

PRO/II Calculations with DDBSP

Short Introduction Tutorial

DDBSP - Dortmund Data Bank Software Package



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Table of Contents

Introduction.....	3
Step 1: Read Components from a PRO/II Database File.....	3
Step 2: Search for Experimental Data in the DDB.....	5
Step 3: Calculate VLE Using the PRO/II Thermodynamics.....	5

Introduction

This document describes briefly in a step-by-step tutorial how to use the PRO/II thermodynamics in the DDB software.

The connection between DDBSP and PRO/II is using a COM interface.

The supported features are:

- Reading components from a PRO/II database file (*.prz)
- Calculation of V(L)LE using the thermodynamics defined in a PRO/II database file

Step 1: Read Components from a PRO/II Database File

In order to compare the experimental data stored in the DDB with a PRO/II model the components in a PRO/II database file must be identified and assigned to DDB components.

To identify the components in a database file start the *Dortmund Data Bank* program.

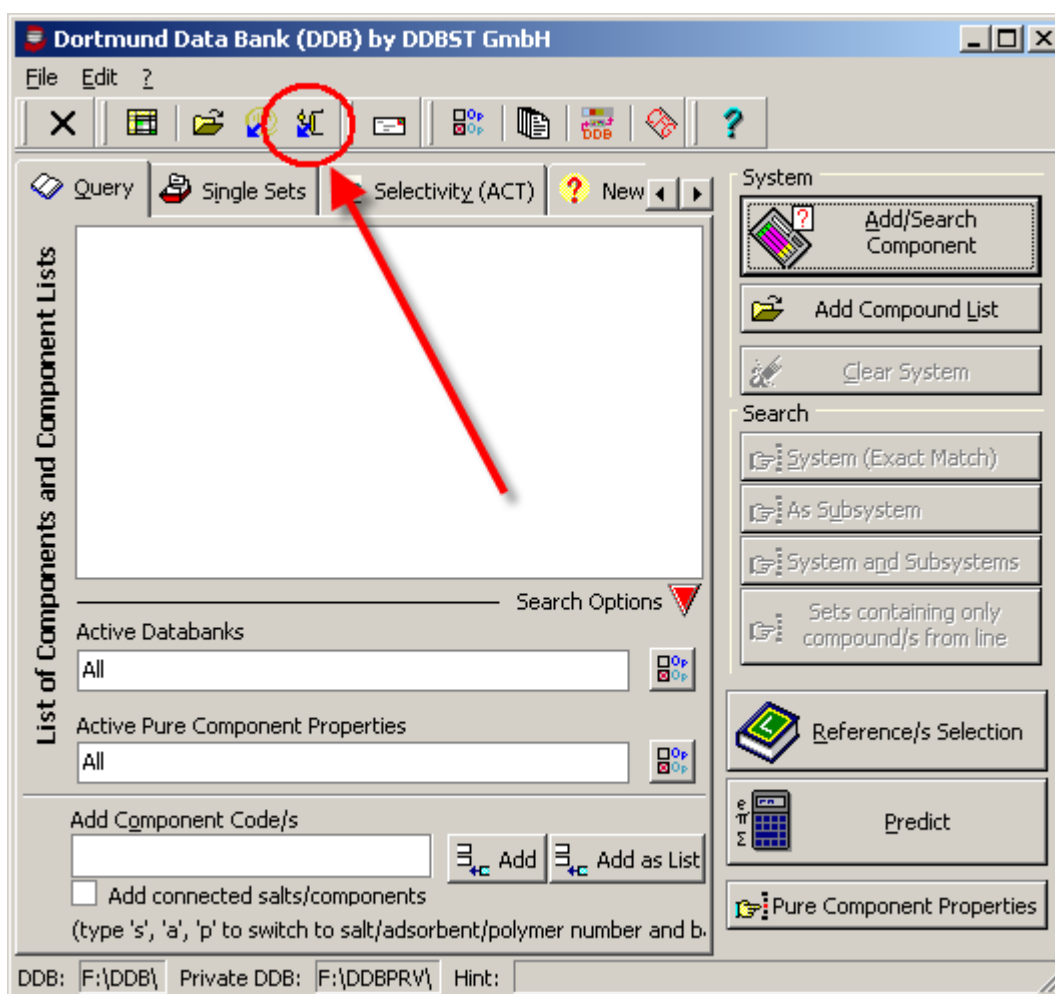


Figure 1: The Dortmund Data Bank Program

Click on the *Import PRO/II Components* button to open a PRO/II database file. After opening the file a component assignment dialog is displayed.

