Pure Component Equations

Fitting of Pure Component Equations

DDBSP – Dortmund Data Bank Software Package

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Introduction

PCPEquationFit fits parameters for a large variety of equations for pure component properties. Parameters can be stored in and retrieved from a parameter database, they can be plotted, and they can be used for calculations.

PCPEquationFit normally uses the pure component properties data bank which is a part of the Dortmund Data Bank. It can also be used to fit data from other data sources since tables can be pasted from the clipboard or loaded from files.

List of Equations

Property	***Equation***
Liquid Viscosity T [K] η [mPa s]	1. Andrade $\eta = e^{A+\frac{B}{T}}$ 2. Vogel $\eta = e^{A+\frac{B}{T+C}}$ 3. DIPPR 101 $\eta = e^{A+\frac{B}{T}+C\ln T+DT^E}$ 4. PPDS 9 $\eta = E\exp\left[A\left(\frac{C-T}{T-D}\right)^{\frac{1}{3}}+B\left(\frac{C-T}{T-D}\right)^{\frac{4}{3}}\right]$ 5. Extended Andrade $\eta = e^{A+\frac{B}{T}+CT+DT^2+ET^3}$
Vapor Viscosity T[K] η [mPa s]	1. DIPPR 102 $\eta = \frac{AT^B}{1+\frac{C}{T}+\frac{D}{T^2}}$ 2. Polynomial $\eta = A+B\cdot T+CT^2+DT^3+ET^4$

Property	***Equation***
Saturated Vapor Pressure T [K] P [kPa]	1. Antoine $P=10^{A-\frac{B}{T+C}}$ (►Other Units: T [°C], P [mmHg]) 2. Wagner 2.5,5 $P=\exp\left(\ln P_c+\frac{A(1-T_r)+B(1-T_r)^{1.5}+C(1-T_r)^{2.5}+D(1-T_r)^5}{T_r}\right)$ 3. Wagner 3,6 $P=\exp\left(\ln P_c+\frac{A(1-T_r)+B(1-T_r)^{1.5}+C(1-T_r)^3+D(1-T_r)^6}{T_r}\right)$ 4. Cox $P=\exp\left[\ln 101.325+e^{A+B\left(\frac{T}{T_B}\right)+C\left(\frac{T}{T_B}\right)^2\left(1-\frac{T_B}{T}\right)}\right]$ 5. DIPPR 101 $P=e^{A+\frac{B}{T}+C\ln T+DT^E}$ (►Other Units: P [Pa]) 6. Extended Antoine (Lonza) $P=\exp\left(A+\frac{B}{T+C}+DT+ET^2+F\ln(T)\right)$ (►Other Units: P [bar]) 7. Extended Antoine (Aspen) $P=\exp\left(A+\frac{B}{T+C}+DT+E\ln(T)+F\,T^G\right)$ G=1 or G=2 8. Extended Antoine (Hysys) $P=\exp\left(A+\frac{B}{T+C}+D\ln(T)+E\,T^F\right)$ F=1 or F=2 9. Short Antoine (Aspen) $P=e^{A-\frac{B}{T}+CT}$ (in preparation) 10. Rarey2P $P=P_{atm}10^{\left[(4.1012+A)\left(\frac{T-B}{T-\frac{B}{8}}\right)\right]}$ $B\approx T_b$ $-1<A<+1$ 11. Xiang/Tan $P=P_c\cdot\exp\left(\ln T_R\cdot\left(A_1+A_2(1-T_R)^{1.89}+A_3\cdot(1-T_R)^{5.67}\right)\right)$

Property	***Equation***
Saturated Vapor Pressure by EOS T [K] P [kPa]	1. Mathias-Copeman Constants for EOS $\alpha=\left(1+m\cdot\left(1-\sqrt{T_r}\right)\right)^2$ $m=c_1+c_2\cdot\left(1-\sqrt{T_r}\right)+c_3\cdot\left(1-\sqrt{T_r}\right)^2$ 2. Twu-Bluck-Cunningham-Coon Constants for EOS $\alpha=T_r^{\left(c_3\cdot\left(c_2-1\right)\right)}\cdot\exp\left(c_1\cdot\left(1-T_r^{\left(c_2\cdot c_3\right)}\right)\right)$ (c_1,c_2,c_3 used in DDB programs) $\alpha=T_r^{\left(N\cdot\left(M-1\right)\right)}\cdot\exp\left(L\cdot\left(1-T_r^{\left(M\cdot N\right)}\right)\right)$ (L,M,N like original authors) 3. Melhem-Saini-Goodwin Constants for EOS $\alpha=\exp\left(c_1\cdot\left(1-T_r\right)+c_2\cdot\left(1-\sqrt{T_r}\right)^2\right)$ 4. Stryjek-Vera Constants for EOS $\kappa=\kappa_0+\kappa_1\left(1+\sqrt{\left(T_r\right)}\right)\left(0.7-T_r\right)$ $\alpha=\left(1+\kappa\left(1-\sqrt{\left(T_r\right)}\right)\right)^2$ 5. Stryjek-Vera-2 Constant for EOS $\kappa=\kappa_0+\left[\kappa_1+\kappa_2\left(\kappa_3-T_r^{0.5}\right)\left(1-T_r^{0.5}\right)\right]\left(1+T_r^{0.5}\right)\left(0.7-T_r\right)$ $\alpha=\left(1+\kappa\left(1-T_r^{0.5}\right)\right)^2$
Liquid Heat Capacity T [K] c_p [J/mol K]	1. Polynomial $c_P=A+BT+CT^2+DT^3+ET^4$ 2. PPDS 15 $c_p=R\left(\frac{A}{\tau}+C\tau+D\tau^2+E\tau^3+F\tau^4\right)$ with $\tau=1-\frac{T}{T_c}$
Ideal Gas Heat Capacity T [K] c_p [J/mol K]	1. Polynomial $c_P=A+BT+CT^2+DT^3+ET^4$ 2. Aly-Lee, DIPPR 107 $c_p=a_0+a_1\left(\frac{\frac{a_2}{T}}{\sinh\frac{a_2}{T}}\right)^2+a_3\left(\frac{\frac{a_4}{T}}{\cosh\frac{a_4}{T}}\right)^2$ 3. PPDS 2 $C_P=R\left(B+\left(C-B\right)y^2\left[1+\left(y-1\right)\left(D+Ey+Fy^2+Gy^3\right)\right]\right)$ with $y=\frac{T}{A+T}$ 4. Shomate $c_P=A+BT+CT^2+DT^3+\frac{E}{T^2}$

Property	***Equation***
Liquid Density T [K] ρ [kg/m³]	1. DIPPR 105 $\rho = \frac{A}{B^{1+\left(1-\frac{T}{C}\right)^{D}}}$ 2. Polynomial $\rho = A + B \cdot T + CT^2 + DT^3 + ET^4$ 3. Tait (pressure-dependent data) $P_{ref} = max(f(T), 1.01325)\,MPa$ (Wagner-Equation) $\rho_{ref} = f(T)\frac{kg}{m^3}$ (DIPPR 105-Equation) $T_{reduced} = 100 \qquad T_R = \frac{T}{T_{reduced}}$ $C = c_0 + c_1 T_R$ $B = b_0 + b_1 T_R + b_2 T_R^2 + b_3 T_R^3 + b_4 T_R^4$ $\rho = \frac{\rho_{ref}}{1 - C \ln\left[\frac{B+P}{B+P_{ref}}\right]}$ 4. DIPPR 116 (with additional addend ρ_C, the critical density) $\rho_L = \rho_c + \left[A\tau^{0.35} + B\tau^{\frac{2}{3}} + C\tau + D\tau^{\frac{4}{3}}\right]$ with $\tau = 1 - \frac{T}{T_c}$
Surface Tension T [K] σ [N/m]	1. Polynomial $\sigma = A + BT + CT^2 + DT^3 + ET^4$ 2. Short DIPPR 106 $\sigma = A(1-T_R)^n$ with $T_R = \frac{T}{T_c}$ 3. $\sigma = A(T - T_C)^B$ 4. Full DIPPR 106 $\sigma = A\left(1-T_r\right)^{B + C T_r + D T_r^2 + E T_r^3}$ with $T_r = \frac{T}{T_c}$
Second Virial Coefficient T [K] B_{ii} [cm³/mol]	1. Polynomial $B_{ii} = A + BT + CT^2 + DT^3 + ET^4$ 2. $B_{ii} = \frac{A}{\sqrt{T}} + \frac{B}{T}$ 3. DIPPR 104 $B_{ii} = A + \frac{B}{T} + \frac{C}{T^3} + \frac{D}{T^8} + \frac{E}{T^9}$

Property	***Equation***
Heat of Vaporization T [K] H_{vap} [J/mol]	1. DIPPR 106 $H_{Vap}=A\left(1-\frac{T}{T_C}\right)^{B+C\left(\frac{T}{T_C}\right)+D\left(\frac{T}{T_C}\right)^2+E\left(\frac{T}{T_C}\right)^3}$ 2. Extended Watson $H_{Vap}=a\left(c-T\right)^b+d$ 3. PPDS 12 $H_{Vap}=R\,T_c\left(A\tau^{\frac{1}{3}}+B\tau^{\frac{2}{3}}+C\tau+D\tau^2+E\tau^6\right)$ with $\tau=1-\frac{T}{T_c}$
Liquid Thermal Conductivity T [K] λ [W/m K]	1. Polynomial $\lambda=A+BT+CT^2+DT^3+ET^4$ 2. PPDS 8 $\lambda=A\left(1+B\tau^{\frac{1}{3}}+C\tau^{\frac{2}{3}}+D\tau\right)$ with $\tau=1-\frac{T}{T_c}$
Vapor Thermal Conductivity T [K] λ [W/m K]	1. PPDS 3 $\lambda=\frac{\sqrt{T_r}}{A+\frac{B}{T_r}+\frac{C}{T_r^2}+\frac{D}{T_r^3}}$ with $T_r=\frac{T}{T_c}$
Isothermal Compressibility	Linear Interpolation
Thermal Expansion Coefficient	Linear Interpolation
Melting Temperature (Pressure Dependency)	Simon-Glatzel Equation $P_m=a\left(\left(\frac{T_m}{T_{m(normal)}}\right)^c-1.\right)$
Dielectric Constants of Liquids, Permittivity T K], ε [.]	1. Polynomial $\lambda=A+BT+CT^2+DT^3+ET^4$

