reference volume ( $V_{ref}$  at  $T_{ref}$ ) is available then

$$Z_{ra} = (P_c V_{ref} / RT_c)^n$$

$$n = 1 / (1 + (1 - T_{ref} / T_c)^m)$$

$m = 2/7$  or other empirical constant

The saturated specific volume is given by,

$$V_s = V_{ref} Z_{ra}^x$$

with

$$x = -(1 - T_{ref} / T_c)^m + (1 - T / T_c)^m$$

In most cases, an experimental value of reference density was available. Where such a value was not available, values were derived from the group contribution method of Le Bas or derived from the critical volume using the Tyn & Calus relation. Tests by Madison Technical Software on over 80 liquids showed that these two methods were significantly more accurate than the Spencer and Danner method for  $Z_{ra}$ . The reader is referred to Reid et al for further details on these methods. With one or more experimental points, the Rackett equation gives errors of about 1% with most values less than 3%. If the reference volumes are estimated, typical errors are 3%.

### Liquid Expansivity

The liquid expansion coefficient is defined as

$$e = (1/V)dV/dT$$

Where  $V$  is the liquid specific volume.

This quantity is important in the study of heat transfer by natural convection and related topics. Liquid expansivity is computed by differentiation of the specific volume functions given by the Lee-Kesler and Wu & Stiel equations of state.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID SPECIFIC VOLUME (Cont./...)

### The Effect of Pressure on Liquid Specific Volume

The effect of pressure on liquid specific volume is derived from the equation of state as follows,

$$V_L = V_{Ls} - V_{Ls,es} + V_{L,es}$$

$V_L$  = specific volume at T and P

$V_{Ls}$  =  $V_L$  at T and  $P_s$  from methods of this section

$V_{Ls,es}$  =  $V_L$  at T and  $P_s$  from the equation of state

$V_{L,es}$  =  $V_L$  at T and P from the equation of state

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID SPECIFIC HEAT

Liquid specific heat can in principle be derived from the equation of state but in practise, direct analytical or group contributions are preferred where experimental data are not available. The majority of compounds have experimentally-derived correlations available for liquid specific heat.

### Rowlinson-Bondi Method

$$(C_{pL} - C_{p0})/R = 1.45 + 0.45/X + 0.25w(17.11 + 25.2X^{0.333}/T_r + 1.742/X)$$

$$X = 1 - T_r$$

w = acentric factor

This method is generally applicable to the range from  $T_f$  to values approaching  $T_c$ . Note that  $C_{pL}$  approaches infinity as T approaches  $T_c$ .

Errors are generally less than 5% except in the case of hydrogen-bonding polar compounds (e.g. alcohols) at low temperatures. For these compounds, the Missenard group contribution method is preferred.

### Missenard Method

The Missenard group contribution method yields values of coefficients in

$$C_{pL} = a + bT + cT^2$$

The accuracy is usually better than 5%. The method cannot deal with double bonds and is not applicable for  $T_r > 0.75$

$$a = \text{Sum}\{a_n\}$$

$$b = \text{Sum}\{b_n\}$$

$$c = \text{Sum}\{c_n\}$$

The group contributions are available in Missenard. See also Reid at al.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID SPECIFIC HEAT (Cont./...)

### The Effect of Pressure on Liquid Specific Heat

As noted above, the equations of state can be employed to estimate liquid specific heat, but the methods presented in 8.4.1 and 8.4.2 are more reliable. The equations of state however can be used to estimate the effect of pressure on liquid specific heat.

$C_{pLs} = C_{pL}$  at  $T_S$  and  $P_S$  determined by the methods of this section.

$C_{po}$  = ideal gas specific heat at  $T_S$

$C_{pL} = C_{pL}$  at  $T_S$  and  $P > P_S$

The equations of state give estimates of

$D_S = (C_{pLs} - C_{po})_{es}$  at  $T_S$  and  $P_S$

$D = (C_{pL} - C_{po})_{es}$  at  $T_S$  and  $P$

The corrected value of the liquid specific heat is

$C_{pL} = C_{pLs} + D - D_S$

The correction is not applied when  $T$  is close to  $T_C$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID VISCOSITY

A majority of the compounds in the database have experimentally-derived correlations for liquid viscosity available.

Liquid viscosity typically varies in magnitude by a factor of 100 or more between the freezing and critical temperatures. No generalized method is available to estimate or represent liquid viscosity adequately over the entire temperature range. Corresponding states methods are applicable above  $T_r = 0.76$ . From the freezing point to the boiling point, the influence of structure is strong.

### Method of Van Velzen

The method of Van Velzen et al is a group contribution method of some complexity and range of applicability. It is the most frequently used group contribution method. The accuracy of the estimation averages about 10% and most estimates are better than 20%. Some of the limitations of the method are:

Larger errors found with the first members of a homologous series  
Only normal and iso substitutions on alkyl chains can be treated  
Heterocyclic compounds cannot be treated  
Application only in the range  $T_f$  to  $T_b$

The method is complex and the reader is directed to the original references for full details.

### Method of Morris

The method of Morris is a group contribution method. This method is useful as a comparison and substitute for the Van Velzen method in cases where the Van Velzen method is not applicable. The accuracy of estimation is of the same order as Van Velzen. The limitations of the method are:

The method is less detailed than the Van Velzen method  
Applicable only in the range  $T_f$  to  $T_b$   
No explicit treatment for heterocyclics or esters (apart from acetates).

The Morris method takes the following form

$$\ln(v/v^*) = 2.3026 J(1/T_r - 1)$$

$$J = (0.577 + \text{Sum}(D_i))^{0.5}$$

The values of  $v^*$  are given for various categories of compounds. The constants  $v^*$  and the group contributions  $D$  are given in Morris.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID VISCOSITY (Cont./...)

### Method of Letsou and Stiel

This is a corresponding states method with applicability over  $0.76 < T_r < 1$ . The method also predicts the viscosity at the critical point ( $T_r = 1$ ). The accuracy is normally better than 5% up to  $T_r = 0.92$  with higher errors encountered as the critical point is approached. Overall this is an excellent estimation method for high-temperature liquid viscosity. The only serious limitation is the restricted range of applicability.

The form of the relation is

$$\nu = (f_0 + w.f_1)/A$$

with

$w$  = acentric factor

$$f_0 = a_0 + b_0 T_r + c_0 T_r^2$$

$$f_1 = a_1 + b_1 T_r + c_1 T_r^2$$

$$A = 0.176 \times 10^6 T_c^{0.1667} / M^{0.5} P_c^{0.667}$$

$$a_0 = 2.648$$

$$a_1 = 7.425$$

$$b_0 = -3.725$$

$$b_1 = -13.39$$

$$c_0 = 1.309$$

$$c_1 = 5.933$$

In the above relations  $P_c$  is in bar and the viscosity is in units of Pa-sec.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID VISCOSITY (Cont./...)

### Method of Przedziecki & Sridhar

In this method, the viscosity is related to changes in the specific volume.

$$\nu = V_0/E(V - V_0) \text{ centipoise}$$

$V$  = liquid molar volume in cc/mol

$$E = -1.12 + V_C/D$$

$$D = 12.94 + 0.1 M - 0.23 P_C + 0.0424 T_f - 11.58 T_f/T_C$$

$$V_0 = 0.0085 wT_C - 2.02 + V_f / \{0.342(T_f / T_C) + 0.894\}$$

with

$T_C$  = critical temperature, K

$P_C$  = critical pressure, bar

$V_C$  = critical volume, cc/mol

$M$  = molecular weight

$T_f$  = freezing point, K

$w$  = acentric factor

$V_f$  = specific volume at  $T_f$

The authors recommend that the volumes be estimated from the Gunn and Yamada equation. The reader is referred to Reid for a discussion on this method. The method is less accurate below reduced temperatures of about 0.55. Errors vary widely but will normally be less than 20% for  $T_r$  greater than 0.55.

This method is used in Delta T Props only where necessary. An error analysis by Reid et al indicates a higher level of error associated with this method than with the Van Velzen method for instance.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID VISCOSITY (Cont./...)

### Interpolation and Extrapolation

Two regions are typically covered well by available experimental data, experimental correlations and by the above relations:

$273 < T < 0.6 T_C$ : this region is normally covered by published data or by one of the methods 8.5.1, 8.5.2, 8.5.4

$0.76 T_C < T < T_C$ : this region is well covered by the method of Letsou and Stiel (section 8.5.3)

This leaves two regions which are often not covered by the above methods

$T_f < T < 273$ : this region may be covered by extrapolation using  $\ln(v)$  versus  $1/T$  extrapolation. The errors due to the extrapolation in practise will not normally exceed 10% with a possible 20% error in the immediate vicinity of the freezing point.

$0.6 T_C < T < 0.76 T_C$ : this region may be covered by interpolation between the  $273 < T < 0.6 T_C$  region and the  $0.76 T_C < T < T_C$  region using  $\ln(v)$  versus  $1/T$  interpolation. The errors due to interpolation in this case rarely exceed 5%.

### The Effect of Pressure on Liquid Viscosity

The method of Lucas is applied:

$$v_L/v_{sL} = (1 + B.FA)/(1 + w.C.F)$$

$v_L$  = viscosity at pressure  $P$

$v_{sL}$  = viscosity at saturation pressure  $P_S$

$$F = (P - P_S)/P_C$$

$w$  = acentric factor

$$A = 0.9991 - 0.0004674/(1.0523/T_r^{0.03877} - 1.0513)$$

$$B = 0.3257/(1.0039 - T_r^{2.573})^{0.2906} - 0.2086$$

$$C = -0.07921 + 2.1616 T_r - 13.404 T_r^2 + 44.1706 T_r^3 - 84.8291 T_r^4 + 96.1209 T_r^5 - 59.8127 T_r^6 + 15.6719 T_r^7$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID THERMAL CONDUCTIVITY

### Method of Latini et al

For specified categories of compounds, the method of Latini et al gives correlations for liquid conductivity for the range  $T_r = 0.3$  to  $0.8$

The correlations are in the form

$$k = A(1 - T_r)^{0.38}/T_r^{0.167}$$

$$A = A_0 T_b^{nM^m T_c^p}$$

Category	$A_0$	n	m	p
Alkanes	0.0035	1.2	-0.5	-0.167
Alkenes	0.0361	1.2	-1.0	-0.167
Cycloalkanes	0.0310	1.2	-1.0	-0.167
Aromatics	0.0346	1.2	-1.0	-0.167
Alcohols/Phenols	0.00339	1.2	-0.5	-0.167
Acids	0.00319	1.2	-0.5	-0.167
Ketones	0.00383	1.2	-1.0	-0.167
Esters	0.0415	1.2	-1.0	-0.167
Ethers	0.0385	1.2	-1.0	-0.167
Halides	0.494	0.0	-0.5	0.167
R20,R21,R22,R23	0.562	0.0	-0.5	0.167

Errors may be large for Diols and Glycols. The Acids equation is not applicable to Formic acid. The reader is referred to Reid for a discussion of the method.

### Method of Sato-Riedel

This method gives the following relation:

$$k = (1.11/M^{0.5})f(T_r)/f(T_{br})$$

with

$$f(X) = 3 + 20(1 - X)^{0.667}$$

This method gives poor results for low molecular weight or branched hydrocarbons. Errors otherwise are likely to be less than 15%. The method should not be applied for  $T_r > 0.8$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID THERMAL CONDUCTIVITY

### Method of Ely and Hanley

The method of Ely and Hanley has application to the high-temperature liquid region ( $T_r > 0.8$ ). There are few data available for high temperature liquid conductivities. The method of Ely and Hanley is probably the best method available. Error estimates are unknown.

This method is used in Delta T Props for  $T_r > 0.8$  with caution. It appears to give reasonable results for non-polar compounds. Errors with polar compounds can be large.

### The Effect of Pressure on Liquid Conductivity

The procedure derived from Missenard as presented in Danner and Daubert is employed:

$$k/k_S = 0.98 + 0.0079 P_r T_r^{1.4} + 0.63 T_r^{1.2} P_r / (30 + P_r)$$

$k$  = conductivity at  $P$

$k_S$  = conductivity at  $P_S$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID SURFACE TENSION

### Method of Brock and Bird

Brock and Bird give the following relation for non-polar liquids:

$$S = A.P_C^{0.667}T_C^{0.333}(0.132 r_C - 0.279)f(T_r)$$

$$f(T_r) = (1 - T_r)^{11/9}$$

$$A = 0.0004601$$

$P_C$  = critical pressure, Pa

$T_C$  = critical temperature, K

$r_C$  = the Riedel parameter at the critical point =  $4.83 w + 5.824$

$w$  = acentric factor

Errors can be expected to be less than 5%. This method is not applicable to quantum liquids.

### Method of Hakim et al

This method by Hakim et al is an extension of the Brock and Bird method to polar compounds.

$$S = A.P_C^{0.667}T_C^{0.333}Q_p((1 - T_r)/0.4)^M$$

with,

$$Q_p = 0.156 + 0.365 w - 1.754 X - 13.57 X^2 - 0.506 w^2 + 1.287 wX$$

$$M = 1.21 + 0.5385 w - 14.61 X - 32.07 X^2 - 1.656 w^2 + 22.03 wX$$

$$X = \text{Stiel Polar Factor} = \log(P_{VR} \text{ at } T_r = 0.6) + 1.70 w + 1.552$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## VAPOUR PRESSURE

The vapour pressure is expressed in its reduced form

$$P_{Vr} = P_V/P_C$$

Reduced vapor pressure varies from very low values at freezing point to unity at the critical point.

### Published Correlations

The experimental correlations are commonly given in the following formats:

Wagner Equation

$$\ln(P_{Vr}) = (aX + bX^{1.5} + cX^3 + dX^6)/T_r$$

with

$$X = 1 - T_r$$

FKT Equation

$$\ln(P_V) = a + b/T + c \ln(T) + dP_V/T^2$$

Antoine Equation

$$\ln(P_V) = a + b/(T + c)$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

VAPOUR PRESSURE (Cont./...)

## Gomez-Thodos Vapour Pressure Equation

Gomez-Nieto and Thodos give the following equation:

$$\ln(P_{VR}) = B(1/T_r^m - 1) + G(T_r^7 - 1)$$

$$G = aH + bB$$

$$a = (1 - 1/T_{br})/(T_{br}^7 - 1)$$

$$b = (1 - 1/T_{br}^m)/(T_{br}^7 - 1)$$

$$H = T_{br} \ln(P_c/P_b)/(1 - T_{br})$$

For non-polar compounds,

$$B = -4.267 - 221.79/(H^{2.5} \exp(0.038 H^{2.5})) + 3.8126/\exp(2272.33/H^3) + D$$

$$m = 0.78425 \exp(0.089315 H) - 8.5217/\exp(0.74826 H)$$

$$D = 0 \text{ except } D = \quad 0.41815 \text{ for He}$$

$$0.19904 \text{ for H}_2$$

$$0.02319 \text{ for Ne}$$

For polar non-hydrogen-bonding compounds (e.g. ammonia and acetic acid),

$$m = 0.466 T_c^{0.1667}$$

$$G = 0.08594 \exp(0.0007462 T_c)$$

$$B = (G - aH)/b$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

LIQUID VISCOSITY (Cont./...)

## Gomez-Thodos Vapour Pressure Equations

For polar hydrogen-bonding compounds (water, alcohols),

$$m = 0.0052 M^{0.29} T_C^{0.72}$$

$$G = (2.464.M) \exp(0.0000098 M T_C)$$

$$B = (G - aH)/b$$

The advantages of this method are,

fit guaranteed at  $T = T_D$  and  $T = T_C$   
good performance with polar compounds  
good performance over  $T_r = 0.5$  to  $1$

In addition, tests carried out by Madison Technical Software show the clear superiority of this method especially at low temperatures over the Lee-Kesler method.

## Lee-Kesler Vapour Pressure Equation

Lee and Kesler give the following vapour pressure equation:

$$\ln(P_{vr}) = f(0) + w.f(1)$$

$w$  = acentric factor

$$f(0) = 5.92714 - 6.09648/T_r - 1.28862 \ln(T_r) + 0.169347 T_r^6$$

$$f(1) = 15.2518 - 15.6875/T_r - 13.4721 \ln(T_r) + 0.43577 T_r^6$$

The characteristics of this equation are,  
guaranteed fit at  $T_r = 1$  and  $0.7$   
accurate for non-polar compounds

This equation is used in the Lee-Kesler and Wu & Stiel equations of state.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID VISCOSITY (Cont./...)

### Interpolation and Extrapolation

In many cases an accurate empirical equation is known which does not extend to the critical point or to the freezing point. The approach taken here is to fit the Wagner equation by least squares to the empirical equation and use the Wagner equation to extrapolate to the freezing point and to the critical point.

Extrapolation by this method to the critical method is a very accurate procedure. Extrapolation to the freezing point is less accurate but it does provide reasonable values.

In Delta T Props, the vapour pressure correlations set out in this section are used to provide the basic data. Empirical relations are used wherever possible.

### Database Vapour Viscosity Values

A majority of compounds in the database have experimentally-derived correlations for vapour viscosity. Where such values are not available, the Lucas methods set out below are used. In all cases, corrections for high pressure are carried out using the Lucas high-pressure correlation.

### The Methods of Lucas

The methods of Lucas are employed here. The equations take two forms:

Low Pressure (< 2 atm)

High Pressure (> 2 atm)

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID VISCOSITY (Cont./...)

### Low-Pressure Equation

$$v_0 = a_0 k_0 \{a_1 + a_2 T_r^n + a_3 \exp(a_4 T_r) + a_5 \exp(a_6 T_r)\} F_{p0} F_{q0}$$

$v_0$  = low pressure viscosity in kg/ms

$$k_0 = M^{0.5} P_c^{0.667} T_c^{0.1667}$$

with  $P_c$  in Pa and  $T_c$  in K

$a_0 = 0.0026373$	$a_1 = 0.018$
$a_2 = 0.807$	$a_3 = -0.357$
$a_4 = -0.449$	$a_5 = 0.340$
$a_6 = -4.058$	$n = 0.618$

The low pressure polar correlation is given by,

$F_{p0} = 1$	$0 < m_r < 0.022$
$F_{p0} = 1 + f(Z_c)$	$0.022 < m_r < 0.075$
$F_{p0} = 1 + f(Z_c) \cdot g(T_r)$	$0.075 < m_r$

$$f(Z_c) = 30.55(0.292 - Z_c)^{1.72}$$

$$g(T_r) = 0.96 + 0.1(T_r - 0.70)$$

$$m_r = 52.46 m^2 P_c / T_c^2$$

$m$  = dipole moment, debye

$P_c$  = critical pressure, bar

$T_c$  = critical temperature, K

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

LIQUID VISCOSITY (Cont./...)