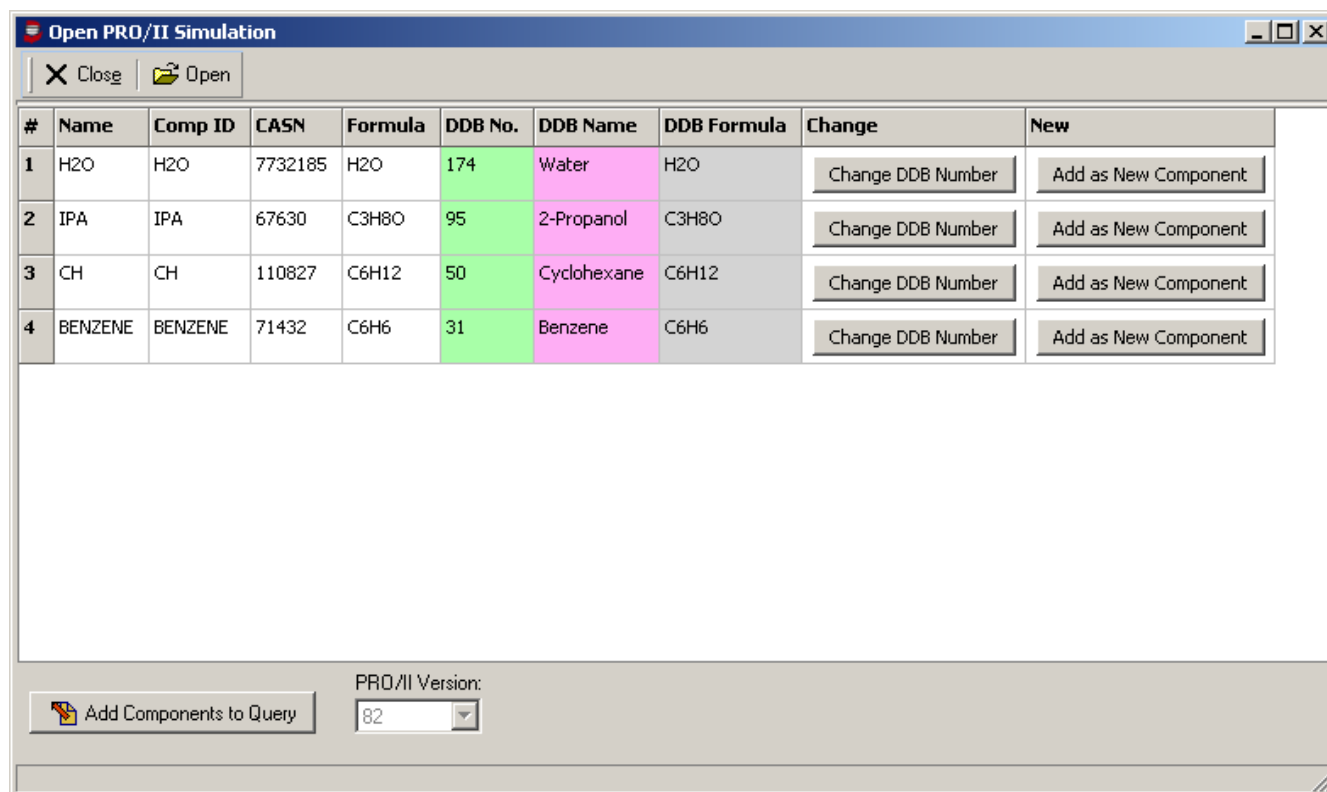


Figure 2: Open PRO/II Database File Dialog

The system tries to assign the components automatically. This is done by the *ChemAbsNum* stored in the PRO/II database.

If a component could not be identified or the identification is wrong the user can select a component from the DDB component list using the *Change DDB Number* button. If the component is not found in the DDB a new component can be defined using the *Add as New Component* button.

After all assignments have been done the components can be added to the query using the *Add Components to Query* button.

Number	Type/ Count	Loc.	Remove	Name
[174]	C	DDB	Remove	[Water]
[95]	C	DDB	Remove	[2-Propanol]
[50]	C	DDB	Remove	[Cyclohexane]
[31]	C	DDB	Remove	[Benzene]

Figure 3: Query Component List

Unwanted components can be removed from the list using the *Remove* button.

Step 2: Search for Experimental Data in the DDB

After the components of interest have been defined within the *Dortmund Data Bank* program the DDB can be searched to find experimental data. In order to search for data for the system Cyclohexane + 2-Propanol the components with the DDB number 50 and 95 have to be added to the query. Click on the button *System (Exact Match)* in the *Search* area to find data for the binary system.