Using the program

Initial Dialog

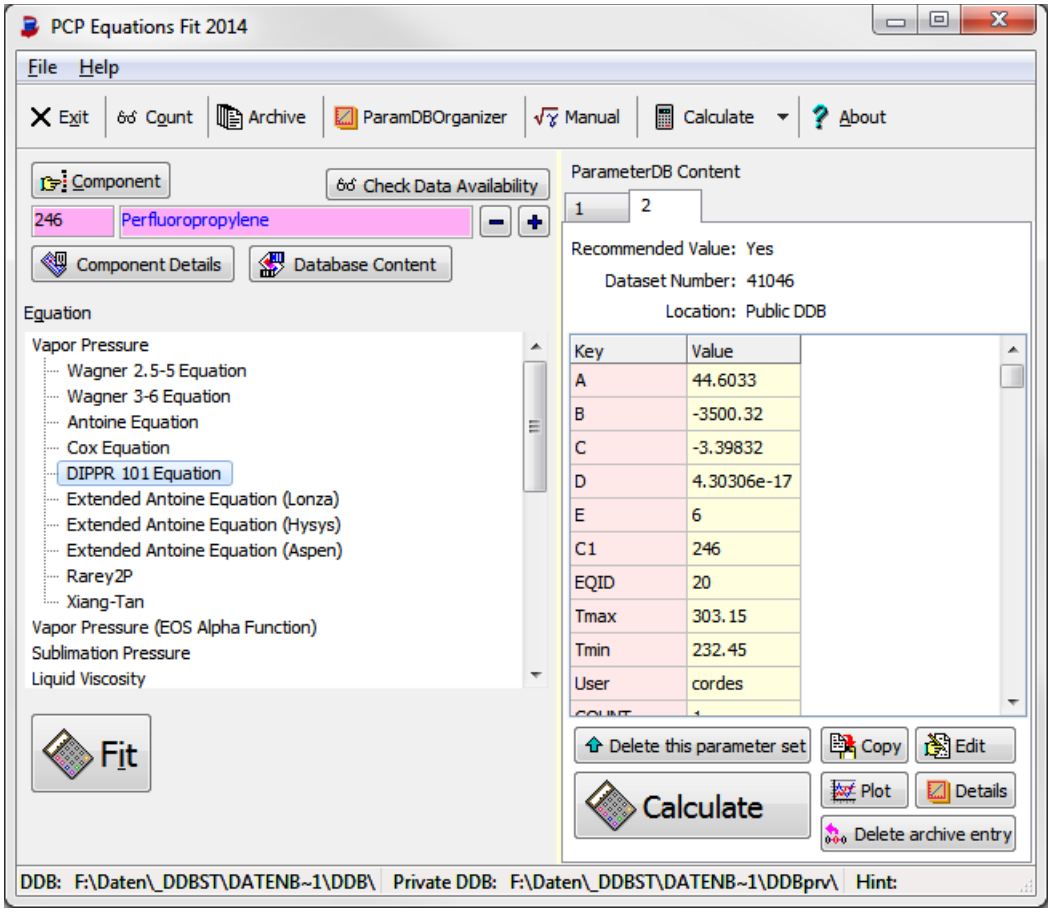


Figure 1 Main PCPEquationFit Dialog

The program's start dialog contains three major parts:

1. The components area allows
    1. selecting components
    2. displaying component details with the component editor
    3. displaying the content of the Dortmund Data Bank for the selected component
    4. verifying if enough data sets or points are available (this is only a hint, since there might be further constraints)
2. The list of equations. The list is organized hierarchically. The methods are summarized below the property they describe.
3. The parameter data set shows the current content of the ParameterDDB.

The toolbar buttons are mainly short cuts for the “File” and “Help” menus.

File Menu

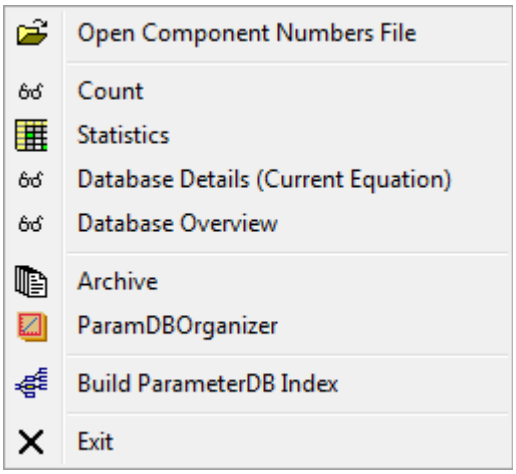
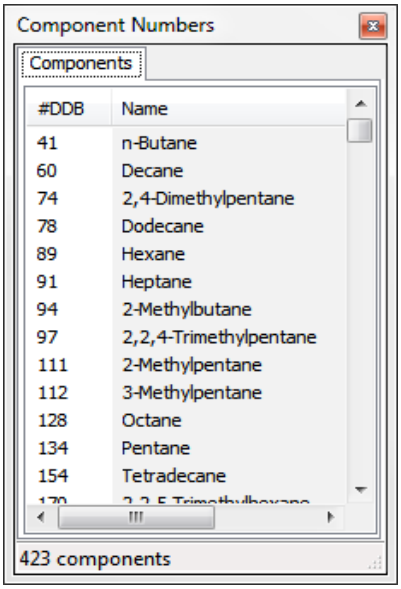


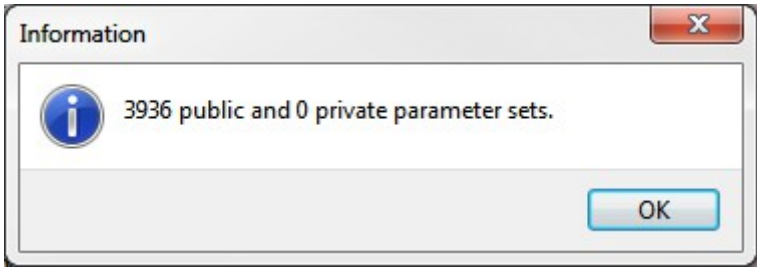
Figure 2: File menu

- **Open Component Numbers File**
  This function allows loading a file with a list of DDB component numbers. Such component files can be created, for example, in the component selection dialog or in the main Dortmund Data Bank program from search results. The data set numbers are shown in a separate window.



  A click on a line sets the component number in the main fit window.

- **Count**
  Count shows the number of available parameter data sets for the current model.



- **Statistics**
  Statistics creates a table with an overview over all equations
- **Database Details (Current Equation)**
  This function creates a table with all data sets available for the current equation.
- **Database Overview**
  This functions creates a table with the number of components for experimental

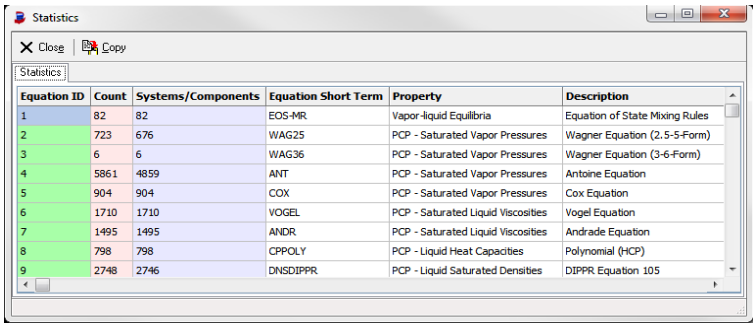


Figure 3: Statistics

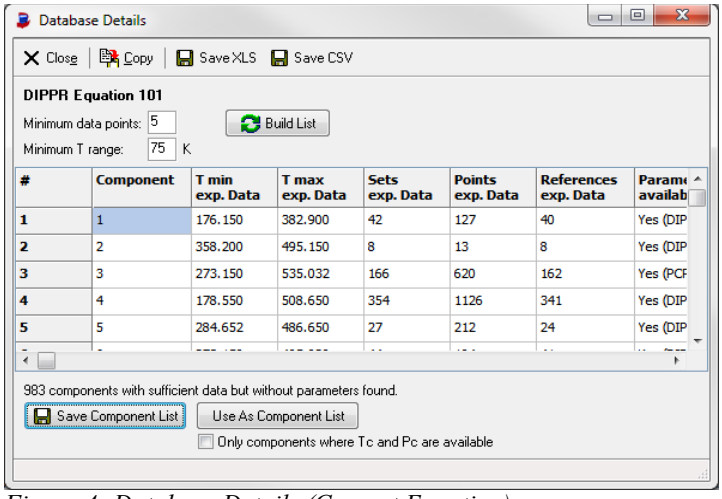


Figure 4: Database Details (Current Equation)

data in the Pure Component Properties part of the Dortmund Data Bank are available for the single equations.

- **Archive**

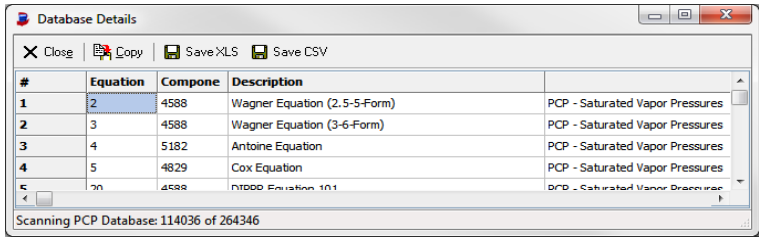


Figure 5: Database Overview

See chapter “Fit Archive” on page 24.

- **ParamDBOrganizer**
  This function call the program for managing the parameter data base. This program is described in a separate PDF (“ParameterDDBOrganizer.pdf”).
- **Build ParameterDB Index**
  This will rebuild the component index of the parameter data base. This is normally done automatically when needed. This function is only needed if changes outside PCPEquationFit have been made.

Help Menu

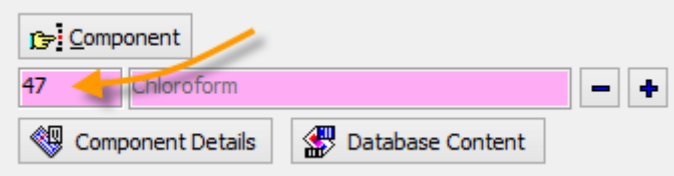
The help menu contains a button which brings this PDF help up and an “About” button which shows some information about the program.

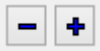
Figure 6: Help menu

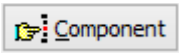
Component Selection

DDB component numbers can be typed directly in the component field.