## Low-Pressure Equation

In the above equations, if  $Z_C > 0.292$  the  $F_{p0}$  is taken as unity. There are only a few compounds that are polar with  $Z_C$  sufficiently larger than 0.292 to make  $F_{p0}$  significantly different from unity. The evidence in any case is scanty.

The low-pressure correction for quantum gases (hydrogen, helium and deuterium),  $F_{q0}$ , is given by,

$$F_{q0} = 1.22 Q^{0.15} \{1 - 0.00385(12 - T_r)^2/M\}$$

with

$$T_r < 12$$

$$Q = 1.38 \text{ for helium}$$

$$0.76 \text{ for hydrogen}$$

$$0.52 \text{ for deuterium}$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## High-Pressure Equation

Define,

$$Z_1 = v_0/a_0k_0$$

For  $T_r \leq 1$ , we define,

$$Z_2 = 0.60 + 0.76 P_r^m + (1 - T_r)(6.99P_r^n - 0.60)$$

$$m = 3.262 + 14.98 P_r^{5.508}$$

$$n = 1.39 + 5.746 P_r$$

For  $T_r > 1$  define,

$$Z_2 = Z_1\{1 + aP_r^e/(bP_r^f + 1/(1 + cP_r^d))\}$$

with,

$$a = (a_1/T_r)\exp(a_2T_r^n)$$

$$b = a(b_1T_r - b_2)$$

$$c = (c_1/T_r)\exp(c_2T_r^m)$$

$$d = (d_1/T_r)\exp(d_2T_r^p)$$

$$e = 1.3088$$

$$f = f_1\exp(f_2T_r^q)$$

$$a_1 = 0.001245 \quad a_2 = 5.1726 \quad n = -0.3286$$

$$b_1 = 1.6553 \quad b_2 = 1.2723$$

$$c_1 = 0.4489 \quad c_2 = 3.0578 \quad m = -37.7332$$

$$d_1 = 1.7368 \quad d_2 = 2.2310 \quad p = -7.6351$$

$$f_1 = 0.9425 \quad f_2 = -0.1853 \quad q = 0.4489$$

then,

$$Y = Z_2/Z_1$$

$$F_p = (1 + (F_{p0} - 1)Y^3)/F_{p0}$$

$$F_q = (1 + (F_{q0} - 1)(1/Y - 0.007(\ln(Y))^4))/F_{q0}$$

$$v = v_0YF_pF_q$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIQUID VISCOSITY (Cont./...)

### Database Vapour Conductivity Values

A majority of compounds in the database have experimentally-derived correlations for vapour conductivity. Where such values are not available, the Ely and Hanley method set out below is used. In all cases, corrections for high pressure are carried out using the Ely and Hanley high-pressure correlation.

### Ely and Hanley Method

The method of Ely and Hanley is adopted for both high and low pressure vapour conductivity. The method is based on hydrocarbon data but gives reasonable values for non-polar non-hydrocarbons. Errors are usually less than 10% except for highly polar compounds. There are few experimental data and no satisfactory correlations for high pressure conductivity for polar compounds.

The vapour conductivity is given by,

$$k = k_1 + k_2 + k_3$$

with,

$$k_1 = 1944 v_0 H (1 + 0.042332(C_{v0} - 3R/2))$$

$$k_2 = r_0 H (b_1 + b_2 (b_3 - \ln(T_0/b_4))^2)$$

$$k_3 = k_{30} k_{31} (k_{32} + k_{33} k_{34}) - 1$$

$$k_{30} = H/1000$$

$$k_{31} = \exp(a_1 + a_2/T_0)$$

$$k_{32} = \exp(a_3 + a_4/T_0^{1.5}) r_0^{0.1}$$

$$k_{33} = 6.1843 (r_0 - 1) r_0^{0.5}$$

$$k_{34} = a_5 + a_6/T_0 + a_7/T_0^2$$

The parameters in the above equations are given by:

$$v_0 = \text{low pressure methane viscosity} = \text{Sum}(c_n T_0^{(n-4)/3})$$

$$c_1 = 2.90774E-01$$

$$c_2 = -3.31287E-01$$

$$c_3 = 1.60810E-01$$

$$c_4 = -4.33190E-02$$

$$c_5 = 7.06248E-03$$

$$c_6 = -7.11662E-04$$

$$c_7 = 4.32517E-05$$

$$c_8 = -1.44591E-06$$

$$c_9 = 2.03712E-08$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## VAPOUR CONDUCTIVITY

### Ely and Hanley Method

$$H = 16.04 f^{0.5} / M h^{0.667}$$

$C_{v0}$  = low pressure specific heat at constant volume in J/mol.K

R = gas constant = 8.314 J/mol.K

M = molecular weight g/mol

$$f = T_c F_1 / 190.4$$

$$h = V_c F_2 / 99.2$$

$T_c$  = critical temperature, K

$V_c$  = critical volume, cc/mol

$$F_1 = 1 + (w - 0.011)(0.56553 - 0.86276 \ln(T^*) - 0.69852/T^*)$$

$$F_2 = \{1 + (w - 0.011)(0.3949(V^* - 1.02355)$$

$$0.93281(V^* - 0.75464)\ln(T^*)\}(0.288/Z_c)$$

w = acentric factor

$Z_c$  = critical compressibility

$$T^* = T_r \text{ for } T_r \leq 2$$

$$= 2 \text{ otherwise}$$

$$V^* = V/V_c \text{ for } 0.5 < V/V_c < 2$$

$$= 0.50 \text{ for } V/V_c \leq 0.50$$

$$= 2 \text{ otherwise}$$

$$b_1 = -2.5276E-04$$

$$b_2 = 3.3433E-04$$

$$b_3 = 1.1200E+00$$

$$b_4 = 1.6800E+02$$

$$a_1 = -7.1977E+00$$

$$a_2 = 8.5678E+01$$

$$a_3 = 1.2472E+01$$

$$a_4 = -9.8463E+02$$

$$a_5 = 3.5947E-01$$

$$a_6 = 6.9798E+01$$

$$a_7 = -8.7288E+02$$

$$r_0 = 16.04 h/V$$

$$T_0 = T/f$$

V = specific volume, cc/mol

T = temperature, K

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## IDEAL GAS THERMODYNAMIC PROPERTIES

Ideal gas thermodynamic properties (i.e. at low pressure) are required for the estimation of the thermodynamic properties of liquids and gases. A majority of the database compounds have experimentally-derived correlations for the ideal gas thermodynamic properties.

### Method of Joback

For those substances not covered by published correlations, the group contribution method of Joback is used to estimate  $C_{p0}$  and the heats of formation.

$$C_{p0} = a + bT + cT^2 + dT^3$$

with,

$$a = \text{Sum}(n_j D_a) - 37.93$$

$$b = \text{Sum}(n_j D_b) + 0.210$$

$$c = \text{Sum}(n_j D_c) - 3.91E-04$$

$$d = \text{Sum}(n_j D_d) + 2.06E-07$$

where  $n_j$  is the number of groups of type  $j$  and the  $D$  contributions are for this type of group.  $T$  is in deg K. The user is referred to Joback for details. Reid et al (1987) gives values of the group contributions. The error associated with this method is usually less than 3%.

### Low-temperature values of $C_{p0}$

To our knowledge, no general estimation method exists for  $C_{p0}$  below about 260 K. In addition, empirical datapoints and correlations in this region are not generally available. In order to extend the applicability of the estimation methods to temperatures below 260 K, extrapolation of known values and correlations was investigated by Madison Technical Software.

Extrapolation as far as 50 K (-223 C) using monotonic power functions fitted to known values at higher temperatures gave estimates whose error did not exceed 10% at 50 K and which averaged about 2% in the range 100 K to 273 K. This extrapolation was tested against known values for over 80 hydrocarbons and non-hydrocarbons. Thermodynamic properties calculated are limited in Delta T Props to temperatures above minus 100 C.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## IDEAL GAS THERMODYNAMIC PROPERTIES (Cont./...)

### Derived Ideal Gas Properties

Ideal gas enthalpy and entropy are derived by integration of the ideal gas specific heat:

The ideal gas enthalpy,  $h_0$ , is given by the integral of  $C_{p0}$  from  $T_0$  to  $T$

$$h_0(T) = [C_0T + C_1T^2/2 + C_2T^3/3 + C_3T^4/4]$$

evaluated between  $T_0$  and  $T$ .

The ideal gas entropy is given by the integral of  $C_{p0}/T$  from  $T_0$  to  $T$

$$s_0(T) = [C_0\ln T + C_1T + C_2T^2/2 + C_3T^3/3]$$

evaluated between  $T_0$  and  $T$ .  $T_0$  is a zero-value reference temperature. The specific heat at constant volume is simply related to the specific heat at constant pressure:

$$C_{v0} = C_{p0} - R$$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## THE EQUATIONS OF STATE

### General

The two equations of state employed in Delta T Props are as follows:

The Lee-Kesler equation of state for non-polar compounds with moderate values of acentric factor

The Wu & Stiel equation of state for polar compounds or those with extreme values of acentric factor

The equations of state are used to predict the following vapor properties:

- Specific Volume
- Compressibility
- Expansion Coefficient
- Specific Heats
- Enthalpy/Internal Energy
- Entropy
- Heat of Vaporisation

The following liquid properties are predicted by this method:

- Heat of Vaporisation
- Pressure Correction to Specific Heat
- Enthalpy/Internal Energy
- Entropy
- Expansion Coefficient
- Pressure Correction to Specific Volume

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## THE EQUATIONS OF STATE (Cont./...)

### The Lee-Kesler Equation of State

The Lee-Kesler equation of state is a three-parameter ( $T_C$ ,  $P_C$  and  $w$ ) equation explicit in pressure with general applicability to compounds with low polarity and moderate acentric factors. The Lee-Kesler equation defines two fluids as follows,

- a simple fluid with zero acentric factor
- a reference fluid with acentric factor = 0.3978

The specific volume and other properties for any fluid are determined by interpolation between the simple fluid properties and the reference fluid properties using acentric factor as the interpolating variable. The properties of the simple and reference fluids are determined by a pair of PVT equations with identical form but with different parameters.

We define,

$$P_r = P/P_C \quad T_r = T/T_C \quad V_r = P_C V / RT_C$$

where  $P$ ,  $P_C$ ,  $T$  and  $T_C$  are the actual and critical pressures and the actual and critical temperatures of the fluid of interest.

First,  $V_r(0)$  is calculated using the constants for the simple fluid. Then  $V_r(r)$  is calculated using the constants for the reference fluid. From these quantities,  $Z(0)$  and  $Z(r)$  are calculated:

$$Z(0) = P_r V_r(0) / T_r \quad Z(r) = P_r V_r(r) / T_r$$

The compressibility of the fluid of interest is calculated using,

$$Z = A(0)Z(0) + A(r)Z(r)$$

$$A(0) = 1 - w/w(r)$$

$$A(r) = w/w(r)$$

$w$  = acentric factor for fluid of interest

$w(r)$  = acentric factor for reference fluid (0.3978)

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## THE EQUATIONS OF STATE (Cont./...)

### The Lee-Kesler Equation of State

The expansion coefficient, specific heat departures, enthalpy and, entropy departures are derived from the simple and reference PVT equations using the relations detailed in Lee and Kesler and in Reid and elsewhere. The component simple fluid and reference fluid values are combined by using relations of the same form shown above for compressibility. Danner & Daubert give typical maximum error values 20 kJ/kg for vapor enthalpy and 70 kJ/kg for liquid enthalpy. Typical errors for specific volume of vapors are 1 to 2%.

### The Wu & Stiel Equation of State

The Wu & Stiel equation of state is a four-parameter equation of state developed as an extension to the Lee-Kesler equation of state to cover polar compounds and compounds with high values of acentric factor. The parameters of this equation of state are,

Critical Temperature,  $T_C$

Critical Pressure,  $P_C$

Acentric Factor,  $w$

Polarity Factor,  $Y$

The Wu and Stiel equation of state uses three reference fluids as follows:

simple fluid with zero acentric factor

reference fluid with acentric factor = 0.3978

polar fluid (water) with acentric factor = 0.344 and polarity factor = 1.0

The specific volume and other properties for any fluid of interest are determined by interpolation between the properties of the reference fluids using acentric factor and polarity factor as interpolating variables.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## THE EQUATIONS OF STATE (Cont./...)

### The Wu and Stiel Equation of State

The properties of the simple and reference fluids are determined from the Lee-Kesler equation of state. The properties of the polar fluid are determined from the Keenan equation of state for water. With  $P_r$  and  $T_r$  for the fluid of interest,

$$Z(0) = P_r V_r(0) / T_r \text{ from simple fluid equation}$$

$$Z(r) = P_r V_r(r) / T_r \text{ from reference fluid equation}$$

$$Z(p) = P_r V_r(p) / T_r \text{ from polar fluid equation}$$

$$Z = A(0)Z(0) + A(r)Z(r) + A(p)Z(p)$$

$$A(0) = (1 - Y) - (w/w(r) - Yw(p)/w(r))$$

$$A(r) = w/w(r) - Yw(p)/w(r)$$

$$A(p) = Y$$

$$A(0) + A(r) + A(p) = 1$$

When  $Y = 0$  these equations reduce to the non-polar Lee-Kesler formula. When  $Y = 1$  and  $w = w(p)$ , they reduce to the Keenan equation of state for water.

The expansion coefficient, specific heat departures, enthalpy, internal energy and entropy departures are derived from the simple, reference and polar PVT equations. The component simple fluid, reference fluid and polar fluid values are combined using relations of the same form as shown above in the case of compressibility. The polarity factor is determined from empirical density data in accordance with the relations set out by Wu and Stiel. Wu & Stiel report excellent results using this equation of state for polar compounds. Errors in specific volume were less than 1 to 2% for example for the vapour phase.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## THE EQUATIONS OF STATE (Cont./...)

### Calculation of Saturation Values

Fluid properties along the saturation line are solved for as follows. For a given value of  $T_r$ ,

The simple fluid component properties are solved at  $T_r, P_{Sr}^{(0)}$  where this latter quantity is the Lee-Kesler reduced saturation pressure at  $T_r$  and  $w = 0$

The reference fluid component properties are solved at  $T_r$  and  $P_{Sr}^{(r)}$  where this latter quantity is the Lee-Kesler reduced saturation pressure at  $T_r$  and  $w = 0.3978$

The polar fluid component properties are solved at  $T_r$  and  $P_{Sr}^{(p)}$  which is the reduced water saturation pressure at  $T_r$  with  $P_{Sr}^{(p)} = P_S^{(p)}/P_C^{(p)}$

The compressibility of the fluid of interest is found by,

$$Z_S = A(0)Z_S(0) + A(r)Z_S(r) + A(p)Z_S(p)$$

This relation gives the saturation state of the fluid of interest by interpolation between the saturation states of the simple, reference and polar fluids at  $T_r$  rather than by interpolation between the three fluids at  $T_r$  and  $P_{Sr}$  where this latter quantity is the reduced vapour pressure of the fluid of interest.

The above relations are presented for the case of the Wu & Stiel equation of state. The relations for the Lee-Kesler equation of state may be obtained by setting the polar contribution equal to zero.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## THE EQUATIONS OF STATE (Cont./...)

### Enthalpy and Entropy Scales

All enthalpy and entropy values are quoted relative to a reference zero-value temperature  $T_0$ . This temperature is taken in all cases to be the higher of 273.15 K and the normal melting point.

Two cases can be distinguished:

If the critical temperature is greater than or equal to 273.15 K then the enthalpy and entropy of the saturated liquid are taken to be zero at  $T_0$ . In this case the enthalpy and entropy functions are,

$$h(T,P) - h_{Ls}(T_0) = [h(T,P) - h_v(T,P_0)]_{es} + [h_0(T_0,T)]_{ig} - [h_{Ls}(T_0) - h_v(T_0,P_0)]_{es}$$

$$s(T,P) - s_{Ls}(T_0) = [s(T,P) - s_v(T,P_0)]_{es} + [s_0(T_0,T)]_{ig} - [s_{Ls}(T_0) - s_v(T_0,P_0)]_{es}$$

If the critical temperature is less than 273.15 then the enthalpy and entropy of the low-pressure vapour are taken to be zero at  $T_0$ . In this case the enthalpy and entropy functions are,

$$h(T,P) - h_v(T_0,P_0) = [h(T,P) - h_v(T,P_0)]_{es} + [h_0(T_0,T)]_{ig}$$

$$s(T,P) - s_v(T_0,P_0) = [s(T,P) - s_v(T,P_0)]_{es} + [s_0(T_0,T)]_{ig}$$

The zero point for water is taken to be 273.16 K in accordance with the Keenan equation of state for water. Liquid enthalpy and entropy are zero at that temperature and saturation conditions.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES OF MIXTURES

### Scope of Correlations

The software provides the user with the facility of defining mixtures of compounds in the database which then may be stored in the database for future use. The properties of mixtures are calculated using the techniques set out in this section. The user should note the following:

A mixture can be formulated using any components in the database except other mixtures, aqueous solutions, heat transfer liquids and User-Defined Liquids.

No check is carried out by the software on the chemical stability, compatibility or miscibility of the selected components or the defined mixture. The user must be satisfied as to the physical reasonableness of the formulation of the mixture.

The accuracy of the calculated properties can be expected to be better when the selected components are chemically similar to each other. The accuracy of the calculated properties of very dissimilar components is not known but may only be order-of-magnitude in some cases. It is to be expected that the errors involved with mixtures of non-polar compounds will be less than with mixtures of polar compounds.

The range of applicability of the correlations is as follows:

A low-limit temperature is defined corresponding to the mole-average of the reduced melting points of the mixture components. Properties cannot be accessed at temperatures lower than this. A high-limit temperature of 1300 K or the pseudocritical temperature (whichever is the greater) is defined for vapour properties. Vapour properties cannot be accessed at temperatures greater than this. The high limit temperature for liquid mixture properties is the pseudocritical temperature of the mixture as defined by the Lee-Kesler rules. Liquid properties cannot be accessed at temperatures higher than this.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES OF MIXTURES (Cont./...)

### Mixture Critical Properties

#### Critical Temperature

$$T_C = \text{Sum}(x_i V_{Ci} T_{Ci}) / \text{Sum}(x_i V_{Ci})$$

where  $x_i$ ,  $V_{Ci}$  and  $T_{Ci}$  are the mole fraction, critical volume and critical temperature of component  $i$ . The reference used here is Li. This method is generally recommended by Reid and by Danner and Daubert. Deviations for binary hydrocarbon mixtures can be expected to be less than 4 K. Errors for multicomponent hydrocarbon mixtures average about 11 K. Errors for binary mixtures of non-hydrocarbons would be of this order.