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Publ.Year	Ref.No.	Reference
[699 0 0]	DDB	11	2	C50 C95	343	353	101 (const.)		Txy(P)	1963	335	[639] Nagata I., Mem.Fac.Techno
[700 0 0]	DDB	13	2	C50 C95	331	340	67 (const.)		Txy(P)	1965	84	[388] Nagata I., J.Chem.Eng.Dat
[1712 0 0]	DDB	11	2	C50 C95	342	350	101 (const.)		Txy(P)	1968	642	[946] Verhoeve L.A.J., J.Chem.E
[2019 0 0]	DDB	42	2	C50 C95	343	356	101 (const.)		Txy(P)	1973	817	[1121] Ocon J., Tojo G., Bao M.
[2091 0 0]	DDB	15	2	C50 C95	343	355	101 (const.)		Txy(P)	1965	841	[1145] Bzhostovskii V.L., Galsk
[3240 0 0]	DDB	26	2	C50 C95	342	352	101 (const.)		Txy(P)	1963	665	[969] Yuan K.S., Ho J.C.K., Kes

Figure 4: Query Result for Binary System

The result is grouped by data types. To see the result for vapor-liquid-equilibrium data click on the *VLE* tab.

Step 3: Calculate VLE Using the PRO/II Thermodynamics

The experimental data in a query result can be used as basis for a calculation.

Set No.	Source	Pts.	Comp's	#DDB	Tmin [K]	Tmax [K]	Pmin [kPa]	Pmax [kPa]	Comment	Publ.Year	Ref.No.	Reference
[699 0 0]	DDB	11	2	C50 C95	343	353	101 (const.)		Txy(P)	1963	335	[639] Nagata I., Mem.Fac.Techno
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Figure 5: Query Result with VLE Predict Button

Select the data of interest and press the *Predict selected datasets* button. The *VLE/HPV Prediction* dialog will be displayed. The components of the first selected dataset will be used as system for the prediction.

Components
50: Cyclohexane
95: 2-Propanol

Figure 6: VLE Prediction Components

The PRO/II database file which has been opened most recently within the DDB software is selected as default file to be used for a calculation with PRO/II.

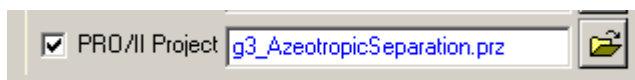


Figure 7

Use the *Select PRO/II Project* button next to the displayed file name to select a different file for the calculation. Then a dialog similar to Figure 2 on page 4 will be displayed. In addition to the dialog in step 1 the thermo set can be selected.

If the mouse is over the *PRO/II Project* checkbox some additional information is displayed.

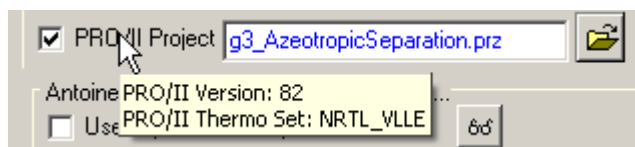


Figure 8: PRO/II File Additional Information

To calculate with PRO/II only all models in the Prediction Method area have to be deselected, just the PRO/II model must be active. All selected models will be used in a calculation.

If several datasets have been selected it is possible to calculate all temperatures (for isothermal calculation) or all pressures (for isobaric calculation).

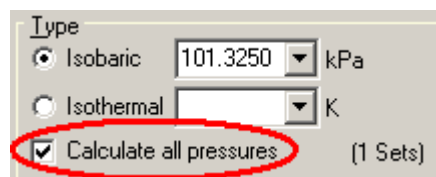


Figure 9: Calculate All Pressures

For a quick comparison between the experimental data and the model(s) the *Predict and Plot* button can be used.

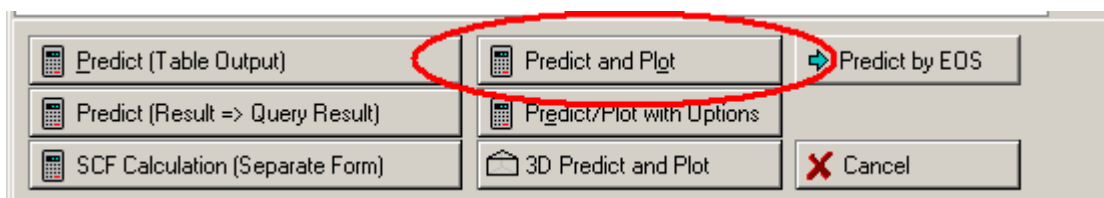


Figure 10

The experimental data together with the calculated results will be displayed in a plot with several diagrams.