After a *Return* the component name is added.



The buttons  allow to navigate through the DDB component list.

The button  calls the component selection dialog

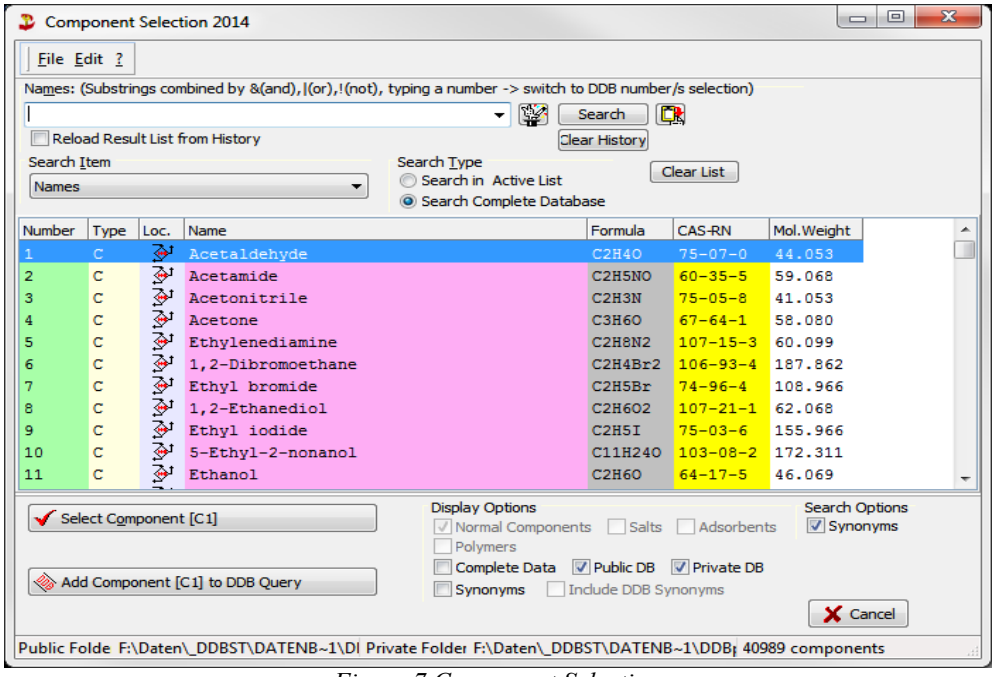
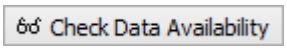


Figure 7 Component Selection

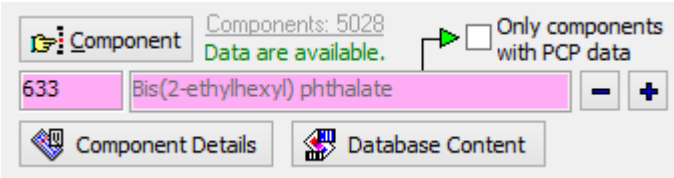
which is described in details in other documents.

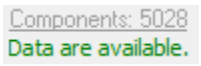
Check Data Availability



This button starts a search in the pure component property data bank for experimental data for the currently selected equation.

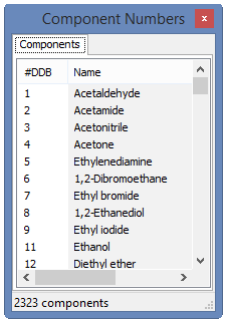
When this search is finished the “Check Data Availability” is hidden and information about the availability of data is shown.



The information lines 

show for how many components the Dortmund Data Bank contains experimental data sets. The example shows the number of components for the Antoine equation (saturated vapor pressures).

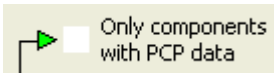
Clicking on the underlined label ("Components 5028") will open a window with the list of components.



The "Data are available" line indicates that there are enough data points for the specific equation. This number is normally set to <number of parameters + 1>.

If no data are available this text will be displayed: 

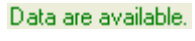
.

The check box 

should be used in "walk-through" mode where a list of components is in work. If checked this will avoid the display of components without experimental data points.

A detailed description of all component selection features is available in the "Component Management" documentation.

Fit

After the component and the equation has been selected and the program indicates that enough data points are available (

) the *Fit* button displays a model specific dialog with **almost** the same content for the different models.

The used example for showing a typical fit is the Wagner 2.5-5 equation for saturated vapor pressures.

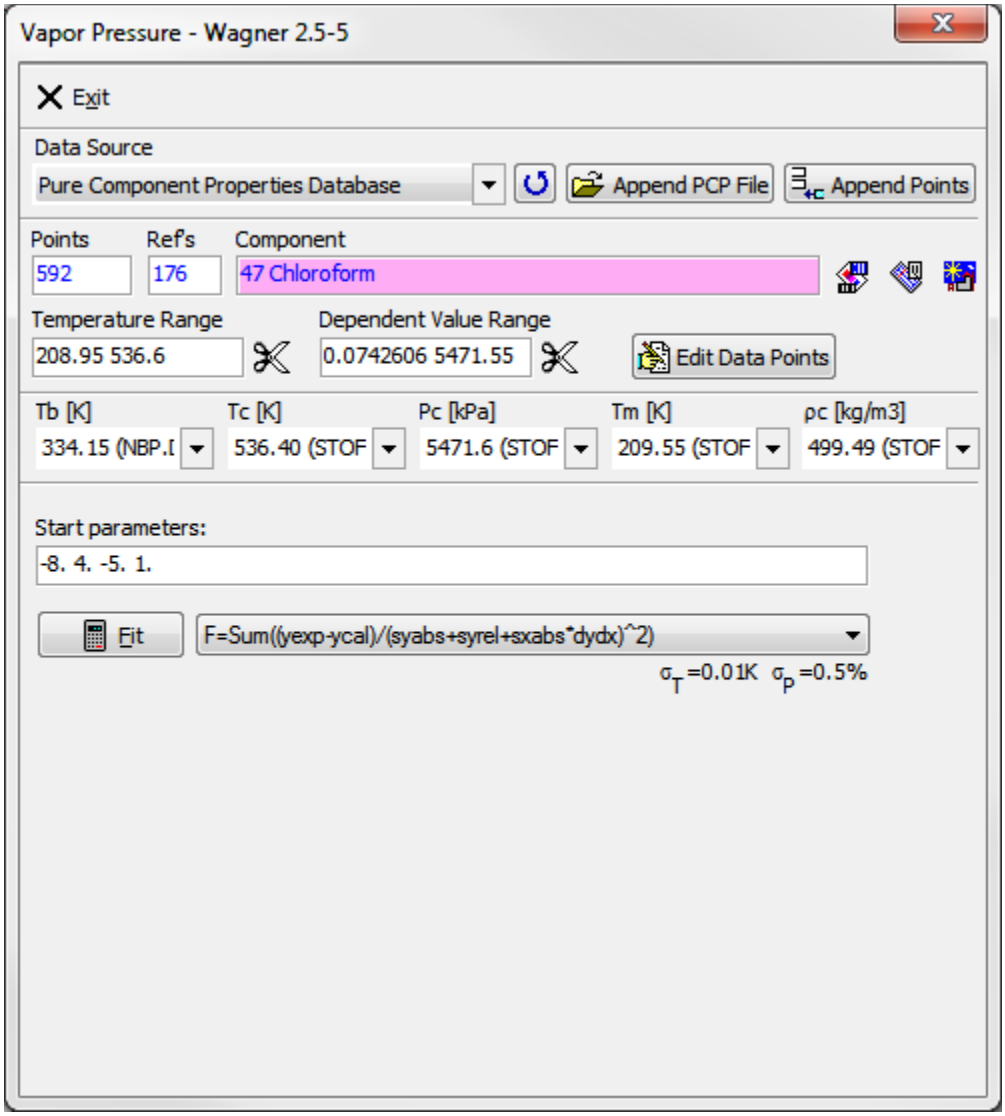
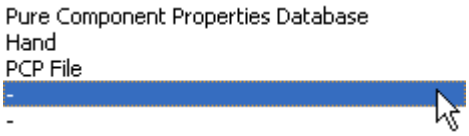


Figure 8 Fit Dialog for Wager 2-5 equation

The dialog displays the data source – which is in most cases the pure component properties data bank. Other possible sources are



1. Input by hand
2. Reading from file
3. Calculated data or stored data points (here marked as '-')

The "Append PCP File" would allow to append data from an external file.

The dialog displays the number of available data points and the number of different references (number of different authors) and repeats the display of the component name. The two buttons besides the name invoke the component editor and the Dortmund Data Bank program.

The temperature and pressure range are also displayed. These limits are editable and can be used to cut points by increasing the lower limit or decreasing the upper limit. The knife buttons will actually throw the points outside the given ranges away. The “Edit Data Points” allows to modify the data from the data sources. It uses the “Input by Hand” dialog.

The normal boiling point (T_b), the critical data (T_c, P_c, ρ_c), and the melting point (T_m) are read from pure component basic files (not from the pure component properties data bank).

The lower part of the dialog is model specific but contains in most cases starting parameters and a selection for an objective function where appropriate.

Input by Hand

If this input mode is selected a dialog with a data grid is shown where the user can either type or paste or load data.