#### Critical Volume

$$V_C = \text{Sum}(a_i V_{Ci}) + \text{Sum}(a_i a_j b_{ij}) \text{ (all } i, j)$$

$$a_i = x_i V_{Ci}^{2/3} / \text{Sum}(x_i V_{Ci})$$

$$b_{ii} = 0 \quad b_{ij} = 2c_{ij}(V_{Ci} + V_{Cj})$$

$$c_{ij} = A_{ij} + B_{ij}d_{ij} + C_{ij}d_{ij}^2 + D_{ij}d_{ij}^3 + E_{ij}d_{ij}^4$$

$$d_{ij} = \text{ABS}\{(V_{Ci}^{2/3} - V_{Cj}^{2/3}) / (V_{Ci}^{2/3} + V_{Cj}^{2/3})\}$$

The binary constants  $A_{ij}$  thru  $E_{ij}$  are given by,

A	B	C	D	E			
Aromatic-Aromatic			all zero				
with a Cycloalkane			all zero				
Alkane-Aromatic			0.0753	-3.332	2.22	0	0
with CO <sub>2</sub> or H <sub>2</sub> S			-0.4957	17.119	-168.56	587.05	-698.89
All others			0.1397	-2.9672	1.8337	-1.536	0

The reference for this method is Schick and Prausnitz. An average error of 10% can be expected for binary mixtures.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES OF MIXTURES (Cont./...)

### Mixture Critical Properties

#### Critical Pressure

$$w_m = \text{Sum}(x_i w_i)$$

$$T_{cm} = \text{Sum}(Z_i T_{ci})$$

$$Z_i = x_i V_{ci} / \text{Sum}(x_i V_{ci})$$

$$T_{cm}^* = \text{Sum}(x_i T_{ci})$$

$$P_{cm}^* = \text{Sum}(x_i P_{ci})$$

$$P_c = P_{cm}^* [1 + (5.808 + 4.93 w_m)(T_{cm} / T_{cm}^* - 1)]$$

This method is based on a simplification of the method of Kreglenski and Kay as amended by Spencer, Daubert and Danner. Errors in the application of this method average about one bar - see Reid et al for details. This method is not applied when the mixture contains inorganic components. In this case the critical pressure is taken equal to the Lee-Kesler pseudocritical pressure.

#### Acentric Factor

In accordance with the Lee-Kesler rules,

$$w = \text{Sum}(x_i w_i)$$

$w_i$  = component acentric factor

$x_i$  = component mole fraction

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES OF MIXTURES (Cont./...)

### Mixture Liquid Specific Volume

The specific volume of a liquid mixture is taken to be the mole-average of the component specific volumes at the same reduced temperature.

The mixture liquid specific volume is given by,

$$V_m = \text{Sum}(x_{ij}M_iV_j) / M_m$$

where,

$V_m$  = mixture specific volume at  $T = T_r T_{cm}$   
 $V_j$  = component specific volume at  $T = T_r T_{cj}$   
 $T_r$  = the reduced temperature  
 $T_{cm}$  = mixture pseudocritical temperature  
 $T_{cj}$  = component critical temperature  
 $M_m$  = mixture molecular weight  
 $M_i$  = component molecular weight  
 $x_i$  = component mole fraction

The specific heat of a liquid mixture is taken to be the mole-average of the component specific heats.

The mixture liquid specific heat is given by,

$$C_m = \text{Sum}(x_j M_j C_j) / M_m$$

where,

$C_m$  = mixture specific heat  
 $C_j$  = component specific heat  
 $M_m$  = mixture molecular weight  
 $M_j$  = component molecular weight  
 $x_j$  = component mole fraction

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES OF MIXTURES (Cont./...)

### Mixture Liquid Viscosity

The mixture liquid viscosity is given by,

$$\ln(v_m) = \text{Sum}\{x_i \ln(v_i)\}$$

where,

$v_m$  = mixture viscosity

$v_i$  = component viscosity

$x_i$  = component mole fraction

### Mixture Liquid Conductivity

The method of Li is adopted for the calculation of conductivities of liquid mixtures.

The mixture liquid conductivity is given by,

$$k_m = \sum_i \sum_j \phi_i \phi_j k_{ij}$$

$$k_{ij} = 2 / (1/k_i + 1/k_j)$$

$$\phi_i = x_i V_i / \sum_j x_j V_j$$

where,

$k_m$  = mixture conductivity

$k_i$  = component conductivity

$x_i$  = component mole fraction

$V_i$  = component molar volume

### Mixture Surface Tension

The methods developed for pure components (Brock & Bird, Hakim et al) are applied directly to mixtures. The mixture pseudocritical properties are used in place of the pure compound critical properties.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROPERTIES OF MIXTURES (Cont./...)

### Vapour Pressure

Accurate determination of the vapour pressures of mixtures normally requires a full vapour-liquid equilibrium model with knowledge of interaction parameters. Such a VLE model is not a part of Delta T Props. In Delta T Props, however, an approximation is used in order to be able to determine the mixture phase for given input T and P. The Lee-Kesler mixing rules give for the acentric factor,

$$w_m = \text{Sum}(x_i w_i)$$

$$w_i = -\log(P_{Vri} \text{ at } T_r = 0.7) - 1$$

$$w_m = -\log(P_{Vrm} \text{ at } T_r = 0.7) - 1 = \text{Sum}(-x_i \log(P_{Vri} \text{ at } T_r = 0.7) - x_i)$$

hence,

$$\log(P_{Vrm} \text{ at } T_r = 0.7) = \text{Sum}(x_i \log(P_{Vri} \text{ at } T_{ri} = 0.7))$$

### Thermodynamic Properties of Mixtures

The Lee-Kesler and Wu & Stiel equations of state are used to calculate the thermodynamic properties of liquid and vapour phases for all pure compounds in the database. To calculate the thermodynamic properties of mixtures, a set of pseudocritical constants are defined for each mixture and the properties are calculated in the usual way.

Delta T Props uses the original Lee-Kesler rules as follows:

$$Z_{ci} = 0.2905 - 0.085 w_i$$

$$V_{ci} = Z_{ci} R_0 T_{ci} / P_{ci}$$

$$V_{cm} = \text{Sum}(x_i x_j (V_{ci}^{1/3} + V_{cj}^{1/3})^3) / 8$$

$$T_{cm} = \text{Sum}(x_i x_j (V_{ci}^{1/3} + V_{cj}^{1/3})^3 (T_{ci} T_{cj})^{1/2}) / (8 V_{cm})$$

$$w_m = \text{Sum}(x_i w_i)$$

$$M_m = \text{Sum}(x_i M_i)$$

$$Z_{cm} = 0.2905 - 0.085 w_m$$

$$P_{cm} = R_0 Z_{cm} T_{cm} / V_{cm}$$

$$R_0 = \text{Gas Constant}$$

The Stiel polarity factor for a polar mixture is computed from the mixture liquid specific volume

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## THERMODYNAMIC AND TRANSPORT PROPERTIES OF MIXTURES

### Vapour Viscosity

The method of Wilke is used to compute the viscosity of vapour mixtures.

$$\mu_m = \sum_j \{x_j \mu_j / \sum_k x_k \phi_{jk}\}$$

with

$$\phi_{jk} = [1 + (\mu_j / \mu_k)^{0.5} (M_k M_j)^{0.25}]^2 / [8(1 + M_j / M_k)]^{0.5}$$

with

$\mu_m$  = mixture viscosity  
 $\mu_j$  = component viscosity  
 $M_j$  = component molecular weight  
 $x_j$  = mole fraction

### Vapour Conductivity

The method of Mason and Saxena is used to compute the conductivity of vapour mixtures

$$k_m = \sum_j \{x_j k_j / \sum_k x_k \phi_{jk}\}$$

with

$$\phi_{jk} = [1 + (\mu_j / \mu_k)^{0.5} (M_k M_j)^{0.25}]^2 / [8(1 + M_j / M_k)]^{0.5}$$

$k_j$  = component conductivity  
 $k_m$  = mixture conductivity  
 $\mu_j$  = component viscosity  
 $M_j$  = component molecular weight  
 $x_j$  = mole fraction

### Ideal-Gas Mixture Properties

Ideal-gas mixture properties are taken as the mole fraction of the pure component properties. The pure component properties are defined per mole of substance.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## NOTATION

C	Specific Heat
e	Expansion Coefficient
h	Enthalpy
log	Logarithm to base 10
ln	Natural Logarithm
m	Dipole Moment
M	Molecular Weight
P	Pressure
R	Gas Constant
r	Riedel Parameter
s	Entropy
S	Surface Tension
T	Temperature
v	Viscosity
V	Specific Volume
w	Acentric Factor
x	Mole Fraction
Y	Wu & Stiel Polarity Factor
Z	Compressibility

## Subscripts

b	Boiling
c	Critical
es	Equation of State
f	Freezing
ig	Ideal Gas
L	Liquid
m	Mixture
Low	Pressure
p	Constant Pressure
ra	Rackett
ref	Reference
r	Reduced
s	Saturated
v	Vapour
v	Constant Volume

## Superscripts

Simple Fluid  
Reference Fluid  
Polar Fluid

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

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Version 5 – Volume 2

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Version 5 – Volume 2

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# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROCESS CALCULATOR

### Introduction

The software offers the user the ability to compute isentropic (efficiency = 100%), non-isentropic (efficiency < 100%) and adiabatic (efficiency = 0%) processes using most compounds drawn from the database. Aqueous Solutions and Heat Transfer Liquids and User-Defined Liquids cannot be used in the Process Calculator. User-Defined Mixtures and User-Defined Compounds (from Delta T Props2) can be used in the Process Calculator.

Processes can be either compressions or expansions.

### Input Screen

Saturated or unsaturated conditions are chosen from the list box. For saturated conditions, the user specifies the initial pressure and quality (Quality = 0 for pure liquid and = 100% for dry vapor). The quality can be any value from 0% to 100%. The user selects the final pressure and the efficiency of the process (Efficiency = 100% for isentropic, < 100% for non-isentropic and 0% for adiabatic). Efficiency is defined in the following way

For expansion processes,

$$h_3 = h_1 + e(h_2 - h_1)$$

For compression processes,

$$h_3 = h_1 + (h_2 - h_1)/e$$

where

$h_1$  = initial enthalpy

$h_2$  = enthalpy after isentropic process

$h_3$  = enthalpy after non-isentropic process

$e$  = efficiency of process

It follows from the definition of efficiency that efficiency cannot be zero for a compressive process. For an expansion process, the efficiency can be zero – in this case an adiabatic expansion is computed (defined by  $h_3 = h_1$ )

### Output Screen

The output screen gives details of properties for both the initial and final states. If either state is saturated, then the output also gives details of the properties for each phase. The properties detailed are pressure, temperature, quality (if saturated), specific volume, enthalpy and entropy. Output can be sent to a printer.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROCESS CALCULATOR (Cont./...)

### Calculation Structure

The outline of the calculation method in the Process Calculator is as follows:

#### Stage 1: Initial Conditions

Initial conditions are set by the user as either saturated or unsaturated.

If conditions are saturated, saturated properties ( $T$ ,  $V$ ,  $h$ ,  $s$ ) are computed at  $P_1$  for both liquid and vapour

If conditions are unsaturated the follows steps are followed:

If  $P_1 < P_c$  and  $T_1 < T_{1sat}$  then subcooled liquid properties are computed at  $P_1$  and  $T_1$

If  $P_1 > P_c$  and  $T_1 < T_c$  then compressed liquid properties are computed.

If  $P_1 > P_c$  and  $T_1 > T_c$  then supercritical fluid properties are computed

#### Stage 2: After Isentropic change from Stage 1

$$s_2 = s_1$$

$$\text{Set } T_2 = T_1$$

If  $P_2 \geq P_c$  then the program iterates for  $T_2$  for the known values of  $P_2$  and  $s_2$  and then computes other properties at  $P_2$ ,  $T_2$

If  $P_2 < P_c$  and  $s_2 < s_{2Lsat}$  the subcooled liquid properties are computed

If  $P_2 < P_c$  and  $s_2 > s_{2Vsat}$  then superheated vapor properties are computed

If  $P_2 < P_c$  and  $s_2 > s_{2Lsat}$  and  $s_2 < s_{2Vsat}$  the saturated vapor and liquid properties are computed, the quality of the vapor/liquid mix and the combined mixture properties.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## PROCESS CALCULATOR (Cont./...)

### Calculation Structure

#### Stage 3: Non-Isentropic change from Stage 1

$$P_3 = P_2$$
$$s_3 \geq s_2$$

$$\text{For } P_2 < P_1, \quad h_3 = h_1 + (h_2 - h_1)e$$

$$\text{For } P_2 > P_1, \quad h_3 = h_1 + (h_2 - h_1)/e$$

where  $e$  is the process efficiency

if  $P_3 \geq P_c$  then the program iterates to  $T_3$  at known  $P_3, s_3$  (with starting value  $T_2$ ) for either compressed liquid or supercritical fluid.

For  $P_3 < P_c$  and  $h_3 < h_{3Lsat}$ , subcooled liquid properties are computed

For  $P_3 < P_c$  and  $h_3 > h_{3Vsat}$  superheated vapour properties are computed

For  $P_3 < P_c$  and  $h_3 > h_{3Lsat}$  and  $h_3 < h_{3Vsat}$ , saturated properties (liquid and vapor) and computed, the mixture quality and the combined mixture properties.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIST OF COMPOUNDS

### Formula-Order List of Names

Air	
Ar	argon
BCl <sub>3</sub>	boron trichloride
Br <sub>2</sub>	bromine
Cl <sub>2</sub>	chlorine
SiCl <sub>4</sub>	silicon tetrachloride
TiCl <sub>4</sub>	titanium tetrachloride
D <sub>2</sub> O	deuterium oxide
F <sub>2</sub>	fluorine
He	helium
Hg	mercury
I <sub>2</sub>	iodine
NO	nitric oxide
NO <sub>2</sub>	nitrogen dioxide
N <sub>2</sub>	nitrogen
N <sub>2</sub> O	nitrous oxide
Ne	neon
O <sub>2</sub>	oxygen
SO <sub>2</sub>	sulfur dioxide
O <sub>3</sub>	ozone
SO <sub>3</sub>	sulfur trioxide
HBr	hydrogen bromide
HCl	hydrogen chloride
HF	hydrogen fluoride
HI	hydrogen iodide
H <sub>2</sub>	hydrogen
H <sub>2</sub> O	water
H <sub>2</sub> S	hydrogen sulfide
NH <sub>3</sub>	ammonia
PH <sub>3</sub>	phosphine
N <sub>2</sub> H <sub>4</sub>	hydrazine
SiH <sub>4</sub>	silane
CBrClF <sub>2</sub>	bromochlorodifluoromethane
CBrCl <sub>3</sub>	bromotrichloromethane
CBr <sub>2</sub> F <sub>2</sub>	dibromodifluoromethane
CBrF <sub>3</sub>	trifluorobromomethane
CClF <sub>3</sub>	chlorotrifluoromethane
CCl <sub>2</sub> F <sub>2</sub>	dichlorodifluoromethane
COCl <sub>2</sub>	phosgene
CCl <sub>3</sub> F	trichlorofluoromethane
CCl <sub>4</sub>	carbon tetrachloride
CF <sub>4</sub>	carbon tetrafluoride
CO	carbon monoxide
COS	carbonyl sulfide

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

CO2	carbon dioxide
CS2	carbon disulfide
CHBr3	tribromomethane
CHClF2	chlorodifluoromethane
CHCl2F	dichloromonofluoromethane
CHCl3	chloroform
CHF3	fluoroform
HCN	hydrogen cyanide
CH2Br2	dibromomethane
CH2BrCl	bromochloromethane
CH2Cl2	dichloromethane
CH2F2	difluoromethane
COH2	formaldehyde
CO2H2	formic acid
CH3Br	methyl bromide
CH3Cl	methyl chloride
CH3F	methyl fluoride
CH3I	methyl iodide
CH3NO	formamide
CH3NO2	nitromethane
CH4	methane
CH4O	methanol
CH4S	methyl mercaptan
CH5N	methyl amine
C2BrF3	bromotrifluoroethylene
2Br2ClF3	1,2-dibromo-1-chlorotrifluoroethane
C2Br2F4	1,2-dibromotetrafluoroethane
C2ClF3	chlorotrifluoroethylene
C2ClF5	chloropentafluoroethane
C2Cl2F4	1,1-dichlorotetrafluoroethane
C2Cl2F4	1,2-dichlorotetrafluoroethane
C2Cl3F3	1,2,2-trichlorotrifluoroethane
C2Cl4	tetrachloroethylene
C2Cl4F2	1,1,2,2-tetrachlorodifluoroethane
C2F3N	trifluoroacetonitrile
C2F4	perfluoroethylene
C2F6	perfluoroethane
C2N2	cyanogen
C2HClF2	1-chloro-2,2-difluoroethylene
C2HClF4	chloro-1,1,2,2-tetrafluoroethane
C2HCl3	trichloroethylene
C2HCl5	pentachloroethane
C2HF3O2	trifluoroacetic acid
C2H2	acetylene
C2H2Cl2	1,1-dichloroethylene
C2H2Cl2	cis-1,2-dichloroethylene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C2H2Cl2	trans-1,2-dichloroethylene
C2H2Cl4	1,1,1,2-tetrachloroethane
C2H2Cl4	1,1,2,2-tetrachloroethane
C2H2F2	1,1-difluoroethene
C2H2O	ketene
C2H3Cl	vinyl chloride
C2H3ClF2	1-chloro-1,1-difluoroethane
C2H3ClO	acetyl chloride
C2H3Cl3	1,1,1-trichloroethane
C2H3Cl3	1,1,2-trichloroethane
C2H3F	vinyl fluoride
C2H3F3	1,1,1-trifluoroethane
C2H3N	acetonitrile
C2H3NO	methyl isocyanate
C2H4	ethylene
C2H4Br2	1,2-dibromoethane
C2H4Cl2	1,1-dichloroethane
C2H4Cl2	1,2-dichloroethane
C2H4F2	1,1-difluoroethane
C2H4O	acetaldehyde
C2H4O	ethylene oxide
C2H4O2	acetic acid
C2H4O2	methyl formate
C2H5Br	ethyl bromide
C2H5Cl	ethyl chloride
C2H5F	ethyl fluoride
C2H5I	ethyl iodide
C2H5NO	acetamide
C2H6	ethane
C2H6O	dimethyl ether
C2H6O	ethanol
C2H6O2	ethylene glycol
C2H6S	ethyl mercaptan
C2H6S	dimethyl sulfide
C2H7N	ethyl amine
C2H7N	dimethylamine
C2H7NO	monoethanolamine
C2H8N2	ethylenediamine
C3ClF5O	chloropentafluoroacetone
C3F6O	perfluoroacetone
C3F8	perfluoropropane
C3H3F3	trifluoropropene
C3H3F5	1,1,1,2,2-pentafluoropropane
C3H3N	acrylonitrile
C3H3NO	oxazole
C3H3NO	isoxazole