For a text output the *Predict (Table Output)* button can be used. The button *Predict (Result => Query Result)* will send the predicted data to the Dortmund Data Bank program.

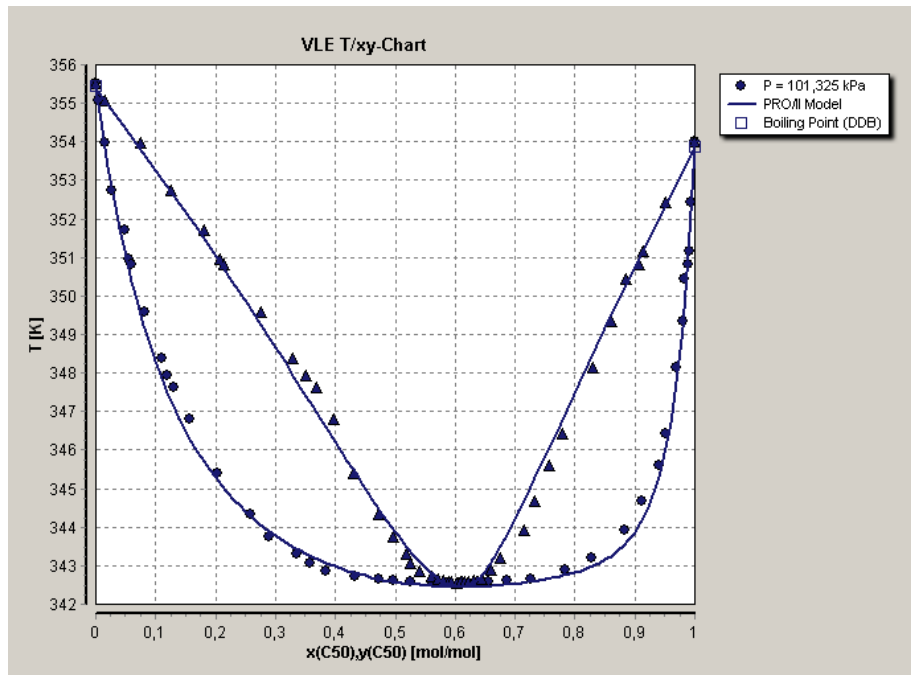


Figure 11: VLE T/x,y Diagram

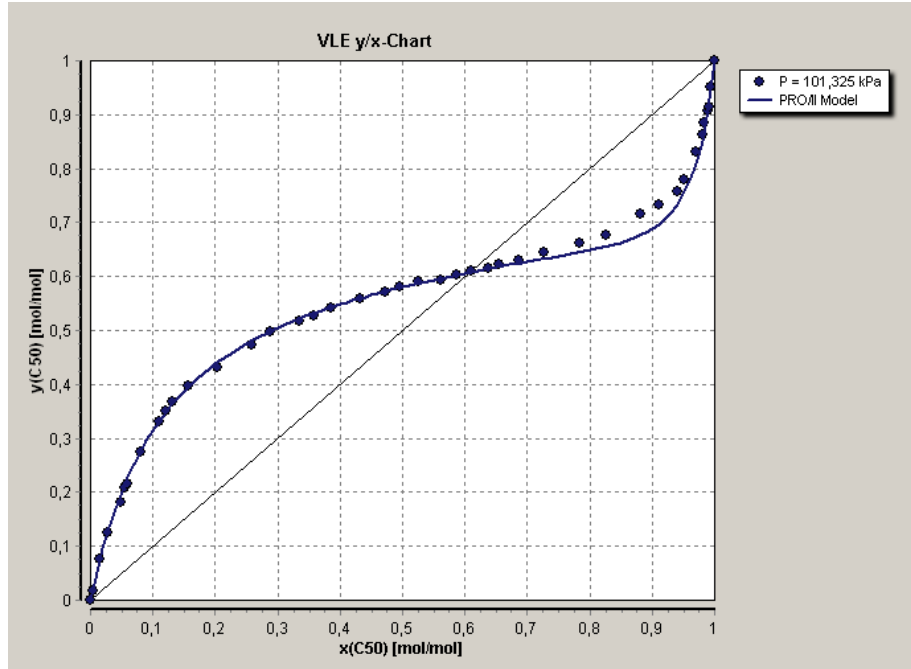


Figure 12: VLE x/y Diagram