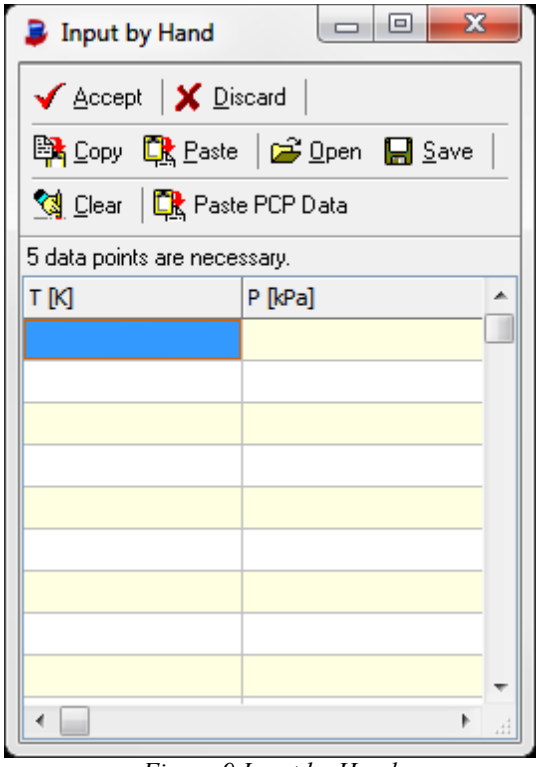


Figure 9 Input by Hand

Fit Results

After pressing the *Fit* button the fit will start and present a "New Parameters" box when it's finished:

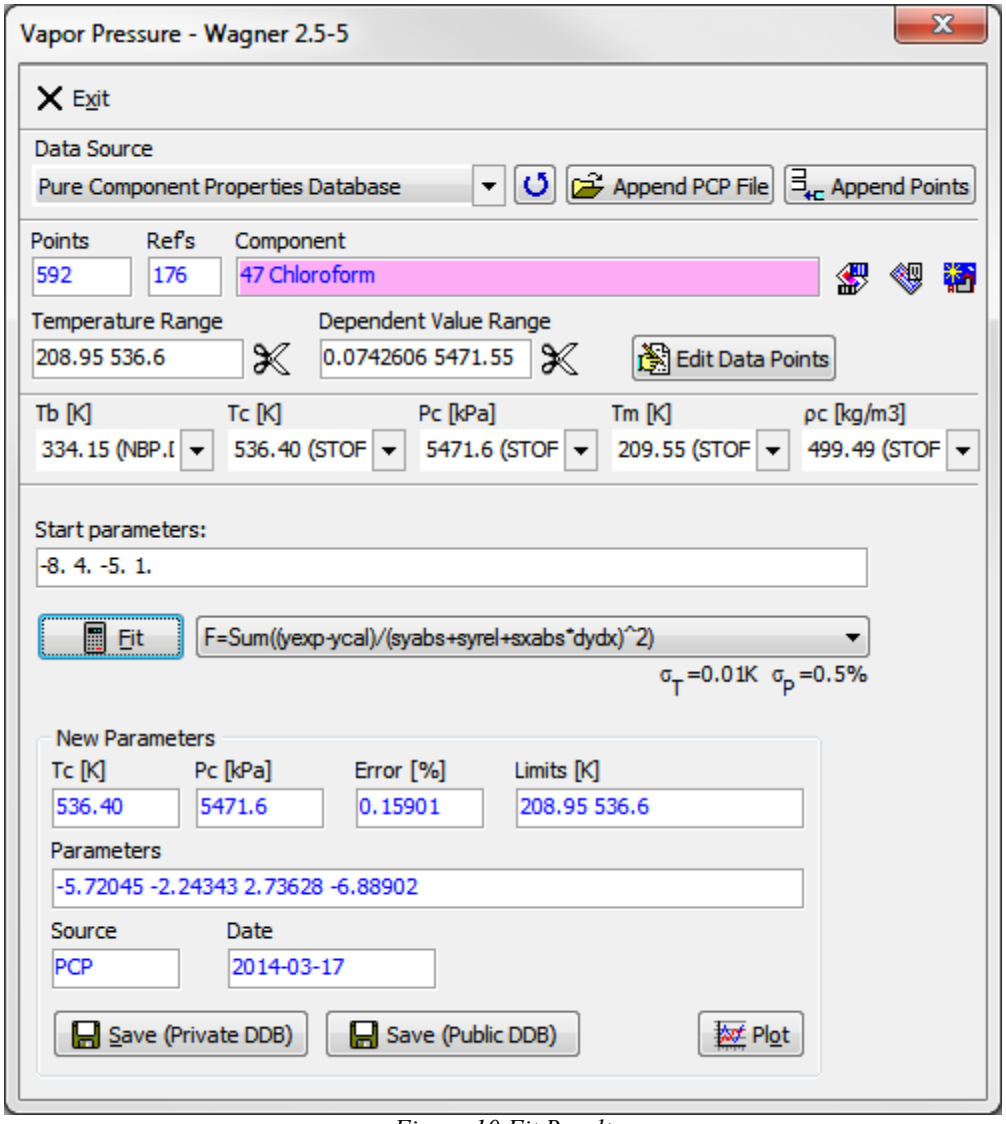


Figure 10 Fit Result

This box shows the new parameters, a mean error, the used temperature limits, the data source and the current date and in some cases additionally used constants like in this example T_c and P_c.

These entries will be stored in the ParameterDDB if one of the "Save" buttons will be pressed.

Plot

For an overview on the fit quality PCPEquationFit provides several plots.

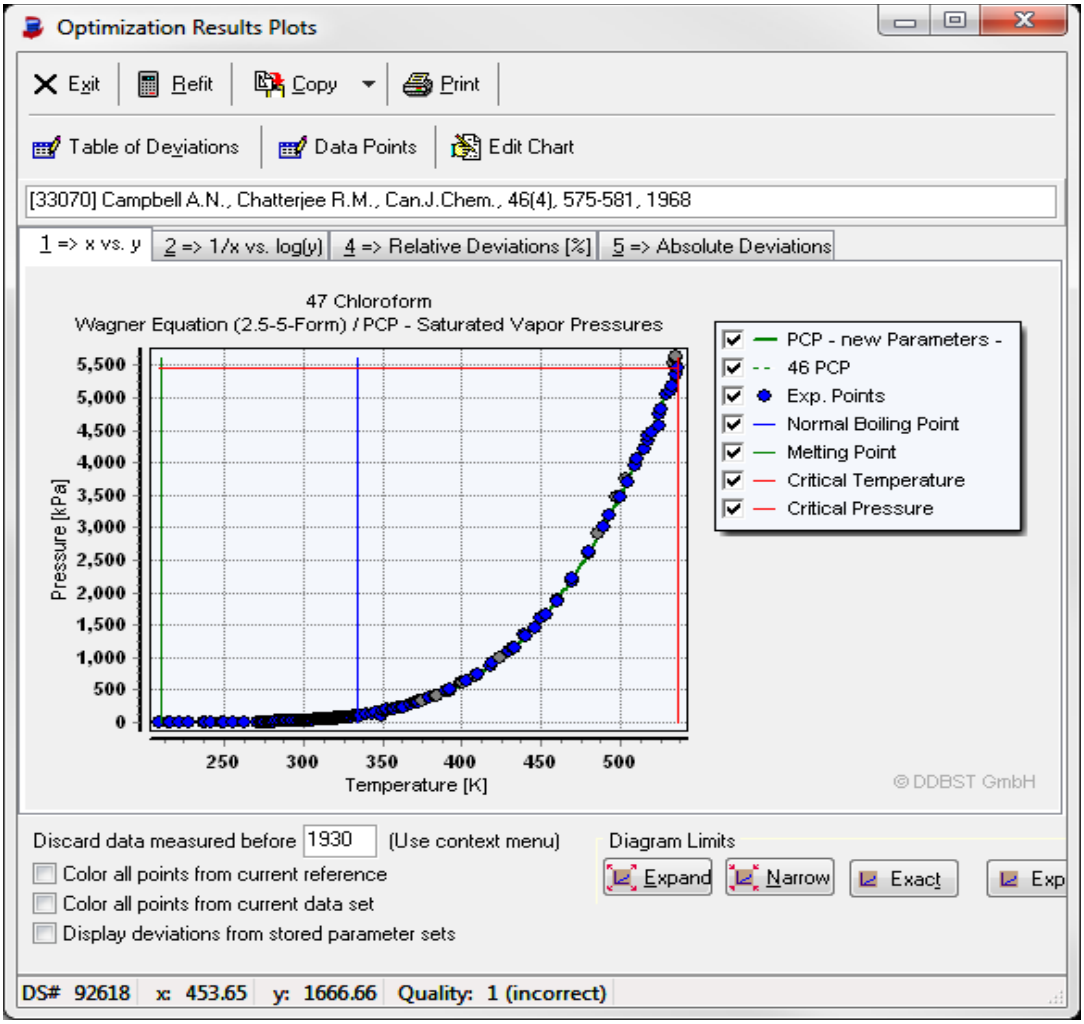
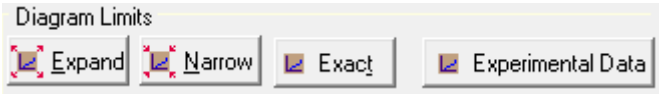


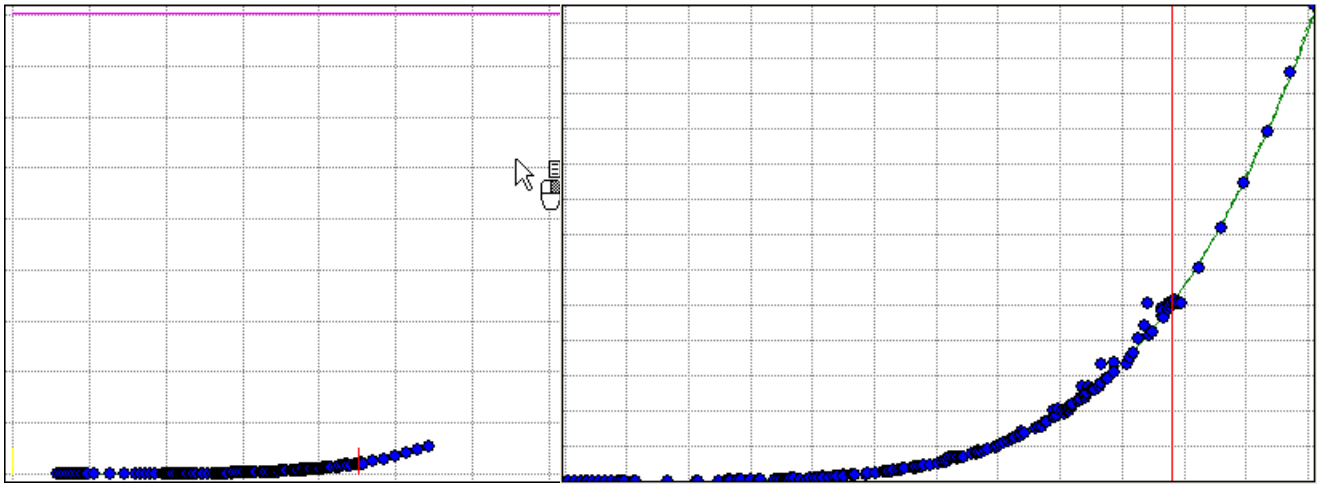
Figure 11 Plot of Fit

The list of plots slightly varies from model to model. Always the same is the rubber band drawn from the mouse cursor to the nearest point. Detailed information of this point are displayed in the status line. Additionally the reference is shown below the tool bar.