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C3H4	propadiene
C3H4	methyl acetylene
C3H4O	acrolein
C3H4O2	acrylic acid
C3H4O2	vinyl formate
C3H5Cl	allyl chloride
C3H5Cl3	1,2,3-trichloropropane
C3H5N	propionitrile
C3H6	cyclopropane
C3H6	propylene
C3H6Cl2	1,2-dichloropropane
C3H6O	acetone
C3H6O	allyl alcohol
C3H6O	propionaldehyde
C3H6O	1,2-propylene oxide
C3H6O	1,3-propylene oxide
C3H6O	vinyl methyl ether
C3H6O2	propionic acid
C3H6O2	ethyl formate
C3H6O2	methyl acetate
C3H7Cl	propyl chloride
C3H7Cl	isopropyl chloride
C3H8	propane
C3H8O	1-propanol
C3H8O	isopropyl alcohol
C3H8O	methyl ethyl ether
C3H8O2	methylal
C3H8O2	1,2-propanediol
C3H8O2	1,3-propanediol
C3H8S	methyl ethyl sulfide
C3H9N	n-propyl amine
C3H9N	isopropyl amine
C3H9N	trimethyl amine
C4F8	perfluorocyclobutane
C4F10	perfluorobutane
C4H4	vinylacetylene
C4H4O	furan
C4H4S	thiophene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIST OF COMPOUNDS

### Formula-Order List of Names

C4H5Cl	chloroprene
C4H5N	allyl cyanide
C4H5N	pyrrole
C4H6	1-butyne
C4H6	2-butyne
C4H6	1,2-butadiene
C4H6	1,3-butadiene
C4H6O2	vinyl acetate
C4H6O3	acetic anhydride
C4H6O4	dimethyl oxalate
C4H6O4	succinic acid
C4H7N	butyronitrile
C4H6O2	methyl acrylate
C4H8	1-butene
C4H8	cis-2-butene
C4H8	trans-2-butene
C4H8	cyclobutane
C4H8	isobutylene
C4H8O	n-butyraldehyde
C4H8O	isobutyraldehyde
C4H8O	methyl ethyl ketone
C4H8O	tetrahydrofuran
C4H8O	vinyl ethyl ether
C4H8O2	n-butyric acid
C4H8O2	isobutyric acid
C4H8O2	1,4-dioxane
C4H8O2	ethyl acetate
C4H8O2	methyl propionate
C4H8O2	n-propyl formate
C4H8S	tetrahydrothiophene
C4H9Cl	1-chlorobutane
C4H9Cl	2-chlorobutane
C4H9Cl	tert-butyl chloride
C4H9N	pyrrolidine
C4H9NO	morpholine
C4H10	n-butane
C4H10	isobutane
C4H10N2	piperazine
C4H10O	1-butanol
C4H10O	2-butanol
C4H10O	isobutanol
C4H10O	tert-butanol
C4H10O	diethyl ether

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C4H10O	methyl propyl ether
C4H10O	methyl isopropyl ether
C4H10O2	1,2-dimethoxyethane
C4H10O2	1,3-butanediol
C4H10O2	1,4-butanediol
C4H10S	diethyl sulfide
C4H10S2	diethyl disulfide
C4H11N	n-butyl amine
C4H11N	isobutyl amine
C4H11N	diethyl amine
C5F12	perfluoropentane
C5H2F6O2	hexafluoroacetylacetone
C5H4O2	furfural
C5H5N	pyridine
C5H6N2	2-methyl pyrazine
C5H6O	2-methyl furan
C5H8	cyclopentene
C5H8	1,2-pentadiene
C5H8	cis-1,3-pentadiene
C5H8	trans-1,3-pentadiene
C5H8	1,4-pentadiene
C5H8	1-pentyne
C5H8	isoprene
C5H8	3-methyl-1,2-butadiene
C5H8O	cyclopentanone
C5H8O	dihydropyran
C5H8O2	ethyl acrylate
C5H10	cyclopentane
C5H10	1-pentene
C5H10	cis-2-pentene
C5H10	trans-2-pentene
C5H10	2-methyl-1-butene
C5H10	2-methyl-2-butene
C5H10	3-methyl-1-butene
C5H10O	valeraldehyde
C5H10O	methyl propyl ketone
C5H10O	methyl isopropyl ketone
C5H10O	diethyl ketone
C5H10O	2-methyl tetrahydrofuran
C5H10O	tetrahydropyran
C5H10O2	n-valeric acid
C5H10O2	isovaleric acid
C5H10O2	isobutyl formate
C5H10O2	n-propyl acetate
C5H10O2	ethyl propionate
C5H10O2	methyl butyrate

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C5H10O2	methyl isobutyrate
C5H11N	piperidine
C5H12	n-pentane
C5H12	2-methyl butane
C5H12	2,2-dimethylpropane
C5H12O	1-pentanol
C5H12O	2-methyl-1-butanol
C5H12O	3-methyl-1-butanol
C5H12O	3-methyl-2-butanol
C5H12O	2-methyl-2-butanol
C5H12O	2,2-dimethyl-1-propanol
C5H12O	ethyl propyl ether
C5H12O	butyl methyl ether
C5H12O	tert-butyl methyl ether
C6BrF5	bromopentafluorobenzene
C6ClF5	chloropentafluorobenzene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIST OF COMPOUNDS

### Formula-Order List of Names

C6Cl2F4	dichlorotetrafluorobenzene
C6Cl3F3	1,3,5-trichlorotrifluorobenzene
C6Cl6	perchlorobenzene
C6F6	perfluorobenzene
C6F12	perfluorocyclohexane
C6F14	perfluoro-n-hexane
C6F14	perfluoro-2-methylpentane
C6F14	perfluoro-3-methylpentane
C6F14	perfluoro-2,3-dimethylbutane
C6HF5	pentafluorobenzene
C6HF5O	pentafluorophenol
C6H2F4	1,2,3,4-tetrafluorobenzene
C6H2F4	1,2,3,5-tetrafluorobenzene
C6H2F4	1,2,4,5-tetrafluorobenzene
C6H4Cl2	o-dichlorobenzene
C6H4Cl2	m-dichlorobenzene
C6H4Cl2	p-dichlorobenzene
C6H4F2	1,4-difluorobenzene
C6H5Br	bromobenzene
C6H5Cl	chlorobenzene
C6H5F	fluorobenzene
C6H5I	iodobenzene
C6H5NO2	nitrobenzene
C6H6	benzene
C6H6O	phenol
C6H7N	aniline
C6H7N	2-methylpyridine
C6H7N	3-methylpyridine
C6H7N	4-methyl pyridine
C6H10	1,5-hexadiene
C6H10	cyclohexene
C6H10O	cyclohexanone
C6H11N	capronitrile
C6H12	cyclohexane
C6H12	methylcyclopentane
C6H12	1-hexene
C6H12	2-hexene,cis
C6H12	2-hexene,trans
C6H12	3-hexene,cis
C6H12	3-hexene,trans
C6H12	2-methyl-1-pentene
C6H12	4-methyl-1-pentene
C6H12	2-methyl-2-pentene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C6H12	3-methyl-2-pentene,cis
C6H12	3-methyl-2-pentene,trans
C6H12	4-methyl-2-pentene,cis
C6H12	4-methyl-2-pentene,trans
C6H12	2,3-dimethyl-1-butene
C6H12	2,3-dimethyl-2-butene
C6H12	3,3-dimethyl-1-butene
C6H12O	cyclohexanol
C6H12O	ethyl propyl ketone
C6H12O	methyl butyl ketone
C6H12O	methyl isobutyl ketone
C6H12O2	n-butyl acetate
C6H12O2	isobutyl acetate
C6H12O2	ethyl butyrate
C6H12O2	ethyl isobutyrate
C6H12O2	n-propyl propionate
C6H12O2	n-amyl formate
C6H12O2	isoamyl formate
C6H12O3	paraldehyde
C6H14	n-hexane
C6H14	isohexane
C6H14	3-methyl pentane
C6H14	2,2-dimethyl butane
C6H14	2,3-dimethyl butane
C6H14O	1-hexanol
C6H14O	2-hexanol
C6H14O	ethyl butyl ether
C6H14O	methyl amyl ether
C6H14O	dipropyl ether
C6H14O	diisopropyl ether
C6H15N	dipropylamine
C6H15N	diisopropylamine
C6H15N	triethylamine
C7F8	perfluorotoluene
C7F14	perfluoromethylcyclohexane
C7F16	perfluoro-n-heptane
C7H3F5	2,3,4,5,6-pentafluorotoluene
C7H5N	benzotrile
C7H6O	benzaldehyde
C7H6O2	benzoic acid
C7H7Cl	benzyl chloride
C7H8	toluene
C7H8O	anisole
C7H8O	benzyl alcohol
C7H8O	o-cresol

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C7H8O	m-cresol
C7H8O	p-cresol
C7H9N	2,3-dimethylpyridine
C7H9N	2,4-dimethylpyridine
C7H9N	2,5-dimethylpyridine
C7H9N	2,6-dimethylpyridine
C7H9N	3,4-dimethylpyridine
C7H9N	3,5-dimethylpyridine
C7H9N	N-methyl aniline
C7H9N	o-toluidine
C7H9N	m-toluidine
C7H9N	p-toluidine
C7H9N	benzylamine
C7H14	cycloheptane
C7H14	1,1-dimethylcyclopentane
C7H14	1,2-dimethylcyclopentane-cis
C7H14	1,2-dimethylcyclopentane-trans
C7H14	ethylcyclopentane
C7H14	methylcyclohexane
C7H14	1-heptene
C7H14	2,3,3-trimethyl-1-butene
C7H14O	methyl amyl ketone
C7H14O2	n-propyl butyrate
C7H14O2	n-propyl isobutyrate
C7H14O2	isoamyl acetate
C7H14O2	isobutyl propionate
C7H16	n-heptane
C7H16	2-methylhexane
C7H16	3-methylhexane
C7H16	2,2-dimethylpentane
C7H16	2,3-dimethylpentane
C7H16	2,4-dimethylpentane
C7H16	3,3-dimethylpentane
C7H16	3-ethylpentane
C7H16	2,2,3-trimethylbutane
C7H16O	1-heptanol
C8H4O3	phthalic anhydride
C8H7N	indole
C8H8	styrene
C8H8O	methyl phenyl ketone
C8H8O2	methyl benzoate
C8H8O3	methyl salicylate
C8H10	o-xylene
C8H10	m-xylene
C8H10	p-xylene
C8H10	ethylbenzene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C8H10O	o-ethylphenol
C8H10O	m-ethylphenol
C8H10O	p-ethylphenol
C8H10O	ethyl phenyl ether
C8H10O	2,3-xylenol
C8H10O	2,4-xylenol
C8H10O	2,5-xylenol
C8H10O	2,6-xylenol
C8H10O	3,4-xylenol
C8H10O	3,5-xylenol
C8H11N	N,N-dimethyl aniline
C8H11N	N-ethyl aniline
C8H14O4	diethylsuccinate
C8H16	1,1-dimethylcyclohexane
C8H16	1,2-dimethylcyclohexane-cis
C8H16	1,2-dimethylcyclohexane-trans
C8H16	1,3-dimethylcyclohexane-cis
C8H16	1,3-dimethylcyclohexane-trans
C8H16	1,4-dimethylcyclohexane-cis
C8H16	1,4-dimethylcyclohexane-trans
C8H16	ethylcyclohexane
C8H16	1,1,2-trimethylcyclopentane
C8H16	1,1,3-trimethylcyclopentane
C8H16	1,2,4-trimethylcyclopentane-c,c,t
C8H16	1,2,4-trimethylcyclopentane-c,t,c
C8H16	1-methyl-1-ethylcyclopentane
C8H16	n-propylcyclopentane
C8H16	isopropylcyclopentane
C8H16	cyclooctane
C8H16	1-octene
C8H16	2-octene-trans
C8H16O2	isoamyl propionate
C8H16O2	isobutyl butyrate
C8H16O2	isobutyl isobutyrate
C8H16O2	n-propyl isovalerate
C8H18	n-octane
C8H18	2-methylheptane
C8H18	3-methylheptane
C8H18	4-methylheptane
C8H18	2,2-dimethylhexane
C8H18	2,3-dimethylhexane
C8H18	2,4-dimethylhexane
C8H18	2,5-dimethylhexane
C8H18	3,3-dimethylhexane
C8H18	3,4-dimethylhexane
C8H18	3-ethylhexane

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C8H18	2,2,3-trimethylpentane
C8H18	2,2,4-trimethylpentane
C8H18	2,3,3-trimethylpentane
C8H18	2,3,4-trimethylpentane
C8H18	2-methyl-3-ethylpentane
C8H18	3-methyl-3-ethylpentane
C8H18	2,2,3,3-tetramethylbutane
C8H18O	1-octanol
C8H18O	2-octanol
C8H18O	4-methyl-3-heptanol
C8H18O	5-methyl-3-heptanol
C8H18O	2-ethyl-1-hexanol
C8H18O	dibutyl ether
C8H18O	di-tert-butyl ether
C8H19N	dibutyl amine
C8H19N	diisobutyl amine
C9H7N	quinoline
C9H7N	isoquinoline
C9H10	indane
C9H10	alpha-methylstyrene
C9H10O2	ethyl benzoate
C9H12	n-propylbenzene
C9H12	isopropylbenzene
C9H12	1-methyl-2-ethylbenzene
C9H12	1-methyl-3-ethylbenzene
C9H12	1-methyl-4-ethylbenzene
C9H12	1,2,3-trimethylbenzene
C9H12	1,2,4-trimethylbenzene
C9H12	1,3,5-trimethylbenzene
C9H13N	N,N-dimethyl-o-toluidine
C9H18	n-propylcyclohexane
C9H18	isopropylcyclohexane
C9H18	1,trans-3,5-trimethylcyclohexane
C9H18	1-nonene
C9H18O	dibutyl ketone
C9H20	n-nonane
C9H20	2-methyloctane
C9H20	2,2-dimethylheptane
C9H20	2,2,3-trimethylhexane
C9H20	2,2,4-trimethylhexane
C9H20	2,2,5-trimethylhexane
C9H20	3,3-diethylpentane
C9H20	2,2,3,3-tetramethylpentane
C9H20	2,2,3,4-tetramethylpentane
C9H20	2,2,4,4-tetramethylpentane

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C9H20	2,3,3,4-tetramethylpentane
C9H20O	1-nonanol
C10F8	perfluoronaphthalene
C10H8	naphthalene
C10H12	1,2,3,4-tetrahydronaphthalene
C10H14	n-butylbenzene
C10H14	isobutylbenzene
C10H14	sec-butylbenzene
C10H14	tert-butylbenzene
C10H14	1-methyl-2-isopropylbenzene
C10H14	1-methyl-3-isopropylbenzene
C10H14	1-methyl-4-isopropylbenzene
C10H14	1,4-diethylbenzene
C10H14	1,2,3,5-tetramethylbenzene
C10H14	1,2,4,5-tetramethylbenzene
C10H14O	thymol
C10H15N	n-butylaniline
C10H18	cis-decalin
C10H18	trans-decalin
C10H18	1,3-decadiene
C10H19N	caprylonitrile
C10H20	butylcyclohexane
C10H20	isobutylcyclohexane
C10H20	sec-butylcyclohexane
C10H20	tert-butylcyclohexane
C10H20	1-decene
C10H20O	menthol
C10H22	n-decane
C10H22	3,3,5-trimethyl heptane
C10H22	2,2,3,3-tetramethylhexane
C10H22	2,2,5,5-tetramethylhexane
C10H22O	1-decanol
C11H10	1-methylnaphthalene
C11H10	2-methylnaphthalene
C11H14O2	butyl benzoate
C11H16	pentamethylbenzene
C11H22	n-hexylcyclopentane
C11H22	1-undecene
C11H24	n-undecane
C12H10	diphenyl
C12H10O	diphenyl ether
C12H18	hexamethylbenzene
C12H24	n-heptylcyclopentane
C12H24	1-dodecene
C12H26	dodecane
C12H26O	dihexylether

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

C12H26O	dodecanol
C12H27N	tributylamine
C13H12	diphenylmethane
C13H26	n-octylcyclopentane
C13H26	1-tridecene
C13H28	n-tridecane
C14H10	anthracene
C14H10	phenanthrene
C14H12O2	benzyl benzoate
C14H28	n-nonylcyclopentane
C14H28	1-tetradecene
C14H30	n-tetradecane
C15H30	n-decylcyclopentane
C15H30	1-pentadecene
C15H32	n-pentadecane
C16H10	pyrene
C16H22O4	dibutyl-o-phthalate
C16H32	n-decylcyclohexane
C16H32	1-hexadecene
C16H34	hexadecane
C17H34	n-dodecylcyclopentane
C17H36O	heptadecanol
C17H36	n-heptadecane
C18H14	o-terphenyl
C18H14	m-terphenyl
C18H14	p-terphenyl
C18H36	1-octadecene
C18H36	n-tridecylcyclopentane
C18H38	octadecane
C18H36O	1-octadecanol
C19H38	1-cyclopentyltetradecane
C19H40	n-nonadecane
C20H40	1-cyclopentylpentadecane
C20H42	n-eicosane
LDB001	calcium chloride 4%
LDB002	calcium chloride 8%
LDB003	calcium chloride 12%
LDB004	calcium chloride 16%
LDB005	calcium chloride 20%
LDB006	calcium chloride 24%
LDB007	calcium chloride 28%
LDB008	Dowtherm A
LDB009	Dowtherm G
LDB010	Dowtherm HT
LDB011	Dowtherm J
LDB012	Dowtherm LF

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

LDB013	Dowtherm Q
LDB014	ethanol 10%
LDB015	ethanol 20%
LDB016	ethanol 30%
LDB017	ethanol 40%
LDB018	ethanol 50%
LDB019	ethanol 60%
LDB020	ethanol 70%
LDB021	ethanol 80%
LDB022	ethanol 90%
LDB023	ethylene glycol 10%
LDB024	ethylene glycol 20%
LDB025	ethylene glycol 30%
LDB026	ethylene glycol 40%
LDB027	ethylene glycol 50%
LDB028	ethylene glycol 60%
LDB029	ethylene glycol 70%
LDB030	ethylene glycol 80%
LDB031	ethylene glycol 90%
LDB032	methanol 10%
LDB033	methanol 20%
LDB034	methanol 30%
LDB035	methanol 40%
LDB036	methanol 50%
LDB037	methanol 60%
LDB038	methanol 70%
LDB039	methanol 80%
LDB040	methanol 90%
LDB041	propylene glycol 10%
LDB042	propylene glycol 20%
LDB043	propylene glycol 30%
LDB044	propylene glycol 40%
LDB045	propylene glycol 50%
LDB046	propylene glycol 60%
LDB047	propylene glycol 70%
LDB048	propylene glycol 80%
LDB049	propylene glycol 90%
LDB050	sodium chloride 4%
LDB051	sodium chloride 8%
LDB052	sodium chloride 12%
LDB053	sodium chloride 16%
LDB054	sodium chloride 20%
LDB055	sodium chloride 24%
LDB056	Therminol LT
LDB057	Therminol 44
LDB058	Therminol 55

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Formula-Order List of Names (Cont./...)

LDB059	Therminol 59
LDB060	Therminol 60
LDB061	Therminol 66
LDB062	Therminol 75
LDB063	Therminol VP-1
LDB064	Syltherm 800
LDB065	Syltherm XLT

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## LIST OF COMPOUNDS

### Alphabetical List of Compound Names and Synonyms

acetylene  
acetylene dichloride  
acetylene dichloride  
acetylene tetrachloride  
acetyl chloride  
acetic chloride  
acetonitrile  
acetene  
acetaldehyde  
acetic acid  
acetamide  
acrylonitrile  
acrolein  
acrylic acid  
acetone  
acetic anhydride  
acetic oxide  
acetic ether  
2-acetylpropane  
1-acetoxypropane  
acetophenone  
adipic ketone  
Air  
allene  
allylene  
allyl aldehyde  
allyl chloride  
allyl trichloride  
allyl alcohol  
allyl cyanide  
alpha-isoamylene  
alpha-chlorotoluene  
alpha-methylstyrene  
ammonia  
aminic acid  
aminomethane  
aminoethane  
2-amino-ethanol  
1-amino-2-methylpropane  
amylene  
amyl aldehyde  
aminobenzene  
amyl carbinol

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

1-amino-2-methylbenzene  
aniline  
anisole  
anthracene  
argon  
argon-40  
Arcton 9  
azole  
azacyclopentane  
azine  
azabenzene  
azacyclohexane  
1-azanaphthalene  
2-azanaphthalene  
beta propylene glycol  
benzene  
benzol  
benzenamine  
benzonitrile  
benzaldehyde  
benzene carbonal  
benzoic acid  
benzene carboxylic acid  
benzyl chloride  
benzyl alcohol  
benzene methanol  
benzylamine  
benzene methanamine  
2-benzene dicarboxylic anhydride  
benzopyrrole  
1-benzazole  
2-benzanine  
benzylbenzene  
benzyl benzoate  
biphenyl  
boron trichloride  
bromine  
bromochlorodifluoromethane  
bromotrichloromethane  
bromoform  
bromochloromethane  
bromotrifluoroethylene  
bromotrifluoroethene  
bromoethane  
bromopentafluorobenzene  
bromobenzene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

1-buten-3-yne  
1-butyne  
2-butyne  
1,2-butadiene  
1,3-butadiene  
butanedioic acid  
butyronitrile  
butanenitrile  
1-butene  
1-butylene  
butanal  
2-butanone  
butylene oxide  
1-butanol  
2-butanol  
1,3-butanediol  
1,4-butanediol  
1-butanamine  
1-butylamine  
butanecarboxylic acid  
butyl methyl ether  
butylethylene  
1-butyl acetate  
butyl ethanoate  
butyl ethyl ether  
butylcyclohexane  
butyl benzoate  
carbon trichlorobromide  
carbonyl chloride  
carbon tetrachloride  
carbon tetrafluoride  
carbon monoxide  
carbonic oxide  
carbonyl sulfide  
carbon oxide sulfide  
carbon oxysulfide  
carbon dioxide  
carbonic acid gas  
carbon disulfide  
carbon bisulfide  
carbamaldehyde  
carbinamine  
carbomethene  
carboxyethane  
carbolic acid  
capronitrile

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

capryl alcohol  
camphor tar  
caprylonitrile  
calcium chloride 4%  
calcium chloride 8%  
calcium chloride 12%  
calcium chloride 16%  
calcium chloride 20%  
calcium chloride 24%  
calcium chloride 28%  
chlorine  
chlorotrifluoromethane  
chloroformyl chloride  
chlorodifluoromethane  
chloroform  
chloromethane  
chlorotrifluoroethylene  
chlorotrifluoroethene  
chloropentafluoroethane  
1-chloro-2,2-difluoroethylene  
chloro-1,1,2,2-tetrafluoroethane  
chloroethene  
1-chloro-1,1-difluoroethane  
chlorothene  
chloroethane  
chloropentafluoroacetone  
3-chloroprene  
3-chloro-1-propene  
1-chloropropane  
2-chloropropane  
chloroprene  
2-chloro-1 3-butadiene  
1-chlorobutane  
2-chlorobutane  
2-chloro-2-methyl propane  
2-chloroisobutane  
chloropentafluorobenzene  
chlorobenzene  
chloromethylbenzene  
chinoline  
cis-1,2-dichloroethylene  
cis-2-butene  
cis-1,3-petadiene  
cis-piperylene  
cis-2-pentene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

cis-beta-amylene  
cis-decalin  
cis-decahydronaphthalene  
crotonylene  
2-cresol  
3-cresol  
4-cresol  
cumene  
cyanogen  
cyanoethylene  
cyclopropane  
cyclobutane  
cyclopentene  
cyclopentanone  
cyclopentane  
cyclohexene  
cyclohexanone  
cyclohexane  
cyclohexanol  
cyanobenzene  
cycloheptane  
cyclooctane  
1-cyclopentyltetradecane  
1-cyclopentylpentadecane  
deuterium oxide  
2-deoxyglycerol  
decafluorobutane  
1,3-decadiene  
1-decene  
1-decanol  
decyl alcohol  
dibromodifluoromethane  
dichlorodifluoromethane  
dithiocarbonic anhydride  
difluorochloromethane  
dichloromonofluoromethane  
dibromomethane  
dichloromethane  
difluoromethane  
1,2-dibromo-1-chlorotrifluoroethane  
1,2-dibromotetrafluoroethane  
1,1-dichlorotetrafluoroethane  
1,2-dichlorotetrafluoroethane  
1,1-dichloroethylene  
1,1-difluoroethene  
1,2-dibromoethane

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

1,1-dichloroethane  
1,2-dichloroethane  
1,1-difluoroethane  
dimethyl  
dimethyl ether  
dimethyl sulfide  
dimethyl thioether  
dimethylamine  
dimethylenediamine  
dimethylenemethane  
1,2-dichloropropane  
dimethyl ketone  
dimethyl methane  
dimethyl carbinol  
dimethoxymethane  
diviyene sulfide  
dimethylacetylene  
divinyl  
dimethyl oxalate  
dimethylethylene  
1,4-dioxane  
diethylene dioxide  
diethylene ether  
diethyleneimide oxide  
diethylene oximide  
diethyl  
diethyl ether  
1,2-dimethoxyethane  
diethyl sulfide  
diethylthioether  
diethyl disulfide  
diethyl amine  
dihydropyran  
diethyl ketone  
dimethyl acetone  
2,2-dimethylpropane  
2,2-dimethyl-1-propanol  
dichlorotetrafluorobenzene  
2-dichlorobenzene  
1 3-dichlorobenzene  
1 4-dichlorobenzene  
1,4-difluorobenzene  
2,3-dimethyl-1-butene  
2,3-dimethyl-2-butene  
3,3-dimethyl-1-butene  
2,2-dimethyl butane

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

2,3-dimethyl butane  
diisopropyl  
dipropyl ether  
diisopropyl ether  
dipropylamine  
diisopropylamine  
diethylaminoethane  
2,3-dimethylpyridine  
2,4-dimethylpyridine  
2,5-dimethylpyridine  
2,6-dimethylpyridine  
3,4-dimethylpyridine  
3,5-dimethylpyridine  
1,1-dimethylcyclopentane  
1,2-dimethylcyclopentane-cis  
1,2-dimethylcyclopentane-trans  
dipropyl methane  
2,2-dimethylpentane  
2,3-dimethylpentane  
diethyldimethylmethane  
2,4-dimethylpentane  
3,3-dimethylpentane  
3-dimethyl phenol  
2 4-dimethyl phenol  
2 5-dimethyl phenol  
2 6-dimethyl phenol  
4-dimethyl phenol  
3 5-dimethyl phenol  
dimethylaminobenzene  
diethylsuccinate  
diethyl butanedioate  
1,1-dimethylcyclohexane  
1,2-dimethylcyclohexane-cis  
1,2-dimethylcyclohexane-trans  
1,3-dimethylcyclohexane-cis  
1,3-dimethylcyclohexane-trans  
1,4-dimethylcyclohexane-cis  
1,4-dimethylcyclohexane-trans  
2,2-dimethylhexane  
2,3-dimethylhexane  
2,4-dimethylhexane  
2,5-dimethylhexane  
3,3-dimethylhexane  
3,4-dimethylhexane  
diethylpropylmethane  
dibutyl ether

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

dibutyl oxide  
di-n-butyl ether  
di-tert-butyl ether  
dibutyl amine  
di-n-butyl amine  
diisobutyl amine  
dibutyl ketone  
2,2-dimethylheptane  
3,3-diethylpentane  
1,4-diethylbenzene  
diphenyl  
diphenyl ether  
dihexylether  
diphenylmethane  
ditane  
dibutyl-o-phthalate  
1 2-diphenylbenzene  
1 3-diphenylbenzene  
1 4-diphenylbenzene  
Dowtherm E  
1-dodecene  
dodecane  
dodecanol  
Dowtherm A  
Dowtherm G  
Dowtherm HT  
Dowtherm J  
Dowtherm LF  
Dowtherm Q  
dry ice  
durene  
epoxyethane  
epoxypropane  
essence of niobe  
ethanedinitrile  
ethane pentachloride  
ethyne  
ethenone  
ethylene monochloride  
ethanoyl chloride  
ethane trichloride  
ethyl nitrile  
ethylene  
ethene  
ethylene dibromide  
ethylidene dichloride

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

ethylene dichloride  
ethylidene difluoride  
ethanal  
ethyl aldehyde  
ethylene oxide  
ethanoic acid  
ethyl bromide  
ethyl chloride  
ethyl fluoride  
ethyl iodide  
ethanamide  
ethane  
ethyl hydride  
ethanol  
ethyl alcohol  
ethylene glycol  
ethylene alcohol  
ethanediol  
ethyl mercaptan  
ethanethiol  
ethyl thioalcohol  
ethyl amine  
ethanamine  
ethylenediamine  
ethenyl methanoate  
ethyl cyanide  
ethyl formate  
ethyl methanoate  
ethylformic ester  
ethyl carbinol  
ethynyl ethene  
ethylacetylene  
ethenyl ethanoate  
ethenyl acetate  
ethanoic anhydride  
ethanedicarboxylic acid  
ethylethylene  
ethoxyethene  
ethyl ethenyl ether  
ethylacetic acid  
ethyl acetate  
ethyl ethanoate  
ethyl methyl carbinol  
ether  
ethoxyethane  
ethylene glycol dimethyl ether

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

ethyl thioethane  
ethyl acrylate  
ethyl propenoate  
ethyl propionate  
ethyl propanoate  
ethyldimethylmethane  
ethyl propyl ether  
1-ethoxypropane  
ethyl propyl ketone  
ethyl n-propyl ketone  
ethyl butyrate  
ethyl butanoate  
ethyl n-butyrate  
ethyl isobutyrate  
ethyl isobutanoate  
ethyl-2-methylpropionate  
ethyl butyl ether  
ethylcyclopentane  
3-ethylpentane  
ethyl benzene  
ethylbenzene  
ethylbenzol  
1-ethyl-2-hydroxybenzene  
1-ethyl-3-hydroxybenzene  
1-ethyl-4-hydroxybenzene  
ethyl phenyl ether  
ethoxybenzene  
ethylaminobenzene  
ethylcyclohexane  
3-ethylhexane  
2-ethyl-1-hexanol  
ethyl benzoate  
2-ethyltoluene  
3-ethyltoluene  
4-ethyltoluene  
ethanol 10%  
ethanol 20%  
ethanol 30%  
ethanol 40%  
ethanol 50%  
ethanol 60%  
ethanol 70%  
ethanol 80%  
ethanol 90%  
ethylene glycol 10%  
ethylene glycol 20%

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

ethylene glycol 30%  
ethylene glycol 40%  
ethylene glycol 50%  
ethylene glycol 60%  
ethylene glycol 70%  
ethylene glycol 80%  
ethylene glycol 90%  
fluorine  
fluoroform  
fluoromethane  
fluoroethene  
fluoroethylene  
fluoroethane  
fluorobenzene  
formonitrile  
formaldehyde  
formic acid  
formamide  
formal  
Freon 12B1  
Freon 12B2  
Freon 13B1  
Freon 13  
Freon 12  
Freon 11  
Freon 10  
Freon 14  
Freon 22  
Freon 21  
Freon 20  
Freon 23  
Freon 30  
Freon 32  
Freon 41  
Freon 114B2  
Freon 115  
Freon 114  
Freon 112  
Freon 116  
Freon 142  
Freon 143  
Freon 152A  
furan  
furanidine  
furfural  
2-furancarboxaldehyde

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

2-furaldehyde  
glycerol trichlorohydrin  
Halon 1211  
Halon 1202  
Halon 1301  
Halon  
Halon 14  
Halon 1011  
heavy water  
helium  
helium-4  
hexafluoroethane  
hexahydropyrazine  
hexafluoroacetylacetone  
hexahydropyridine  
hexafluorobenzene  
1,5-hexadiene  
hexahydrobenzene  
hexamethylene  
1-hexene  
2-hexene,cis  
2-hexene,trans  
3-hexene,cis  
3-hexene,trans  
2-hexanone  
hexane  
1-hexanol  
2-hexanol  
1-heptene  
1-heptylene  
2-heptanone  
heptane  
1-heptanol  
heptyl alcohol  
hemimellitene  
hexamethylbenzene  
1-hexadecene  
hexadecane  
heptadecanol  
hydrogen bromide  
hydrobromic acid  
hydrogen chloride  
hydrochloric acid  
hydrogen fluoride  
hydrofluoric acid  
hydrogen iodide

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

hydroiodic acid  
hydrogen  
hydrogen sulfide  
hydrazine  
hydrogen cyanide  
hydroxymethane  
2-hydroxyethylamine  
1-hydroxymethylpropane  
hydroxybenzene  
1-hydroxyhexane  
i-butane  
imidole  
indole  
indane  
iodine  
iodomethane  
iodoethane  
iodobenzene  
isoxazole  
isopropyl chloride  
isopropyl alcohol  
isopropyl amine  
isobutylene  
isobutene  
isobutyraldehyde  
isobutanal  
isobutyric acid  
isobutane  
isobutanol  
isopropyl methyl ether  
isobutyl amine  
isoprene  
isopentadiene  
1-isoamylene  
isopropylethylene  
isovaleric acid  
isopentanoic acid  
isobutyl formate  
isopentane  
isoamyl alcohol  
isopentyl alcohol  
isopropylacetone  
isobutyl acetate  
isoamyl formate  
isohexane  
2-isopropoxypropane

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

isoamyl acetate  
isopentyl acetate  
isobutyl propionate  
isobutyl n-propionate  
isoheptane  
1 3-isobenzofurandione  
isopropylcyclopentane  
isoamyl propionate  
isopentyl propionate  
isobutyl butyrate  
isobutyl isobutyrate  
isooctane  
isopropylmethylpropylmethane  
isoquinoline  
isopropylbenzene  
isopropylcyclohexane  
isobutylbenzene  
isobutylcyclohexane  
ketene  
kelene  
ketoexamethylene  
2-ketoheptane  
laughing gas  
lemonene  
m-dichlorobenzene  
m-phenylene dichloride  
m-cresol  
m-methylphenol  
m-toluidine  
m-xylene  
m-xylol  
m-methyltoluene  
m-ethylphenol  
m-ethylbenzene  
m-cymene  
m-isopropyltoluene  
m-terphenyl  
marsh gas  
mercury  
methynyl tribromide  
methylene bromide  
methylene dibromide  
methylene chlorobromide  
methylene chloride  
methylene fluoride

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

methanal  
methyl aldehyde  
methanoic acid  
methyl bromide  
methyl chloride  
methyl fluoride  
methyl iodide  
methanamide  
methane  
methyl hydride  
methanol  
methyl alcohol  
methyl mercaptan  
methanethiol  
methyl sulfhydrate  
methyl amine  
methyl chloroform  
methyl fluoroform  
methyl cyanide  
methyl isocyanate  
methanecarboxylic acid  
methyl formate  
methyl methanoate  
methanecarboxamide  
methyl carbinol  
methyl methanamine  
methyl acetylene  
methyl ethene  
methyl acetaldehyde  
methyl oxirane  
methoxyethene  
methoxyethylene  
methylacetic acid  
methyl acetate  
methyl ethanoate  
methyl ethyl ether  
methoxyethane  
methylal  
methylethylene glycol  
methyl ethyl sulfide  
methylallene  
methyl acrylate  
methyl propenate  
2-methylpropene  
2-methyl propanal

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

methyl ethyl ketone  
methyl acetone  
methyl propionate  
methyl propanoate  
methyl propylate  
methylethylmethane  
2-methylpropane  
2-methyl-1-propanol  
2-methyl-2-propanol  
methyl propyl ether  
methyl isopropyl ether  
methyltrimethylene glycol  
2-methyl-1-propanamine  
2-methyl pyrazine  
2-methyl furan  
2-methylbutadiene  
3-methyl-1,2-butadiene  
2-methyl-1-butene  
2-methyl-2-butene  
3-methyl-1-butene  
methyl propyl ketone  
methyl n-propyl ketone  
methyl isopropyl ketone  
3-methyl-2-butanone  
2-methyl tetrahydrofuran  
2-methyl butanoic acid  
methyl butyrate  
methyl n-butyrate  
methyl n-butanoate  
methyl isobutyrate  
2-methyl butane  
2-methyl-1-butanol  
3-methyl-1-butanol  
3-methyl-2-butanol  
methyl isopropyl carbinol  
2-methyl-2-butanol  
methyl n-butyl ether  
methyl tert-butyl ether  
2-methoxy-2-methyl-propane  
2-methylpyridine  
3-methylpyridine  
4-methyl pyridine  
methylcyclopentane  
2-methyl-1-pentene  
4-methyl-1-pentene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