The diagram limit can be widened and narrowed.



The “Experimental Data” button adjusts the diagram so that the experimental data are filling the chart window. This is useful in the cases where critical data and melting points are shown and the experimental data are available only for a smaller range.



Through a context menu on the plot it is possible to

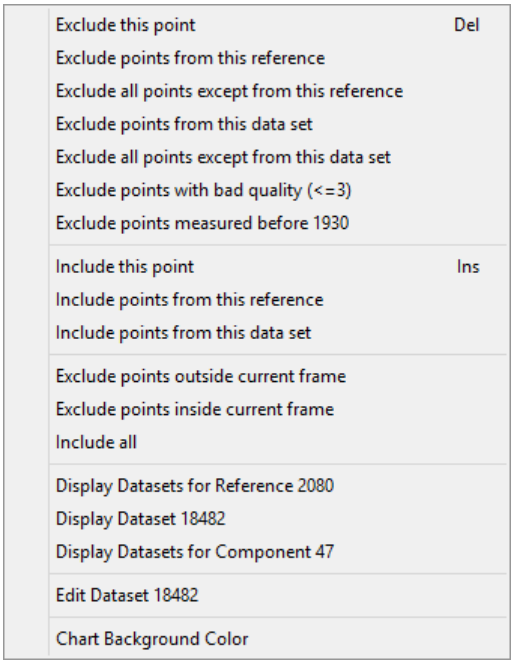
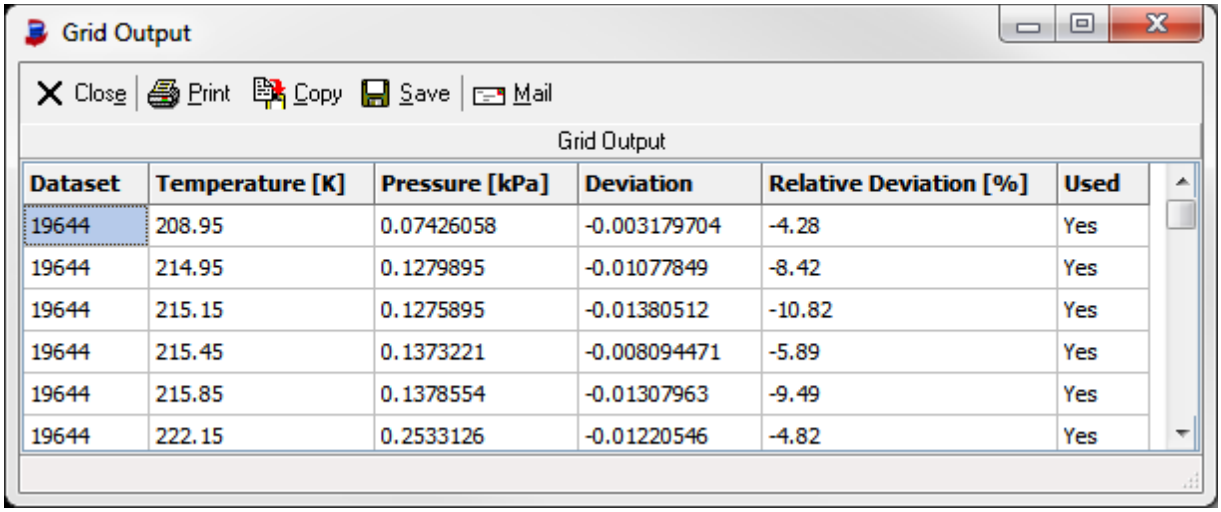


Figure 12 Plot Context Menu

1. Exclude points (either single or by criteria)
2. Include formerly excluded points
3. Display data sets shown in the chart (either single or a list of data sets for the current component or reference)
4. Call the data sets editor
5. Change the background color

Additionally a complete list of deviations can be created (“Table of Deviations” tool button) and the diagram can be copied to the Windows clipboard or printed.

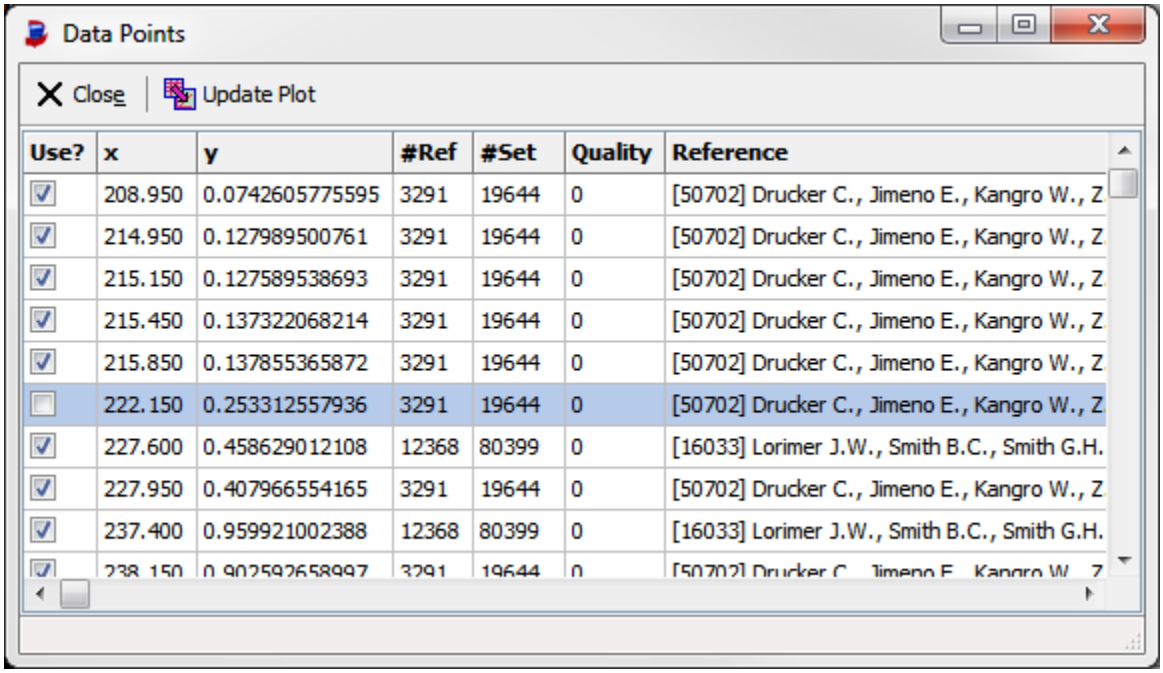


Dataset	Temperature [K]	Pressure [kPa]	Deviation	Relative Deviation [%]	Used
19644	208.95	0.07426058	-0.003179704	-4.28	Yes
19644	214.95	0.1279895	-0.01077849	-8.42	Yes
19644	215.15	0.1275895	-0.01380512	-10.82	Yes
19644	215.45	0.1373221	-0.008094471	-5.89	Yes
19644	215.85	0.1378554	-0.01307963	-9.49	Yes
19644	222.15	0.2533126	-0.01220546	-4.82	Yes

Figure 13 Table of Deviations

The "Data Points" tool button 

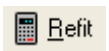
opens a dialog where all data points are listed. This dialog can be used to include and exclude data points.



Use?	x	y	#Ref	#Set	Quality	Reference
☑	208.950	0.0742605775595	3291	19644	0	[50702] Drucker C., Jimeno E., Kangro W., Z
☑	214.950	0.127989500761	3291	19644	0	[50702] Drucker C., Jimeno E., Kangro W., Z
☑	215.150	0.127589538693	3291	19644	0	[50702] Drucker C., Jimeno E., Kangro W., Z
☑	215.450	0.137322068214	3291	19644	0	[50702] Drucker C., Jimeno E., Kangro W., Z
☑	215.850	0.137855365872	3291	19644	0	[50702] Drucker C., Jimeno E., Kangro W., Z
☐	222.150	0.253312557936	3291	19644	0	[50702] Drucker C., Jimeno E., Kangro W., Z
☑	227.600	0.458629012108	12368	80399	0	[16033] Lorimer J.W., Smith B.C., Smith G.H.
☑	227.950	0.407966554165	3291	19644	0	[50702] Drucker C., Jimeno E., Kangro W., Z
☑	237.400	0.959921002388	12368	80399	0	[16033] Lorimer J.W., Smith B.C., Smith G.H.
☑	238.150	0.902592658997	3291	19644	0	[50702] Drucker C., Jimeno E., Kangro W., Z

Figure 14: Data Points Selection

This function has been added because of points occupying exactly the same position (exactly same data) which makes it impossible to select all these points by mouse.

If points have been excluded it is necessary to start a new fit by the "Refit" button 

. This will return us to the fit dialog allowing to store the modified parameters.

Understanding the ParameterDDB Dataset Display

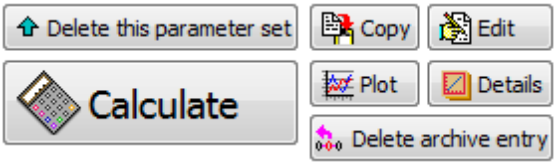
Key	Value
A	-8,41515
B	4,65592
C	-6,26863
D	1,7655
C1	12
Pc	3637,57
Tc	466,7
EQID	2
Tmax	466,74
Tmin	250,046
User	Cordes
COUNT	1
DateD	16
DateM	6
DateY	1994
Error	0,092
SETNUM	12
Source	PCP
LOCATION	0
AUTOSELECT	true
SourceFile	PARAM.WAG

Figure 15 Parameter Data Set

The ParameterDDB contains key/value pairs. The keys describe the values. The grid shows the list of keys and the values belonging to them.

1. The keys “A”, “B”, “C”, “D” and so on are the parameters of the equations.
2. “C1” is the DDB component number. Its name can be found in the component editor.
3. “Pc”, “Tc” are critical temperature and pressure. Other possible entries are e.g. “Tb”.
4. “EQID” is the internal equation number.
5. “Tmax” and “Tmin” are the upper and lower temperature limits of the experimental data used. Please regard these values also as validity range for the equation.
6. “User” specifies the person who stored the parameter dataset.
7. “DateD”, “DateM”, “DateY” specify the date when the dataset has been stored.
8. “Error” gives the model and fit specific error.
9. “Source” specifies the source of the data points which have been used for the fit.
10. “Location” specifies if the parameter set is stored in the public DDB (0) or in the private DDB (1) or, if missing or another number, some other location.
11. “AUTOSELECT” is necessary if more than one dataset is available for a component and a single equation. It specifies the preferred parameter set.
12. “SourceFile” is given in some cases and specifies a file from which the set has been imported.