2-methyl-2-pentene  
3-methyl-2-pentene,cis  
3-methyl-2-pentene,trans  
4-methyl-2-pentene,cis  
4-methyl-2-pentene,trans  
methyl butyl ketone  
methyl n-butyl ketone  
methyl isobutyl ketone  
4-methyl-2-pentanone  
2-methylpentane  
3-methyl pentane  
methyl amyl ether  
methylbenzene  
methyl phenyl ether  
methoxybenzene  
methylphenylamine  
2-methyl-benzenamine  
3-methylaniline  
3-methyl-benzeamine  
4-methylaniline  
4-methyl-benzeamine  
methylcyclohexane  
methyl amyl ketone  
2-methylhexane  
3-methylhexane  
methyl phenyl ketone  
methyl benzoate  
methyl benzene carboxylate  
methyl salicylate  
methyl-o-hydroxybenzoate  
1-methyl-1-ethylcyclopentane  
2-methylheptane  
3-methylheptane  
4-methylheptane  
2-methyl-3-ethylpentane  
3-methyl-3-ethylpentane  
methyl hexyl carbinol  
4-methyl-3-heptanol  
5-methyl-3-heptanol  
1-methyl-1-phenyl-ethylene  
1-methyl-2-ethylbenzene  
1-methyl-3-ethylbenzene  
1-methyl-4-ethylbenzene  
2-methyloctane  
2-methyl-2-phenylpropane  
1-methyl-2-isopropylbenzene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

1-methyl-3-isopropylbenzene  
1-methyl-4-isopropylbenzene  
menthol  
1-methylnaphthalene  
2-methylnaphthalene  
methanol 10%  
methanol 20%  
methanol 30%  
methanol 40%  
methanol 50%  
methanol 60%  
methanol 70%  
methanol 80%  
methanol 90%  
monobromomethane  
monochloromethane  
monoethanolamine  
morpholine  
n-propyl chloride  
n-propane  
n-propanol  
n-propyl amine  
n-butyraldehyde  
n-butyl aldehyde  
n-butyric acid  
n-butanoic acid  
n-propyl formate  
n-butyl chloride  
n-propylcarbinyl chloride  
n-butane  
n-butanol  
n-propyl methyl ether  
n-butyl amine  
n-ethyl ethanamine  
n-valeric acid  
n-propyl acetate  
n-pentane  
n-amyl alcohol  
n-butyl methyl ether  
n-propyl ethyl ketone  
n-butyl acetate  
n-propyl propionate  
n-amyl formate  
n-hexane  
n-butyl ethyl ether

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

n-propyl ether  
n-propyl-1-propanamine  
N-(1-methylethyl)-2-propanamine  
N-methyl aniline  
N-methyl-benzenamine  
n-hept-1-ene  
n-propyl butyrate  
n-propyl n-butanoate  
n-propyl n-butyrate  
n-propyl isobutyrate  
n-propyl isobutanoate  
n-heptane  
n-heptanol  
N,N-dimethyl aniline  
N-ethyl aniline  
n-propylcyclopentane  
n-propyl isovalerate  
n-octane  
n-butyl-1-butanamine  
n-propylbenzene  
N,N-dimethyl-o-toluidine  
n-propylcyclohexane  
n-nonane  
n-nonyl alcohol  
n-butylbenzene  
n-butyraniline  
n-decane  
n-hexylcyclopentane  
n-undecane  
n-heptylcyclopentane  
n-octylcyclopentane  
n-tridecane  
n-nonylcyclopentane  
n-tetradecane  
n-decylcyclopentane  
n-pentadecane  
n-decylcyclohexane  
n-dodecylcyclopentane  
n-heptadecane  
n-tridecylcyclopentane  
n-nonadecane  
n-eicosane  
naphthalene  
neon

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

neopentane  
neopentanol  
neohexane  
nitric oxide  
nitrogen dioxide  
nitrogen  
nitrous oxide  
nitromethane  
nitrocarbol  
nitrobenzene  
niobe oil  
1-nonene  
1-nonanol  
nonyl carbinol  
o-dichlorobenzene  
o-cresol  
o-methylphenol  
o-toluidine  
o-xylene  
o-xylol  
o-methyl toluene  
o-ethylphenol  
o-xylenol  
o-ethyltoluene  
o-cymene  
o-isopropyltoluene  
o-terphenyl  
octafluoropropane  
octafluorocyclobutane  
1-octene  
2-octene-trans  
1-octanol  
octyl alcohol  
2-octanol  
octyl carbinol  
1-octadecene  
octadecane  
1-octadecanol  
oil of mirbane  
oxygen  
oxalic acid dinitrile  
oxirane  
oxazole  
oxetane  
oxole  
oxacyclopentadiene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

ozone  
p-dichlorobenzene  
p-cresol  
p-methylphenol  
p-toluidine  
p-xylene  
p-xylol  
p-methyltoluene  
p-ethylphenol  
p-xilenol  
p-ethylbenzene  
p-cymene  
p-isopropyltoluene  
p-diethylbenzene  
p-terphenyl  
paraldehyde  
paracetaldehyde  
perfluoroethyl chloride  
perclene  
perfluoroethylene  
perfluoroethane  
pentachloroethane  
perfluoroacetic acid  
perfluoroacetone  
perfluoropropane  
1,1,1,2,2-pentafluoropropane  
perfluorocyclobutane  
perfluorobutane  
perfluoropentane  
perfluoro-n-pentane  
1,2-pentadiene  
1,4-pentadiene  
1-pentyne  
pentamethylene  
1-pentene  
pentanal  
2-pentanone  
3-pentanone  
pentanoic acid  
pentane  
1-pentanol  
pentyl alcohol  
perchlorobenzene  
perfluorobenzene  
perfluorocyclohexane  
perfluoro-n-hexane  
perfluoro-2-methylpentane

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

perfluoro-isohexane  
perfluoro-3-methylpentane  
perfluoro-2,3-dimethylbutane  
pentafluorobenzene  
pentafluorophenol  
perfluorotoluene  
perfluoromethylcyclohexane  
perfluoro-n-heptane  
2,3,4,5,6-pentafluorotoluene  
perfluoronaphthalene  
pentamethylbenzene  
1-pentadecene  
phosphine  
phosgene  
phenyl bromide  
phenyl chloride  
phenyl fluoride  
phenyl iodide  
phenol  
phenyl cyanide  
phenyl formic acid  
phenyl carbinol  
phenylmethanamine  
phthalic anhydride  
phenyl ethylene  
1-phenyl-ethanone  
phenylethane  
phenetole  
2-phenylpropane  
2-phenyl butane  
phenyloxybenzene  
phenanthrene  
piperazine  
piperazine  
piperidine  
2-picoline  
3-picoline  
4-picoline  
pimelin ketone  
prussic acid  
propadiene  
1-propyne  
2-propenal  
2-propenoic acid  
propionitrile  
propyl nitrile

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

propylene  
1-propene  
propylene chloride  
propylene dichloride  
2-propanone  
2-propen-1-ol  
propionaldehyde  
propenal  
1,2-propylene oxide  
1,3-propylene oxide  
propionic acid  
propyl chloride  
propane  
1-propanol  
2-propanol  
1,2-propanediol  
propylene glycol  
1,3-propanediol  
1-propanamine  
1-propyl amine  
2-propanamine  
propyl cyanide  
propyl methanoate  
propyl carbinol  
propyl methyl ether  
propylethylene  
propyl ethanoate  
propionic ester  
propyl ethyl ether  
1-propyl-2-methylphenol  
propylene glycol 10%  
propylene glycol 20%  
propylene glycol 30%  
propylene glycol 40%  
propylene glycol 50%  
propylene glycol 60%  
propylene glycol 70%  
propylene glycol 80%  
propylene glycol 90%  
pseudocumene  
pyrrole  
pyrrolidine  
pyridine  
pyrene  
quicksilver  
quinoline

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

R 21  
R 4081  
sec-butyl chloride  
sec-butanol  
sec-butyl carbinol  
sec-caprylic alcohol  
sec-butylbenzene  
sec-butylcyclohexane  
silicon tetrachloride  
silane  
sodium chloride 4%  
sodium chloride 8%  
sodium chloride 12%  
sodium chloride 16%  
sodium chloride 20%  
sodium chloride 24%  
styrene  
sulfur dioxide  
sulfur trioxide  
succinic acid  
synthetic wintergreen oil  
Syltherm 800  
Syltherm XLT  
tetrachloromethane  
tetrachloroethylene  
tetrachloroethene  
1,1,2,2-tetrachlorodifluoroethane  
tetrafluoroethene  
tetrafluoroethylene  
1,1,1,2-tetrachloroethane  
1,1,2,2-tetrachloroethane  
tetramethylene  
tetrahydrofuran  
tetrahydrothiophene  
tert-butyl chloride  
tetrahydropyrrole  
tert-butanol  
tetramethylene glycol  
tetrahydropyran  
tert-pentane  
tert-amyl alcohol  
tert-pentanol  
tert-butyl carbinol  
tert-butyl methyl ether  
1,2,3,4-tetrafluorobenzene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

1,2,3,5-tetrafluorobenzene  
1,2,4,5-tetrafluorobenzene  
2,2,3,3-tetramethylbutane  
2,2,3,3-tetramethylpentane  
2,2,3,4-tetramethylpentane  
2,2,4,4-tetramethylpentane  
2,3,3,4-tetramethylpentane  
1,2,3,4-tetrahydronaphthalene  
tetralin  
tert-butylbenzene  
1,2,3,5-tetramethylbenzene  
1,2,4,5-tetramethylbenzene  
tert-butylcyclohexane  
2,2,3,3-tetramethylhexane  
2,2,5,5-tetramethylhexane  
1-tetradecene  
thiobismethane  
thiophene  
thiole  
thiacyclopentane  
thiophane  
thymol  
Therminol LT  
Therminol 44  
Therminol 55  
Therminol 59  
Therminol 60  
Therminol 66  
Therminol 75  
Therminol VP-1  
titanium tetrachloride  
toluene  
toluol  
trichloroborane  
trichloromethyl bromide  
trifluorobromomethane  
trifluoromethyl chloride  
trichlorofluoromethane  
tribromomethane  
trichloromethane  
trifluoromethane  
trifluorovinyl bromide  
trifluorovinyl chloride  
1,2,2-trichlorotrifluoroethane  
trifluoroacetonitrile  
trichloroethylene

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

trichloroethene  
triclene  
trifluoroacetic acid  
trifluoroethanoic acid  
trans-1,2-dichloroethylene  
1,1,1-trichloroethane  
1,1,2-trichloroethane  
1,1,1-trifluoroethane  
trifluoropropene  
1,2,3-trichloropropane  
trimethylene  
trimethylene oxide  
trimethyl amine  
trans-2-butene  
trimethyl carbinol  
trans-1,3-pentadiene  
trans-piperylene  
trans-2-pentene  
trans-beta-amylene  
trimethylethylene  
1,3,5-trichlorotrifluorobenzene  
trimethyltrioxymethylene  
triethylamine  
2,3,3-trimethyl-1-butene  
2,2,3-trimethylbutane  
trimethylisopropylmethane  
1,1,2-trimethylcyclopentane  
1,1,3-trimethylcyclopentane  
1,2,4-trimethylcyclopentane-c,c,t  
1,2,4-trimethylcyclopentane-c,t,c  
2,2,3-trimethylpentane  
2,2,4-trimethylpentane  
2,3,3-trimethylpentane  
2,3,4-trimethylpentane  
1,2,3-trimethylbenzene  
1,2,4-trimethylbenzene  
1,3,5-trimethylbenzene  
1,trans-3,5-trimethylcyclohexane  
2,2,3-trimethylhexane  
2,2,4-trimethylhexane  
2,2,5-trimethylhexane  
trimethylphenylmethane  
trans-decalin  
trans-decahydronaphthalene  
3,3,5-trimethyl heptane  
tributylamine

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Alphabetical List of Compound Names and Synonyms (Cont./...)

1-tridecene  
1-undecene  
valeraldehyde  
vinylidene chloride  
vinylidene fluoride  
vinyl chloride  
vinyl trichloride  
vinyl fluoride  
vinyl cyanide  
vinylformic acid  
vinyl formate  
vinyl carbinol  
vinyl methyl ether  
vinylacetylene  
vinylethylene  
vinyl acetate  
vinyl ethyl ether  
water  
2,3-xylenol  
2,4-xylenol  
2,5-xylenol  
2,6-xylenol  
3,4-xylenol  
3,5-xylenol

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## **USER-DEFINED COMPOUNDS (Delta T Props2)**

### **Contents**

General

Installation of Delta T Props2

Outline Procedure

Compound Selection

Constant Properties

Low-Pressure Vapor Specific Heat

Joback Group Contribution Estimation Method

Vapor Pressure

Liquid Specific Volume

Liquid Viscosity

Liquid Conductivity

Liquid Specific Heat

Liquid Surface Tension

Gas Viscosity

Gas Conductivity

Units Selection

Sample Calculation

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2)

### General

*Delta T Props2 is not a standard component of the Delta T package. It may be purchased separately as an optional add-on.*

There are over 600 compounds in the Delta T Props database. The database gives physical properties for many of the common chemical used in industry; however, no matter how many compounds are included in a database like Delta T Props, there will always be some compounds not represented in the database and which are required by the user.

To aid the user in this respect, Delta T Props to date has allowed the user to define the following:

- User-Defined Liquids: limited properties and liquid-only properties
- User-Defined Mixtures: components drawn from the database

With Delta T Props2, the limitations of these features are overcome: now users can define User-Defined Compounds which have the same range of properties found in the regular Delta T Props database. The properties are available for liquid and vapor phases and both saturated and unsaturated just like in the regular Delta T Props database. The methods and techniques available to the user within Delta T Props2 are the same as those used by Madison Technical Software in the formulation of the Delta T Props database.

### Installation of Delta T Props2

If the software has been downloaded from email, simply run the executable file. The program and data files will automatically unzip from this file.

Note that all Delta T Props2 files must be installed to the same directory as Delta T Props. Delta T Props2 cannot run without Delta T Props.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Outline Procedure

Delta T Props2 allows the user to estimate and define the properties of arbitrary compounds and add these to the Delta T Props database for future recall and calculation. Up to 100 new compounds may be defined and stored at any one time.

The user does not have to be an expert in physical properties estimation to operate Delta T Props2 successfully. Help screens are available to assist the user in evaluation of the estimation methods and further details are given here in this manual.

Some basic information is required to be able to use Delta T Props2 most effectively:

- Type of Compound: the user should be able to categorize the compound in accordance with the category list in Delta T Props
- To take full advantage of the resident estimation methods, the user should sketch out on paper the structural formula of the compound.
- If the user can locate published values of the compound physical properties so much the better (particularly critical properties and boiling point); however, default estimation methods are available for all physical properties

### Constant Properties

These are required to define both liquid and vapor properties. If published values of boiling point and critical constants are available, these should be used. In the absence of published values, the user can use the Joback Estimation Method to estimate these values. All constant properties must be specified.

### Outline Procedure

The method number should be defined first. A list of methods and method numbers is available from the Help menu. If the Joback values have been defined and method number 2 specified, pressing the Calculate button displays the Joback estimates.

### Vapor and Liquid Properties

Seven liquid properties are represented within the Delta T Props database as arrays of 11 property values at equally-spaced temperature intervals from the Melting Point to the Critical Point. Low pressure vapor specific heat is represented by 11 values at equally-spaced temperature intervals from 50 K to 1300 K. Property values are calculated in Delta T Props by multi-point interpolation and by applying a pressure correction if appropriate.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

The user must complete the estimation of the seven liquid properties and the low-pressure vapor specific heat.

The method numbers should be specified first. For each property a list of methods and method numbers is available from the Help menu. Certain methods need additional parameters to be specified; these are defined by accessing the Parameters menu. For these methods, the word “defined” or “undefined” is attached to the method name that appears in the Comments column when the method number is entered. When the methods have been defined, pressing the Calculate button displays the property values.

### Other Vapor and Liquid Properties

Other vapor and liquid thermodynamic and transport properties not directly estimated by the user are derived from an equation of state within Delta T Props which uses the constant properties as scaling factors.

### Calculate Function

When all the method numbers have been specified and all methods appropriately defined, pressing the Calculate button causes each property value to be calculated and displayed in accordance with the specified method.

### Graphics Display

When all of the property values have been calculated, Delta T Props2 provides screen graphical display of the calculated values versus temperature as well as showing by a continuous curve the interpolated values that would be calculated during normal Delta T Props operation. The graphical display will easily reveal any discontinuities in the property function which then can be amended by the user until a satisfactory function is obtained. The graphical display is accessed from the Local Menu. The graphical display can be sent to a Windows-compatible printer by selecting the Print Screen option on the graphical display screen

### Save Data Function

At any time the user can access the Save Data function from the Local Menu. Note that this function saves to file all of the data, selected method numbers and corresponding method parameters for all properties and not just the current property.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

## Compound Selection

### Compound Selection List

The compound list gives the user access to 100 locations to define new compounds. To select a compound/location the user clicks on the compound name in the list.

### Compound Naming

Initially all compound names are set to “not in use”. To name a new compound, click on the desired location in the Compound List and enter the new compound name in the Compound Name Text Box

### Compound Data Saving & Recall

The Local Menu gives access to Compound Data Recall and Saving. When compound data is recalled, the data status is updated and reported on this screen. Saving compound data will write over the compound data previously stored at the chosen location.

### Clearing Compound Data

The Local Menu gives access to the Clear Data function. This function clears all compound data at the selected location. Note that the corresponding file locations on disk are also cleared.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Constant Properties

#### Specification of Methods

It is necessary to specify the compound constant properties before attempting to specify any of the other properties. The property values can be published values directly input by the user or alternatively estimated using the Joback method. The user specifies the selected methods by entering the method numbers in the method text boxes for each property as follows. When the method numbers are entered, method names are displayed alongside.

Method 0: Undefined

Method 1: User-Defined Values

The user enters the values directly to the property text boxes.

Method 2: Joback Estimate

The user accesses the Joback estimation screen thru the Estimates Menu and specifies the molecular structure of the compound. Method number 2 is specified in the method text boxes as appropriate. Pressing the Calculate button computes and displays the estimated property values. Values computed by the Joback estimation procedure are reasonably accurate; the use of published experimental data is to be preferred where these data are available. See Section 10.7 for details on the application of the Joback method. Technical details may be found in Section 8.2.7

#### Note on Accuracy

The accuracy of the constant properties is vital to the overall accuracy of the property estimations in Delta T Props2. In particular, the values of the normal boiling point, critical temperature and critical pressure are used throughout the estimation procedures for the liquid and vapor properties. The use of accurate published values for these parameters will increase the overall accuracy of the property values. Typical error levels for the Joback method are (from Reid et al)

Critical Temperature	5 K	
Critical Pressure		5%
Critical Volume	2%	
Boiling Point		13 K
Melting Point		23 K

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Low-Pressure Vapor Specific Heat

The low-pressure vapor specific heat is required for the calculation of many liquid and vapor thermal and transport properties. For technical details see Section 8.11

In Delta T Props, low-pressure vapor specific heat is calculated by cubic interpolation from an array of 11 data values at equal temperature intervals from 50 K thru 1300 K. To define the specific heat function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from published literature, known correlations or use the resident estimation technique. In addition, Delta T Props2 provides methods to estimate values at the high and low end of the temperature scale.