Working with a Parameter Data Set



Copy

The data set grid will be copied to the windows clipboard as it is displayed in Figure 15 (source) and Figure 16 (destination).

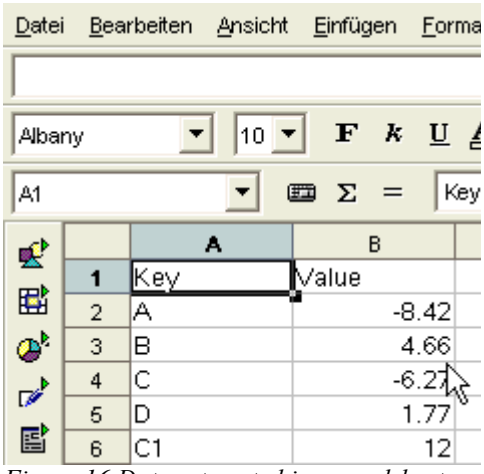


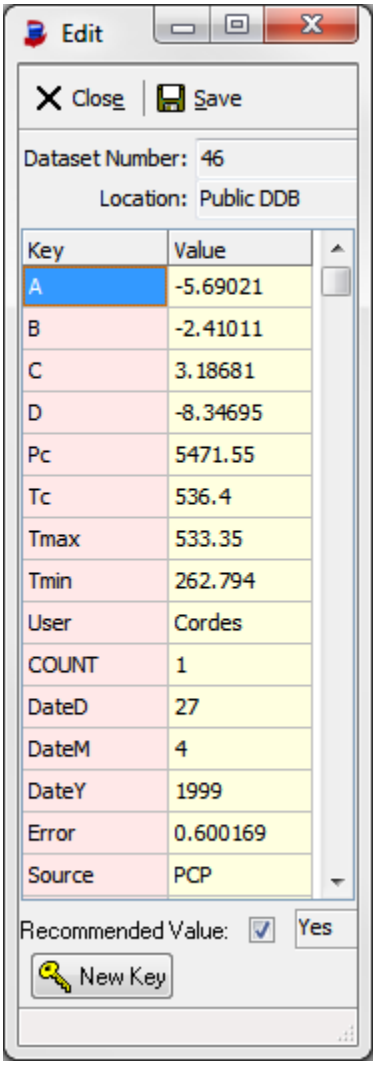
Figure 16 Data set pasted in spreadsheet program

Edit

The editor is another view on the parameter data set grid. The grid is now editable and new values can be typed in the Value column.

The Key column is not directly editable but new keys (New Key) can be added and keys with empty values will be removed automatically when the data set is saved.

The "Recommended Value" check mark should be set if more than one data set is available for the same component and equation and the current data set should be preferred over all others.



Plot

This plot shows the stored equation parameters together with points from the pure component properties data bank. It's the same plot as used in the fit procedure with the exception that some editing functions are not available – like removal of data points.

Details

This function displays a more detailed and explanatory view on the current parameter set. It is part of the ParamDDBOrganizer program.

This program is described in detail in the separate document "ParameterDDBOrganizer.pdf".

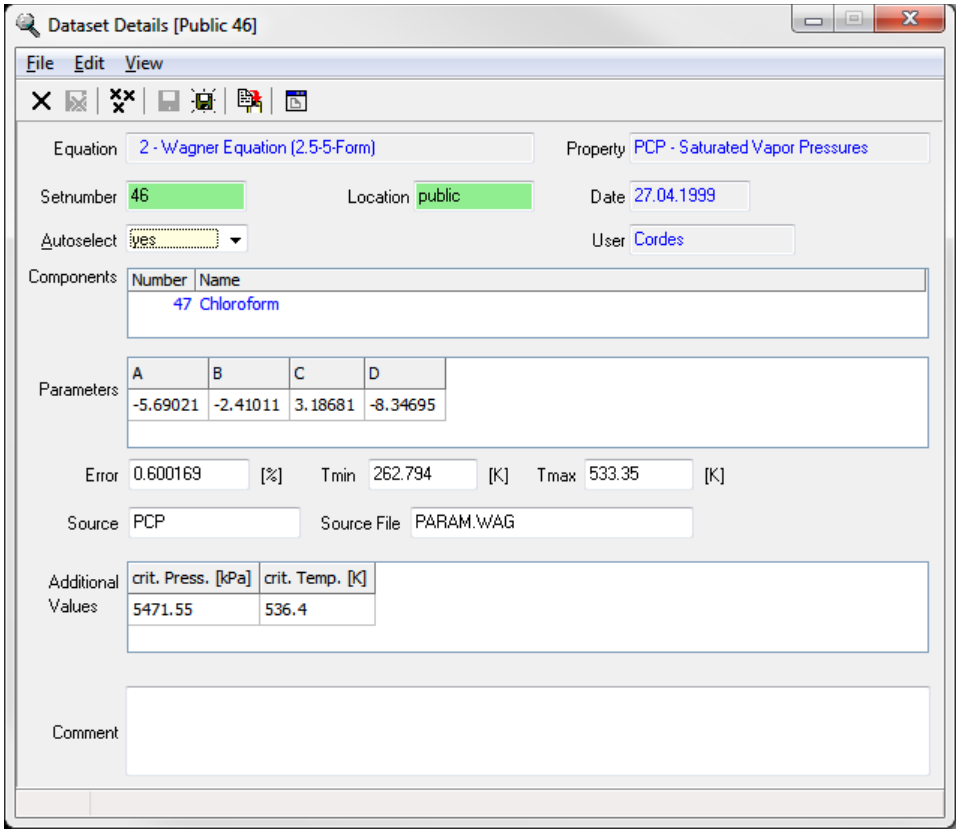


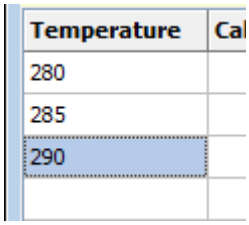
Figure 17 Data set details

Calculate

Stored parameter sets can be used to calculate the property at arbitrary temperatures.

It is either possible to calculate values in a temperature range where start and end temperature as well as a step width can be specified

or single values typed in the data grid.



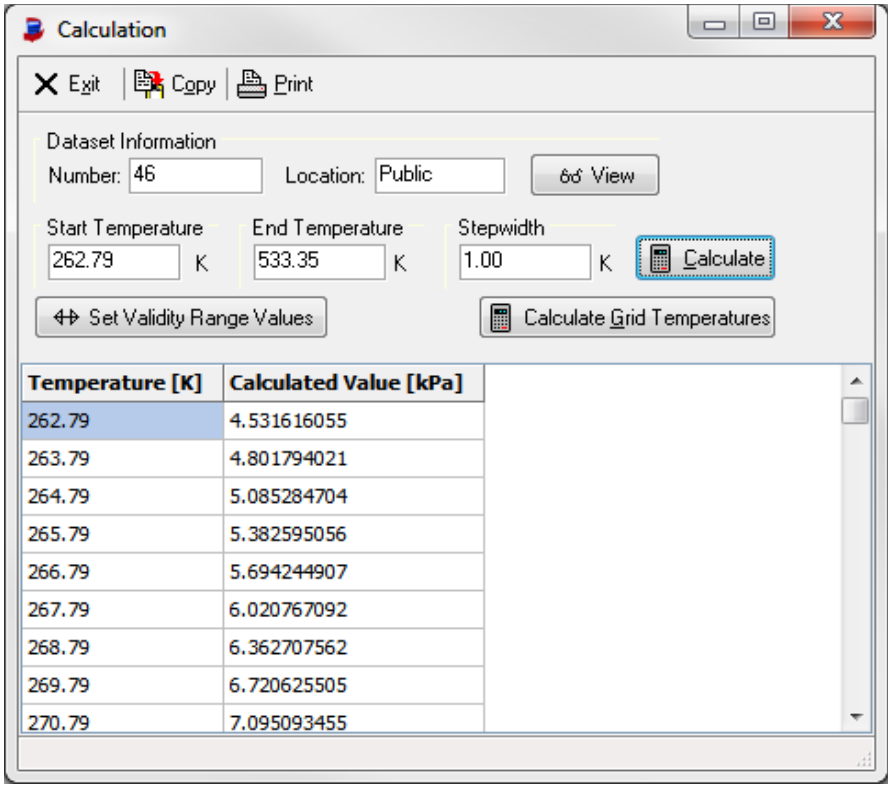


Figure 18: Calculate properties with stored parameters

Fit Archive

PCPEquationFit stores a history of fitted parameters and used datasets. This archive is accessible through the tool bar button Archive .

The archive is intended to be the memory of all fits. It should allow to save the data which have been used for the fit and to restore them and perform a full re-fit under the same conditions as done originally. This goal is currently not perfectly achieved.

The archive dialog itself (Figure 19) shows a list of of parameter sets identified by component number and model description separated for the public and private data banks.

The details grid shows the x and y, the reference number and the dataset number and in the "Used" column a "+" if the value has been used in the fit or a "-" if the point has been excluded.

The "Refit" button creates a fit dialog for the given equation and component with the stored data points (Figure 20).

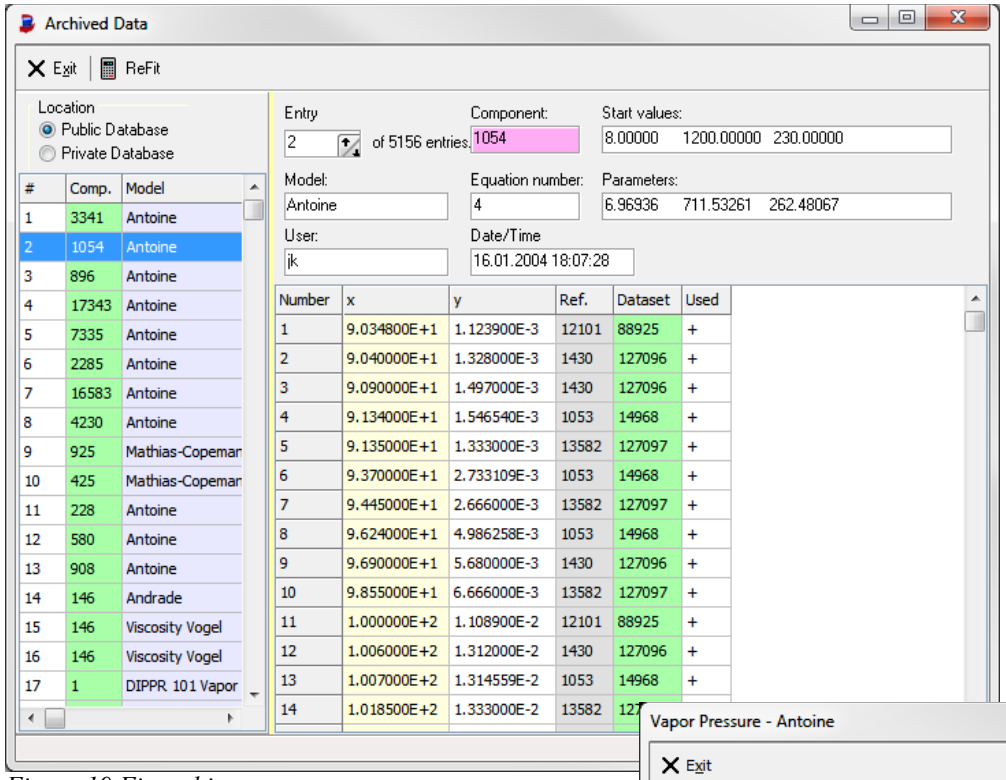


Figure 19 Fit archive

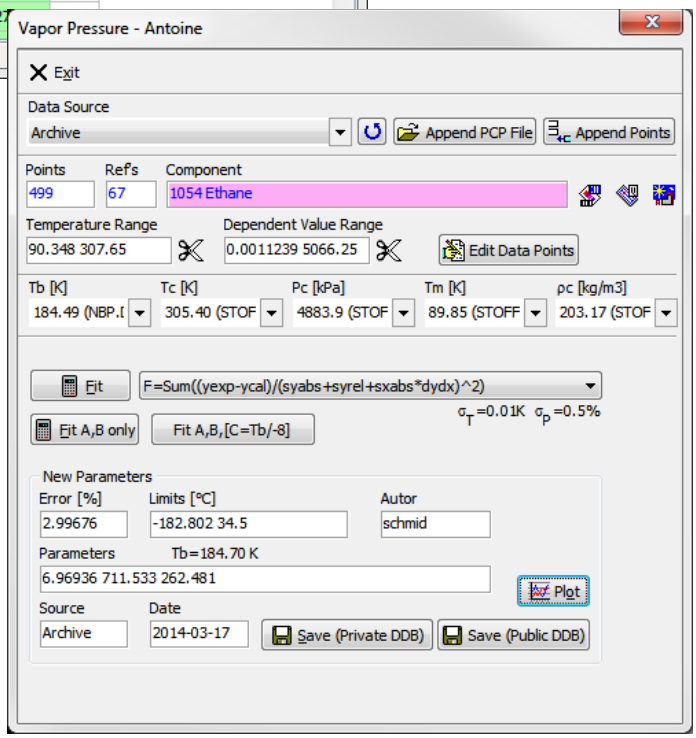
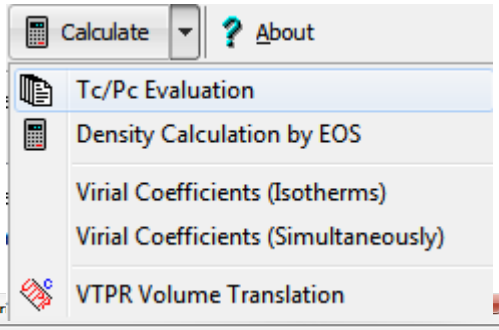


Figure 20 Refit with archived data

T_c/P_c Evaluation

PCPEquationFit allows with this function the evaluation of experimental pure component critical data and saturated vapor pressures together with calculated and estimated values.

For a full investigation it is necessary to have at least a parameter set for a vapor pressure equation and the Artist program package should also be present since it is used for displaying estimated critical data.



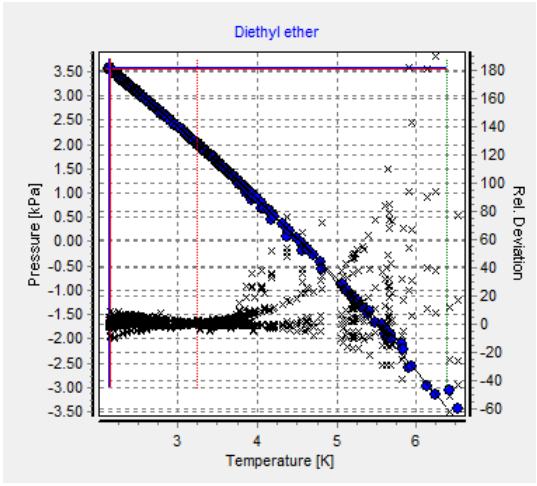
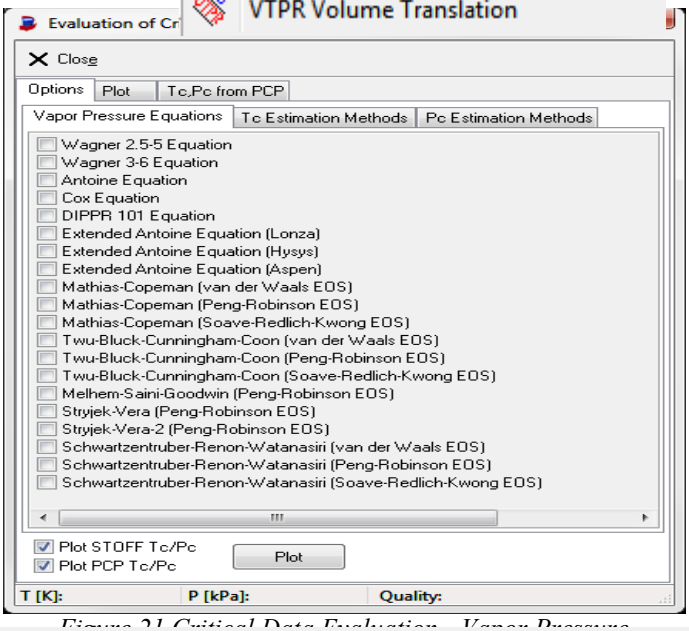


Figure 22 Critical Data Evaluation - Plot

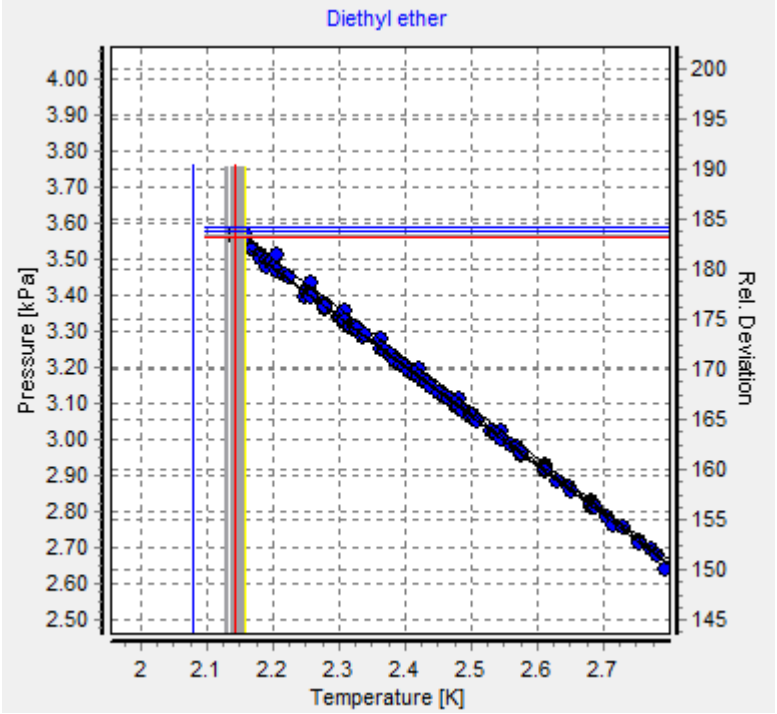


The "Options" page allows selecting vapor pressure equations from PCPEquationFit and T_c and P_c estimation methods from Artist.

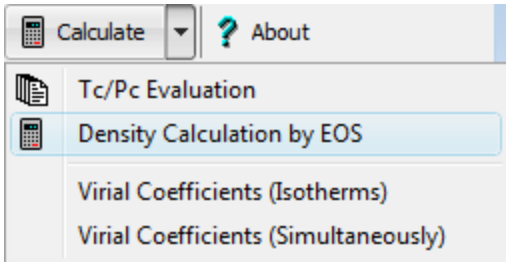
The resulting diagram shows all experimental, calculated, and estimated data points in a Temperature vs. Pressure plot. Deviations are shown in the same diagram with its scale on the diagram's right side.

The diagram allows switching between "T vs. P" and "1000/T vs. $\log_{10}$ P" and the display of the deviations can be switched on and off.

The important point is the end point of the vapor pressure curve. The experimental and estimated critical T_c and P_c are shown as horizontal and vertical line. The intersections give a hint where the correct critical point lies.



Density Prediction by Equation of State



This dialog

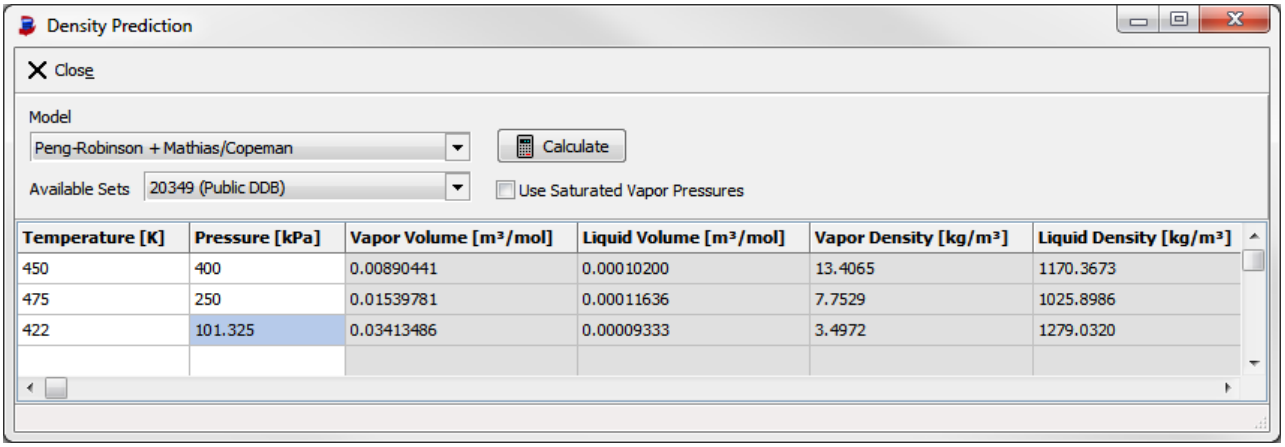


Figure 23: Density Prediction

can be used to calculate liquid and vapor densities and volumes of pure components by equation of states. The supported equations of state are the same which can be used to regress α function parameters in the main dialog and the regressed α function parameters are used also for this density calculation.