### Specification of Methods

The user first specifies the methods to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When the method numbers are thus entered, the method name is displayed in the comments column. A list of available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the specific heat text boxes.

#### Method 2: User-Defined Polynomial

The user accesses the estimate screen and specifies the coefficients of a polynomial

#### Method 3: Joback Method

The user accesses the Joback estimation screen and specifies the molecular structure of the compound. The Joback method is a generally applicable method which yields accurate (average errors in the range 1% to 2%) values of the vapor specific heat over the temperature range 273 K to 1000 K. For technical details see Section 8.11.1

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Method 4: Low-End Extrapolation

This method allows the estimation of vapor specific heat at Location 1 (50 K) and Location 2 (175 K) from known values at Location 3 thru Location 6. The method of extrapolation was developed by MTS as a modified power-law extrapolation derived from analysis of low-temperature specific heat data for a range of compounds. To apply the method to Locations 1 and 2, the user simply specifies method 4 in the method text boxes for Locations 1 and 2. Do not use this method for any locations other than 1 or 2. The rationale for including this feature is that many published correlations and the Joback estimation method may not be valid much below 273 K. This extrapolation is reasonably accurate; at 50 - 100 K the error level is about 5%. In the region 100K thru 250 K, the average error is less than 2%.

### Method 5: High-End Extrapolation

This method allows the estimation of vapor specific heat at Location 9 (1050 K), Location 10 (1175 K) and Location 11 (1300 K) from values at Location 7 (800 K) and Location 8 (925 K). The method used is a power-law extrapolation. To apply the method to Locations 9 thru 11, the user simply specifies method 5 in the method text boxes for Locations 9 thru 11. Do not use this method for any locations other than 9 thru 11. The rationale for including this feature is that many published correlations and the Joback estimation method may be unreliable above 1000 K. The average error for this extrapolation in the region 1000 K to 1300 K is probably not more than 2%.

### Method 6: Datafit to User Data

The user access the Datafit screen through the Parameters Menu and specifies between 2 and 10 datapoints comprising temperature and specific heat values. For two data points, the routine fits a straight line. For three datapoints, the routine fits a quadratic. For four datapoints, the routine fits a cubic. For more than four datapoints, the routine fits a cubic by least squares. Selecting the Calculate option after the datapoints have been entered causes the specific heat values predicted by the fitting function to be printed to the screen alongside the actual specific heat values. For 2, 3 and 4 datapoints, the function fit to the entered datapoints will be exact. For more than 4 datapoints, the function will be a least squares smooth cubic fit to the datapoints. The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

The Joback group contribution estimation method allows the user to estimate selected compound properties from a specification of the molecular structure of the compound.

When called from the Low Pressure Vapor Specific Heat Module, the Joback method yields estimates of the low pressure vapor specific heat as a function of temperature. The general applicability of the method is in the range 270 to 1000 K. Errors usually average 2 or 3%. For technical details see Section 8.11.1

When called from the Constant Properties Module, the Joback method yields estimates for the normal boiling point, normal melting point, critical temperature, critical pressure, critical volume, Enthalpy of Formation and Gibbs Free Energy of Formation. For technical details see Section 8.2.7.

Typical error levels for the Joback method are (from Reid et al)

Critical Temperature	5 K	
Critical Pressure		5%
Critical Volume	2%	
Boiling Point		13 K
Melting Point		23 K

To apply the method, the user should draw the structural formula of the compound in question. The structural formula is expressed as the sum of a number of Joback groups. The relevant numbers of each group present in the molecule are entered into the appropriate text boxes on the screen. As these numbers are entered, the Compound Formula box displays the accumulated compound formula. When all the numbers of groups have been entered, the formula displayed in the Compound Formula box must be the correct formula.

Note that the molecular groups are in three categories: Non-Ring Groups (i.e. not in a Benzene or other carbon ring), Ring Groups (i.e. in a Benzene or other carbon ring) and General Groups.

When all numbers of groups have been entered, pressing the Calculate button causes the Joback parameters to be calculated and saved. The relevant property values can then be called up by entering the appropriate estimate method number in the main screen.

From the Local Menu, the user can return to the calling module and can clear current input values. Two examples are as follows:

Ethanol is C<sub>2</sub>H<sub>5</sub>OH and can be represented as CH<sub>3</sub>-CH<sub>2</sub>-OH. The user enters 1 for CH<sub>3</sub>(non-ring), 1 for CH<sub>2</sub> (non-ring) and 1 for OH (non-ring)

Dichlorobenzene is C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub> and can be represented as 4 x (-CH<) (ring) + 2 x (=C<) ring + 2 x (Cl). The user enters 4 for -CH< (ring), 2 for =C< (ring) and 2 for Cl (general)

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Vapor Pressure

In Delta T Props, vapor pressure is calculated by interpolation from an array of 11 data values at equal temperature intervals from the Melting Point thru the Critical Temperature. The interpolation is a cubic function of the logarithm of the reduced vapor pressure at the data points. To define the vapor pressure function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from the published literature, known correlations or use the resident estimation techniques. The user may also compute datafit functions from known datapoints and use these to predict the required values. Technical aspects of vapor pressure are discussed in Section 8.8

### Specification of Methods

The user first specifies the methods to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When the method numbers are thus entered, the method name is displayed in the comments column. A list of available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the specific heat text boxes

#### Method 2: User-Defined Wagner Equation

The user accesses the estimate screen and specifies the coefficients as a Wagner Equation, a functional form often used to represent experimental vapor pressure data accurately over wide temperature ranges. The Wagner Equation takes the following form:

$$P_v = P_c \text{Exp}\{(aq + bq^{1.5} + cq^3 + dq^6)/T_r\}$$

with

$P_v$  = Vapor pressure

$P_c$  = Critical pressure

$T_r$  = Reduced temperature ( $T/T_c$ )

$q = 1 - T_r$

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Method 3: Antoine Equation

This equation is a popular functional form to represent vapor pressure data over limited temperature ranges. The Antoine equation takes the form:

$$P_v = \text{Exp}\{a + b/(T + c)\}$$

The user accesses the estimate screen and specifies the coefficients of the Antoine equation.

### Method 4: Lee-Kesler Equation

The Lee Kesler vapor pressure equation needs no specific user definition of equation parameters. The correlation gives a good representation of vapor pressure for non-polar compounds from low temperatures thru the critical point. Reid et al note that this method predicts vapor pressure within about 2% from the normal boiling point thru the critical point; below the normal boiling point, this method may under-predict by a few percent.

### Method 5: Gomez-Thodos Equations

The Gomez-Thodos vapor pressure equations need no specific user definition of equation parameters apart from the classification of the compound as non-polar, polar or alcohol which is specified in the Constant Properties Module. The Gomez-Thodos equations usually give excellent representation of the vapor pressure for most compounds from low temperatures thru the critical point. Tests by MTS using published data for a large number of compounds showed that this method was superior to the Lee Kesler method even for non-polar compounds.

### Methods 6 & 7: Interpolation

The user accesses the estimate screen and specifies two locations for the interpolation. Delta T Props2 will compute interpolated values based on a linear relation between  $\ln(P_v)$  and  $1/T$ . Delta T Props2 allows two such interpolations to be defined.

### Method 8: Datafit to User Data

The user accesses the Datafit screen through the Parameters Menu and specifies between 2 and 10 datapoints comprising temperature and vapor pressure values.

For two data points, the routine fits a  $P_v = \text{Exp}\{a + b/T\}$  function. For three datapoints, the routine fits an Antoine function. For more than three datapoints, the routine fits an Antoine function by least squares. Selecting the Calculate option after the datapoints have been entered causes the property values predicted by the fitting function to be printed to the screen alongside the actual property values. The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Critical Point

For consistency within the database, the vapor pressure at the critical temperature (Location 11) is set equal to the critical pressure as defined in the Constant Properties Module.

### Liquid Specific Volume

In Delta T Props, liquid specific volume (reciprocal of liquid density) is calculated from an array of 11 data values at equal temperature intervals from the Melting Temperature thru the Critical Temperature. The interpolation is a cubic function of the liquid density at the data points. Technical aspects of liquid specific volume are discussed in Section 8.3

To define the liquid specific volume function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from the published literature, known correlations or use the resident estimation techniques. The user may also compute datafit functions from known datapoints and use these to predict the required values.

### Specification of Methods

The user first specifies the methods to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When the method numbers are thus entered, the method name is displayed in the comments column. A list of available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the specific volume text boxes

#### Method 2: Linear Equation

The user accesses the estimate screen from the Parameters Menu and specifies the coefficients of a linear equation.

#### Method 3: Polynomial

The user accesses the estimate screen from the Parameters Menu and specifies the coefficients of a cubic polynomial.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### **Method 4: Rackett Equation**

This is a power law function computed from critical constants specified in the Constant Properties Module. No specific user input is required. The method yields reasonable values for specific volume. If an experimental volume point is known use the next method. Typical errors are in the range 1 to 3%. For a technical discussion of the Rackett method see Section 8.3.2

### **Method 5: Rackett Equation with an experimental point.**

This method allows the user to input an experimental or other well-established datapoint to fix certain parameters of the Rackett equation. Assuming an accurate datapoint, this method will give improved accuracy over Method 4. The datapoint is entered in the estimate screen accessed thru the Parameters Menu

### **Methods 6 & 7: Interpolation**

The user accesses the estimate screen and specifies two locations for the interpolation. Delta T Props2 will compute interpolated values based on a linear relation between volume and temperature. Delta T Props2 allows two such interpolations to be defined.

### **Method 8: Datafit to User Data**

The user access the Datafit screen through the Parameters Menu and specifies between 2 and 10 datapoints comprising temperature and specific volume values. The routine fits a linear function either by direct fit (for two datapoints) or by least squares (for more than two datapoints). Selecting the Calculate option after the datapoints have been entered causes the property values predicted by the fitting function to be printed to the screen alongside the actual property values. The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Liquid Viscosity

In Delta T Props, liquid viscosity is calculated from an array of 11 data values at equal temperature intervals from the Melting Temperature thru the Critical Temperature. The interpolation is a cubic function of the logarithm of the liquid viscosity at the data points. Technical aspects of liquid viscosity are discussed in Section 8.5

To define the liquid viscosity function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from the published literature, known correlations or use the resident estimation techniques. The user may also compute datafit functions from known datapoints and use these to predict the required values.

Liquid viscosity is difficult to estimate from any one general scheme. Group contribution methods are used at lower temperatures; corresponding states methods work quite well at higher temperatures. No single approach works for all compounds over all temperatures. For this reason, MTS has presented a greater number of methods for estimating liquid viscosity than for other properties.

### Specification of Methods

The user first specifies the methods to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When the method numbers are thus entered, the method name is displayed in the comments column. A list of available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the viscosity text boxes

#### Method 2: Power Function

The user accesses the estimate screen from the Parameters Menu and specifies the coefficients of a power function:  $\text{Viscosity} = a T^b$

#### Method 3: Exponential Function #1

The user accesses the estimate screen from the Parameters Menu and specifies the coefficients of an exponential function as follows:

$$\text{Viscosity} = \text{Exp}\{a + b/T + c.\ln(T) + dT^{10}\}$$

This functional form is used in a number of literature sources

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Method 4: Exponential Function #2

The user accesses the estimate screen from the Parameters Menu and specifies the coefficients of an exponential function as follows:  $\text{Viscosity} = \text{Exp}\{a + b/T + cT + dT^2\}$  This functional form is used in a number of literature sources

### Method 5: Van Velzen Estimation

The Van Velzen method is a relatively accurate group contribution method of some complexity in its original published form. The MTS software implementation of the method has simplified its use from the standpoint of the user without deviating from the detail of the method. The user accesses the Van Velzen estimate screen from the Parameters Menu. The user specifies aspects of the molecular structure of the compound. For absolute temperatures less than 0.75 of the critical temperature and in the absence of published data, this method is recommended. Above this limit, the method is not recommended. Typical errors are in the 5 to 15% range. See Section 8.5.1 and Section 8 References for details.

### Method 6: Przedziecki Method

This method does not require specific user input. The method uses changes in liquid volume to estimate liquid viscosity values - hence the user must define the liquid specific volume before specifying this method. The absolute temperature should lie between 0.5 and 0.8 of the critical temperature. This method has only fair accuracy; some large errors greater than 20 to 25% can be expected. The advantage of the method is that it does provide a reasonable default method in the mid-temperature range. See Section 8.5.4 for details.

### Method 7: Letsou & Stiel

This method is applicable to absolute temperatures in excess of 0.75 of the critical temperature. This method is based on corresponding states theory and requires no user specification of parameters. Errors should lie in the range 5% to 10% but may be larger in the immediate vicinity of the critical point. See Section 8.5.3 for technical details

### Methods 8 & 9: Interpolation

The user accesses the estimate screen from the Parameters Menu and specifies two locations for the interpolation; Delta T Props2 will compute interpolated values based on a linear relation between log viscosity and inverse temperature. Delta T Props2 allows two such interpolations to be defined.

### Method 10: Datafit to User Data

The user access the Datafit screen through the Parameters Menu and specifies between 2 and 10 datapoints comprising viscosity and temperature values. The routine fits a linear function of log viscosity versus inverse temperature either by direct fit (for two datapoints) or by least squares (for more than two datapoints). Selecting the Calculate option after the datapoints have been entered causes the property values predicted by the fitting function to be printed to the screen alongside the actual property values. The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Van Velzen Group Contribution Estimation Method

The Van Velzen group contribution estimation method allows the user to estimate liquid viscosity as a function of temperature from a specification of the molecular structure of the compound. See Section 8.5.1 and Section 8 References for technical details of the Van Velzen method.. The application and calculation of the method is generally complex but MTS has put together a data entry screen for this method which makes the application a reasonably straightforward task. The expected errors from the method are in the 5 to 15% range.

To apply the method, the user should sketch the structural formula of the compound in question. The structural formula is then characterized by numbers of active groups and other structural parameters. The relevant number of each group present in the molecule are entered into the appropriate text boxes on the screen. The data required is in the following categories:

Primary Data: this data should be filled in first

Ring Groups and Non-Ring Groups: the molecular structure is expressed in terms of the Van Velzen groups where relevant

Ring Configuration: this is specified for aromatic rings with substitutions in the ortho, para or meta positions.

Non-Ring Corrections: these corrections are specified when certain halogen groups occur in the non-ring portion of the molecule. Note that the occurrence of the halogens themselves must be entered as well as the non-ring corrections.

When all numbers of groups have been entered, pressing the Calculate button causes the Van Velzen parameters to be calculated and stored. The relevant viscosity values can then be computed and displayed by entering the appropriate estimate number (4) in the main screen method text boxes and pressing the Calculate button.

From the Local Menu, the user can return to the calling module and can clear current input values. Some examples of Van Velzen input are as follows:

Ethanol is C<sub>2</sub>H<sub>5</sub>OH or CH<sub>3</sub>-CH<sub>2</sub>-OH. The user enters 2 for # Carbons and 1 for Primary Alcohol (non ring)

Ortho-dichlorobenzene is C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>. The user enters 6 for # Carbons, 1 for # Benzene Rings and 2 for Cl (ring). The ring configuration list box is set to "ortho"

Perfluoroethane is CF<sub>3</sub>-CF<sub>3</sub>. The user enters 2 for # Carbons, 6 for Fluorine (non-ring) and 2 for CF<sub>3</sub> (non-ring corrections)

Isobutane is CH<sub>3</sub>-CH(CH<sub>3</sub>)-CH<sub>3</sub>. The user specifies 4 for # Carbons and 1 for # Iso-methyls

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Liquid Conductivity

In Delta T Props, liquid thermal conductivity is calculated from an array of 11 data values at equal temperature intervals from the Melting Temperature thru the Critical Temperature. The interpolation is a cubic function of the liquid conductivity at the data points. Technical aspects of liquid conductivity are discussed in Section 8.6

To define the liquid conductivity function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from the published literature, known correlations or use the resident estimation techniques. The user may also compute datafit functions from known datapoints and use these to predict the required values.

### Specification of Methods

The user first specifies the methods to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When the method numbers are thus entered, the method name is displayed in the comments column. A list of available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the conductivity text boxes

#### Method 2: Polynomial

The user accesses the estimate screen thru the Parameters Menu and specifies the coefficients of a polynomial function:  $k = a + bT + cT^2 + dT^3$

#### Method 3: Sato-Riedel Estimate

This method requires no user specification of parameters. Errors usually lie in the range 5 to 15%. Poor results are noted for low molecular weight hydrocarbons and branched hydrocarbons; the predicted value is generally larger than the actual value. Better results are noted for non-hydrocarbons. This method should not be used for absolute temperature greater than 0.75 of the critical temperature. See Section 8.6.3

#### Method 4: Latini Estimate

The user accesses the estimate screen from the Parameters Menu and specifies the compound category. Best results are found when the molecular weight lies between 50 and 250. Errors are usually less than 10%. Nitrogen and Sulfur compounds and aldehydes cannot be estimated by the Latini method. This method should not be used for absolute temperatures in excess of 0.75 of the critical temperature. See Section 8.6.1

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### **Method 5: Ely and Hanley Method**

This is a corresponding states method which gives estimates of liquid conductivity for absolute temperatures in excess of 0.8 of the critical temperature. No user specification of parameters is required. For hydrocarbons, errors less than 10% can be expected. Errors for non-hydrocarbons and particularly for polar compounds. This method will underpredict the conductivity at the critical point. See Section 8.6.4 and Section 8.10 for a detailed discussion on this method.

### **Methods 8 & 9: Interpolation**

The user accesses the estimate screen from the Parameters Menu and specifies two locations for the interpolation; Delta T Props2 will compute interpolated values based on a linear relation between conductivity and temperature. Delta T Props2 allows two such interpolations to be defined.

### **Method 10: Datafit to User Data**

The user access the Datafit screen through the Parameters Menu and specifies between 2 and 10 datapoints comprising temperature and specific volume values. The routine fits a linear function of conductivity versus temperature either by direct fit (for two datapoints) or by least squares (for more than two datapoints). Selecting the Calculate option after the datapoints have been entered causes the property values predicted by the fitting function to be printed to the screen alongside the actual property values. The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Liquid Specific Heat

In Delta T Props, liquid specific heat is calculated from an array of 11 data values at equal temperature intervals from the Melting Temperature thru the Critical Temperature. The interpolation is a cubic function of a special function of liquid specific heat at the data points.

To define the liquid specific heat function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from the published literature, known correlations or use the resident estimation techniques. The user may also compute datafit functions from known datapoints and use these to predict the required values.