Input for the calculation by the equation of state are temperatures and pressures. The pressure can either be given directly or the saturated vapor pressure can be used. The saturated vapor pressure would be determined by the equation of state.

Temperature [K]	Pressure [kPa]
450	1541.280771
475	2318.513690
422	922.802849

Figure 24: Using saturated vapor pressures

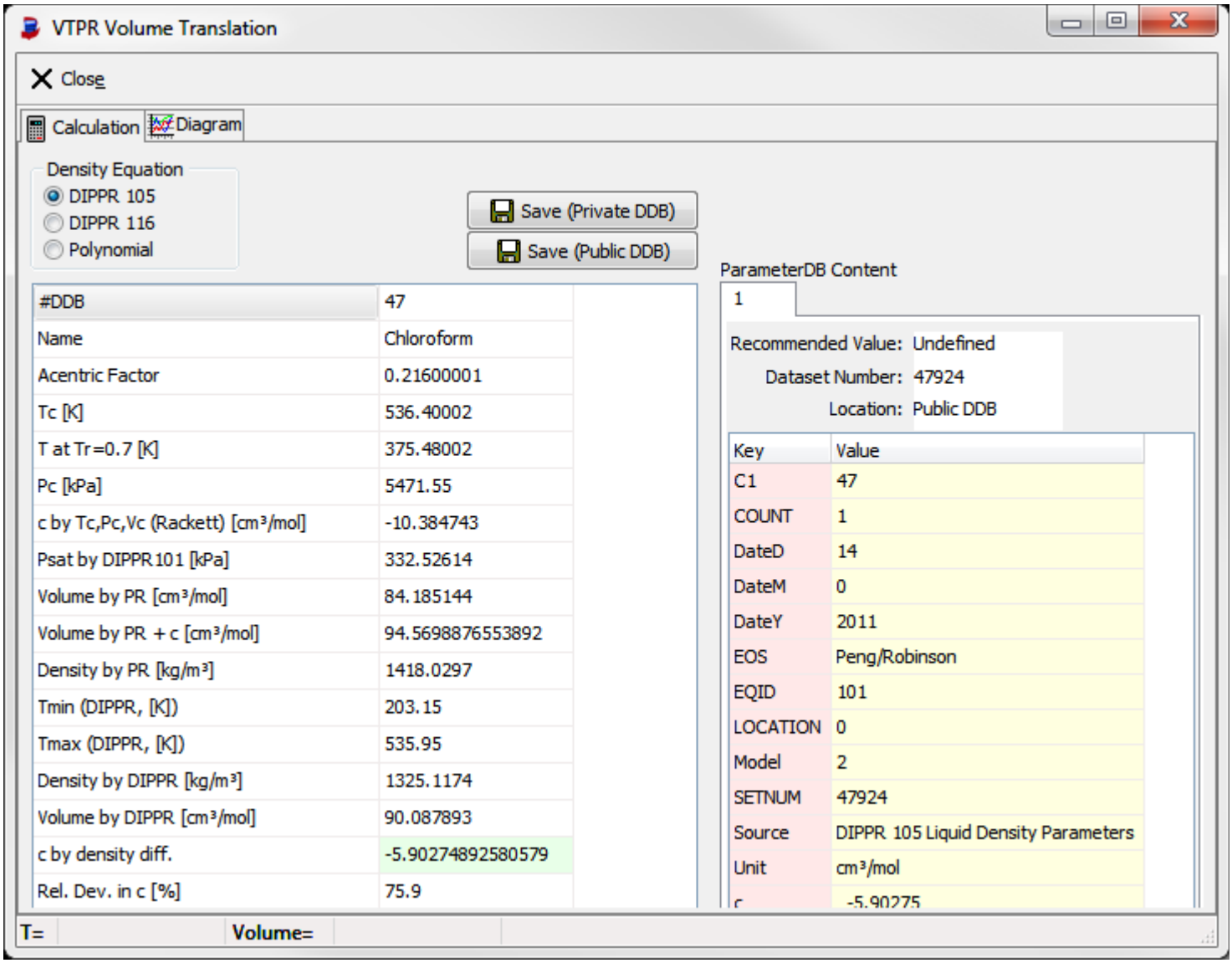
Virial Coefficients

Both calculation methods for virial coefficients are described in separate documents (“IsothermManual.pdf” and “SimultanManual.pdf”) .

VTPR Volume Translation

VTPR uses a volume translation based on the difference between the experimental volume and the volume calculated by the Peng-Robinson equation of state at $T=T_c*0.7$. This temperature is normally quite close to the normal boiling point.

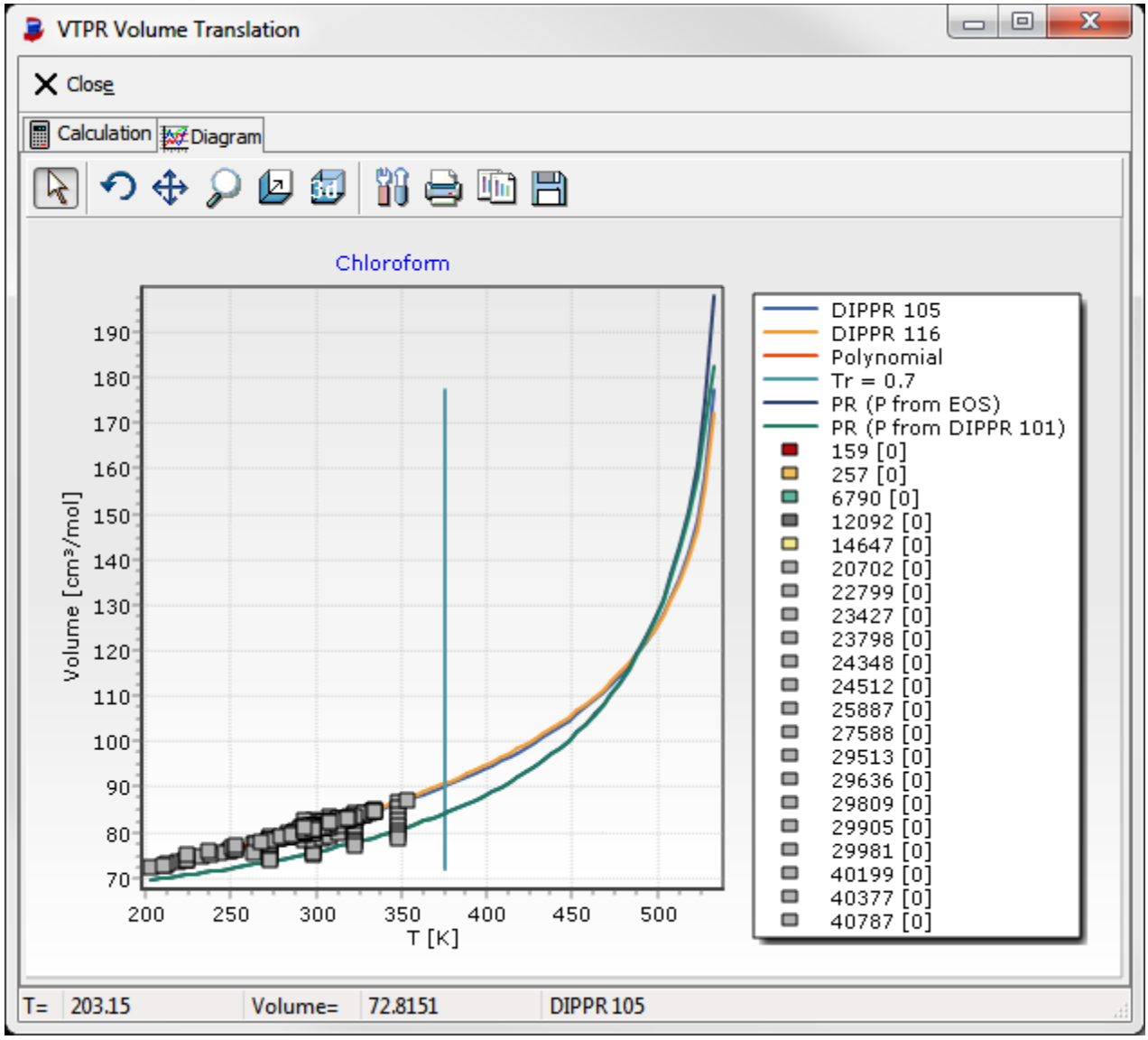
In this dialog



the volumes calculated by the equations DIPPR 105, DIPPR 116, and Polynomial are used as source for the experimental volume. The left table shows the calculation result with the volume translation value c in light green.

The right table shows the already stored values in the parameter data bank.

The “Diagram” page shows the different calculated volume ($1/\rho$) curves, a vertical line at $T_c*0.7$ and experimental values from the pure component property data base.


VTPR Volume Translation
Close
Calculation
Diagram
Chloroform
Volume [cm³/mol]
T [K]
DIPPR 105
DIPPR 116
Polynomial
Tr = 0.7
PR (P from EOS)
PR (P from DIPPR 101)
159 [0]
257 [0]
6790 [0]
12092 [0]
14647 [0]
20702 [0]
22799 [0]
23427 [0]
23798 [0]
24348 [0]
24512 [0]
25887 [0]
27588 [0]
29513 [0]
29636 [0]
29809 [0]
29905 [0]
29981 [0]
40199 [0]
40377 [0]
40787 [0]
T= 203.15
Volume= 72.8151
DIPPR 105