### Specification of Methods

The user first specifies the methods to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When the method numbers are thus entered, the method name is displayed in the comments column. A list of available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the specific heat text boxes

#### Method 2: Polynomial

The user accesses the estimate screen thru the Parameters Menu and specifies the coefficients of a polynomial function:  $C = a + bT + cT^2 + dT^3$

#### Method 3: Missenard Estimate

The user accesses the Missenard Group Contribution Method from the Parameters Menu. The molecular structure of the compound is specified by the user. This method is valid for temperatures up to 0.75 of the critical temperature. Details of this method are given below.

#### Method 4: Rowlinson-Bondi Estimate

This is a corresponding states method of general application. No parameters need be specified by the user. This method is valid over the entire temperature range except in the case of alcohols where it should not be used if the absolute temperature is below 0.75 of the critical temperature.

#### Methods 5 & 6: Interpolation

The user accesses the estimate screen from the Parameters Menu and specifies two locations for the interpolation; Delta T Props2 will compute interpolated values based on a linear relation between a special function of specific heat (see below) and temperature. Delta T Props2 allows two such interpolations to be defined.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Method 7: Datafit to User Data

The user access the Datafit screen through the Parameters Menu and specifies between 2 and 10 datapoints comprising temperature and specific heat values. The routine fits a linear function of specific heat versus temperature either by direct fit (for two datapoints) or by least squares (for more than two datapoints). Selecting the Calculate option after the datapoints have been entered causes the property values predicted by the fitting function to be printed to the screen alongside the actual property values. The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

### Special Specific Heat Function

As with other Delta T Props properties, liquid specific heat is computed by interpolation of an array of 11 values from the melting point to the critical point. In the case of liquid specific heat, a particular problem occurs at the critical point: for all substances, the liquid specific heat approaches infinity as the temperature approaches the critical point; thus the value at the critical point is useless for interpolation.

The problem is solved as follows: though the specific heat approaches infinity as temperature approaches the critical point, the enthalpy which is the integral of the specific heat does not exhibit a singularity; nor does the function  $C_p \cdot (1 - T/T_c)$  where  $T_c$  is the critical temperature and  $C_p$  is the liquid specific heat. The function  $C_p \cdot (1 - T/T_c)$  is a well-behaved function which varies relatively slowly over the temperature range and which approaches a finite limit at the critical point. Thus, in Delta T Props, the liquid specific heat values are actually stored as  $C_p \cdot (1 - T/T_c)$ . Interpolation is carried out on these values and not on the untransformed  $C_p$  values.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Liquid Specific Heat

#### Missenard Group Contribution Method

The Missenard group contribution method allows the user to estimate liquid specific heat from a specification of the molecular structure of the compound. See Section 8.4.2 for a technical discussion of this method.

To apply the method, the user should sketch the structural formula of the compound in question. The structural formula is then expressed as the sum of a number of Missenard groups. The relevant numbers of each group present in the molecule are entered into the appropriate text boxes on the screen. As these numbers are entered, the compound formula box displays the accumulated compound formula. When all the numbers of groups have been entered, the formula displayed in the compound formula box must be the correct compound formula. When all numbers of groups have been entered, pressing the calculate button causes the Missenard parameters to be calculated and stored. The relevant specific heat values can then be called up by entering the appropriate estimate method number in the main screen.

From the Local Menu, the user can return to the calling menu and can clear current input values.

Some examples are:

Ethanol is C<sub>2</sub>H<sub>5</sub>OH or CH<sub>3</sub>-CH<sub>2</sub>-OH. The user enters 1 for CH<sub>3</sub>, 1 for CH<sub>2</sub> and 1 for OH

Acetone is CH<sub>3</sub>-CO-CH<sub>3</sub>. The user enters 2 for CH<sub>3</sub> and 1 for CO (ketone)

Chlorobenzene is C<sub>6</sub>H<sub>5</sub>Cl. The user enters 1 for C<sub>6</sub>H<sub>5</sub> and 1 for Cl

### Liquid Surface Tension

In Delta T Props, liquid surface tension is calculated from an array of 11 data values at equal temperature intervals from the Melting Temperature thru the Critical Temperature. The interpolation is a cubic function of a special function of liquid surface tension at the data points. Technical aspects of liquid surface tension are discussed in Section 8.7

To define the liquid surface tension function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from the published literature, known correlations or use the resident estimation techniques. The user may also compute datafit functions from known datapoints and use these to predict the required values.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Specification of Methods

The user first specifies the methods to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When the method numbers are thus entered, the method name is displayed in the comments column. A list of available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the surface tension text boxes

#### Method 2: Polynomial

The user accesses the estimate screen thru the Parameters Menu and specifies the coefficients of a polynomial function:  $s = a + bT + cT^2 + dT^3$

#### Method 3: Power Function

The user accesses the estimate screen from the Parameters Menu and specifies the coefficients of a power function:  $s = a(1 - T_r)^{(b + cT + dT^2)}$

#### Method 4: Brock & Bird/Hakim Method

The Brock & Bird method is a corresponding states method with general applicability to non-polar compounds. The Hakim method is an extension of the Brock & Bird method to polar compounds. The program chooses the correct method in accordance with the polarity specification in the Constant Properties Module. No user specification of parameters is required.

#### Methods 5 & 6: Interpolation

The user accesses the estimate screen from the Parameters Menu and specifies two locations for the interpolation; Delta T Props2 will compute interpolated values based on a linear relation between surface tension and temperature. Delta T Props2 allows two such interpolations to be defined.

#### Method 7: Datafit to User Data

The user access the Datafit screen through the Parameters Menu and specifies between 2 and 10 datapoints comprising temperature and surface tension values. The routine fits a function of surface tension versus temperature [ $s = a(1 - T_r)^b$ ] either by direct fit (for two datapoints) or by least squares (for more than two datapoints). Selecting the Calculate option after the datapoints have been entered causes the property values predicted by the fitting function to be printed to the screen alongside the actual property values. The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Gas Viscosity

In Delta T Props, low-pressure gas viscosity is calculated by interpolation from an array of 11 data values at equal temperature intervals from 50 K thru 1300 K. The interpolation is a cubic interpolation of gas viscosity at the data points versus temperature. To define the gas viscosity function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from the published literature or use the resident estimation techniques. The user may also compute datafit functions from known datapoints and use these to predict the required values.

### Specification of Methods

The user should first specify the method to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When method numbers are thus entered, the method name is displayed in the comments column. A list of the available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the viscosity text boxes.

#### Method 2: Lucas Method

The Lucas method is a corresponding states method with general applicability. No user specification of parameters is required.

#### Methods 3 and 4: Interpolation

The user accesses the estimate screen from the Parameters Menu and specifies two locations for the interpolation; Delta T Props2 will compute interpolated values based on a linear relation between gas viscosity and temperature. Delta T Props2 allows two such interpolations to be defined.

#### Method 7: Datafit to User Data

The user accesses the Datafit screen from the Parameters Menu and specifies between 2 and 10 datapoints comprising temperature and viscosity values.

The routine fits a linear function of viscosity versus temperature either by direct fit (for two datapoints) or by least squares (for more than two datapoints). The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Gas Viscosity

#### Calculate Function

When all method numbers have been specified and all methods appropriately defined, pressing the Calculate button causes each property value to be calculated and displayed in accordance with the specified method.

#### Graphics Display

When the all of the property values have been calculated, Delta T Props2 provides screen graphical display of the calculated values versus temperature as well as showing by a continuous curve the interpolated values that would be calculated during normal Delta T Props operation. The graphical display will easily reveal any discontinuities in the property function which then can be amended by the user until a satisfactory function is obtained.

The graphical display is accessed from the Local Menu. The graphical display can be sent to a Windows-compatible printer by selecting the Print Screen option on the graphical display screen.

#### Save Data Function

At any time the user can access the Save Data function from the Local Menu. Note that this function saves to file all of the data, selected method numbers and corresponding method parameters for all properties and not just the current property.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Gas Thermal Conductivity

In Delta T Props, low-pressure gas conductivity is calculated by interpolation from an array of 11 data values at equal temperature intervals from 50 K thru 1300 K. The interpolation is a cubic interpolation of gas conductivity at the data points versus temperature. To define the gas conductivity function within Delta T Props2, the user must specify each of these 11 values. The user can enter known values from the published literature or use the resident estimation techniques. The user may also compute datafit functions from known datapoints and use these to predict the required values.

### Specification of Methods

The user should first specify the method to be employed for each of the eleven datapoints required by entering the method numbers into the method text boxes. When method numbers are thus entered, the method name is displayed in the comments column. A list of the available methods and the corresponding method numbers is available from the Help menu. The available methods are:

#### Method 0: Undefined

#### Method 1: User-Defined Values

The user enters values directly to the conductivity text boxes.

#### Method 2: Ely and Hanley Method

The Ely and Hanley method is a corresponding states method with general applicability. No user specification of parameters is required.

#### Methods 3 and 4: Interpolation

The user accesses the estimate screen from the Parameters Menu and specifies two locations for the interpolation; Delta T Props2 will compute interpolated values based on a linear relation between gas conductivity and temperature. Delta T Props2 allows two such interpolations to be defined.

#### Method 7: Datafit to User Data

The user accesses the Datafit screen from the Parameters Menu and specifies between 2 and 10 datapoints comprising temperature and conductivity values.

The routine fits a linear function of conductivity versus temperature either by direct fit (for two datapoints) or by least squares (for more than two datapoints). The Local Menu on the Datafit screen allows the user to save the calculated parameters to file.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Gas Thermal Conductivity

#### Calculate Function

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#### Graphics Display

When the all of the property values have been calculated, Delta T Props2 provides screen graphical display of the calculated values versus temperature as well as showing by a continuous curve the interpolated values that would be calculated during normal Delta T Props operation. The graphical display will easily reveal any discontinuities in the property function which then can be amended by the user until a satisfactory function is obtained.

The graphical display is accessed from the Local Menu. The graphical display can be sent to a Windows-compatible printer by selecting the Print Screen option on the graphical display screen.

#### Save Data Function

At any time the user can access the Save Data function from the Local Menu. Note that this function saves to file all of the data, selected method numbers and corresponding method parameters for all properties and not just the current property.

#### Units Selection

In Delta T Props, the user may select from a range of US and Metric units for all relevant physical units for input and display of data. For each physical unit (temperature, pressure etc), the user clicks on the unit list box and again on the desired unit selection. The selected units may then be saved to file by accessing the Local Menu.

When Delta T Props boots up, this units file is accessed automatically and the previously selected and saved units are used for input and display.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Sample Calculation

In this section, a sample definition of Ethanol physical properties is demonstrated. It is assumed within each section (apart from the Constant Properties Module as discussed below) that no experimental property data is known. This is a good way to start; experimental or published values can be added later once a good first estimate has been made.

### Compound Name

Click on an empty location on the Compound Selection List. Enter “ethanol” in the Compound Name Text Box

### Constant Properties

Access Constant Properties from the Module Menu. Choose Joback Estimate from the Local Menu. Ethanol is CH<sub>3</sub>-CH<sub>2</sub>-OH: enter 1 for CH<sub>3</sub>, 1 for CH<sub>2</sub> and 1 for OH (all non-ring contributions). Press Calculate/Save. Return to the Constant Properties screen via the Local Menu

For each property enter 2 for Method Number. Method 2 is the Joback Method (see List of Methods in the Help Menu). The caption “defined Joback Method” appears opposite each property in the comments column. When the method numbers have been defined, press the Calculate button. The Joback estimate values will be displayed.

Click on the Relative Polarity list box and select “alcohols/glycols”

At this point, let us assume that we do in fact have access to some published data on the constant properties of Ethanol. The use of good published values for the constant properties will improve the quality of the physical property estimates. Suppose that we have the following values:

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Sample Calculation

	Published	Joback
Critical Temperature	513.9 K	499.1 K
Critical Pressure	61.4 bara	57.6 bara
Normal Boiling Point	351.4 K	337.3 K
Normal Melting Point	159.1 K	172.6 K

As can be seen, the Joback estimates are reasonable but use of the published values will improve accuracy greatly.

In the method number boxes for each of the above properties, enter 1 (the method number for user-defined values). Into the property value boxes enter the published values of the known properties. Press Calculate. Save the data to disk via the Local Menu.

### Low-Pressure Vapor Specific Heat

Access this module from the Module Menu. We have to define the Vapor Specific Heat at 11 temperature values ranging from 50 K to 1300 K. The default method is the Joback method. Access the Joback Method from the Parameters Menu. As before, enter 1 for CH<sub>3</sub>, 1 for CH<sub>2</sub> and 1 for OH. Press Calculate. Return to the Vapor Specific Heat screen by using the Local Menu.

Enter 3 to each method number box. Press Calculate. The Joback estimates are displayed.

We can improve the accuracy of the values at high and low temperatures by using the high and low temperatures extrapolation. Enter method 4 at locations 1 and enter method 5 at locations 9, 10 and 11 (see List of Methods from Help Menu). Press Calculate. Save the data via the Local Menu. The smoothness of the fit can be seen by choosing Graphical Display from the Local Menu.

### Vapor Pressure

Method number 5 (Gomez-Thodos Method) is recommended. This set of equations has a special equation for alcohols. Note that the value of the vapor pressure at the critical temperature equals the critical pressure already specified in the Constant Properties Module and cannot be changed here.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## Liquid Specific Volume

The default method is number 4 (Rackett Estimate). This method gives reasonable values for Specific Volume. Note that the value at the critical temperature is equal to the critical volume defined in the Constant Properties Module.

## Liquid Viscosity

Here we will have to use two different default methods. Up to location 7 (372 K) we will use the Van Velzen method. Access to this method is through the Parameters Menu. Only two entries are required: enter 2 for the number of carbon atoms and enter 1 for Primary Alcohol. Press Calculate and then return to the Liquid Viscosity screen.

Enter method 5 (Van Velzen) in the method boxes for locations 1 thru 7. The Van Velzen method is not applicable much above the normal boiling point.

For high-temperature values of viscosity, the choice is the Letsou and Stiel Method (number 7). Enter 7 in the method number boxes for locations 8 thru 11.

Press calculate. It will be noted from the graphical display that the values predicted by the two methods transition into each other quite smoothly.

## Liquid Conductivity

There are a number of default methods available at low temperatures (less than the normal boiling point approximately). The Latini method has a specific correlation for alcohols, so this method will be used up to location 7 (372 K). Select the Latini method from the Parameters Menu; click on the list box and select "alcohols". Return to the main screen and enter method number 4 in the method boxes for locations 1 thru 7.

High temperature conductivity presents a problem: the only method with any applicability to high temperatures is the Ely and Hanley method (number 5). The method was developed for alkanes and does not perform well for polar substances. Our suggestion here is simply to extrapolate from locations 6 and 7 to locations 8 thru 11. The results may not be very accurate but at least should be reasonable.

Select one of the interpolation functions from the Parameters Menu; enter 6 and 7 for the two 'anchor' points for the extrapolation. Return to the main screen and enter 7 in the method number boxes for locations 8 thru 11.

If we had specified the Ely & Hanley method for locations 8 thru 11, we would have got a serious discontinuity between the Latini and the Ely and Hanley values. This can be shown by entering 5 in the method number boxes for locations 8 thru 11, pressing Calculate and viewing the Graphical Display.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Liquid Specific Heat

The Rowlinson-Bondi method is the usual default method for Liquid Specific Heat. In the case of alcohols, however, this method is applicable only at high temperatures. To estimate the values at low temperatures, we use the Missenard group contribution method.

Access the Missenard method from the Parameters Menu. Enter 1 for CH<sub>3</sub>, 1 for CH<sub>2</sub> and 1 for OH. Press Calculate and return to the main screen. Enter method number 3 in the method number boxes for locations 1 thru 7.

Enter method number 5 (Rowlinson Bondi) for locations 8 thru 10. Press Calculate. Note that the value at the critical point is infinite and cannot be changed by the user.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Liquid Surface Tension

The default method is Brock & Bird/Hakim which covers the cases of polar and non-polar compounds reasonably well. Enter method 4 for locations 1 thru 10. The value at the critical point is always zero.

### Comparison of Results

The version of Ethanol as defined here is stored and recalled in Delta T Props under User-Defined Compounds. We can compare the values calculated for this with the values calculated for the normal version of Ethanol within Delta T Props (Category = Alcohols). The following comparison of selected properties is given at the normal boiling point (saturated conditions). The Delta T Props2 estimated values are given in brackets:

#### *Ethanol*

Temperature	351.4 K	
Vapor Pressure (bar)	1.0140 (1.0144)	
	Liquid	Vapor
Volume (cc/gram)	1.365 (1.368)	614.3 (616.1)
Expansivity (per K)	0.00179 (0.00184)	0.00318 (0.00318)
Compr Factor	0.00200 (0.00201)	0.982 (0.985)
Sp Heat Cp (kJ/kgK)	3.007 (3.023)	1.675 (1.648)
Latent Heat (kJ/kg)		839.6 (849.8)
Viscosity (cP)	0.428 (0.559)	0.0105 (0.0104)
Conductivity (W/mk)	0.155 (0.137)	0.0159 (0.0157)
Surf Tension (dyne/cm) 1	7.24 (13.2)	

With the exception of Liquid Viscosity and Surface Tension, the errors are typically less than a few percent with several errors virtually zero. The liquid viscosity has an error of about 25% and the surface tension of about 25%. Note that the vapor properties are all close to the regular Delta T Props values principally due to the setting of the constant properties to the published values. Ethanol being polar, hydrogen-bonding and near the beginning of the alcohol series is a tough test for any estimation scheme that relies on such a small amount of data. All in all, the estimation performed very well. For other compounds, the user can expect significantly better results on average. The results show that if the user can get any published data on the liquid properties of the compound of interest, accuracy will be greatly enhanced.

# The new batch reactor heat transfer and chemical properties calculator



Version 5 – Volume 2

## USER-DEFINED COMPOUNDS (Delta T Props2) (Cont./..)

### Sample Calculation

A similar estimation was carried out on normal hexane. This compound is non-polar and we expect a very good quality estimation. The results are summarized below.

#### *Hexane*

Temperature	341.9 K	
Vapor Pressure (bar)	1.0134 (1.0133)	
	Liquid	Vapor
Volume (cc/gram)	1.627 (1.622)	308.8 (309.3)
Expansivity (per K)	0.00172 (0.00172)	0.00347 (0.00348)
Compr Factor	0.00513 (0.00509)	0.949 (0.950)
Sp Heat Cp (kJ/kgK)	2.479 (2.428)	1.900 (1.909)
Latent Heat (kJ/kg)		333.7 (338.5)
Viscosity (cP)	0.212 (0.199)	0.0074 (0.0078)
Conductivity (W/mK)	0.104 (0.102)	0.0169 (0.0169)
Surf Tension (dyne/cm)	13.31 (13.55)	

The agreement between Delta T Props2 and Delta T Props values is excellent