Dortmund Data Bank (DDB)
DDB Software Package (DDBSP)

An Introductory Course for DDB/DDBSP
Dortmund Data Bank (DDB)

DDB Software Package (DDBSP)

Chemical Thermodynamics and Physical Properties with DDB and DDBSP

Contents

- Parts of DDB/DDBSP
- Components and Component Lists in DDB
- DDB Literature Management (Lear)
- Pure Component Data Estimation (Artist)
- Pure Component and Mixture Data - Retrieval and Output
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- Mixture Data Estimation
- Check Parameters Prior to Process Simulation
- DDB Parameter Data Bank
- Process Synthesis
- Data Input
- Data Import and Export
- DDBSP and Programming
Parts of DDB and DDBSP

**Lesson Objectives**
- become familiar with how to start DDBSP
- some data in DDB (exp. and basic data)
- component types in DDB
- ways to select components and component lists
- store, retrieve and edit component lists
- component lists by substructure
Component Types and their Basic Data

- normal components (organic and inorganic)
  - name, emp. formula, CAS#
  - Antoine constants, critical data, acentric factor, ...
  - melting point, heat of fusion
  - molecular weight, dipole moment
  - density (Wilson), R and Q values, ...
- salts
  - thermodynamic data, heat capacity
  - dielectric constant, ions, ...
- polymers
  - further specifications together with exp. data
- adsorbents
  - further specifications together with exp. data
- ions
  - ...

Start Dortmund Data Bank and select Add/Search Component to display the following Dialog:

Please look at the menu for further options!

Component types:
- Normal Components
- Salts
- Adsorbents
- Polymers

Data banks
- Public DB (DDB)
- Private DB
Same component may be **normal component** or **salt**.

**Sodium Chloride**
- as a normal component
  - density, vapor pressure, heat of vaporization, melting point, surface tension, viscosity, thermal conductivity
  - VLE, AZD, LLE, SLE, ...
- as a salt
  - electrolyte VLE
  - electrolyte SLE

Checking "add connected salts/components" will always select both.

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**Search for Pure Components**

**query expression**  |  **query syntax**
--- | ---
activate history |  reload
Select previous query from history |  search in all components or only those found in the active search
|  what to search for

Search for „name“ searches also the alternative name.
Search for „formula“ allows any order of the elements (H2SO4, SH2O4, …).
Select Components, Component Identification

As in the Windows Explorer:
- select or unselect components by mouse-click while pressing ctrl
- select from ... to by pressing shift when selecting the second item
- ctrl-a to select all components
- remove selected component(s) from the list; right mouse button and "remove component" or "remove selected components"

Clicking on table header will sort for this item.

Search for Pure Components - Synonyms

Search for synonyms
- synonyms
- component names and identifiers from Aspen Tech
- ...

Companies can add special names and identifiers for their inhouse systems.
Searching synonyms is much slower ......
Basic Data (Usually Without Source Reference)

Basic Data - Normal Components

Molecular Structures (ChemDB)

Literature Sources, Documents (LEAR)

Basic Data - Salts

Model Parameters (ParamDB)

COSMO α-Profiles

Different Sheets for Each Data Bank

Experimental Data (Nearly Strictly Only from Primary Reference)

Try out the small pics in the dialog boxes!
Component Selection Workshop

- Workshop
  - bring up the Jumpstart menu
  - start "Dortmund Data Bank" under the "Dortmund Data Bank" header
  - in the dialog window, click "Add/Search Component"
  - de-select search option synonyms
  - de-select display of synonyms
  - search for component R134a
  - click once on the component in the list and bring up the context menu (right mouse button)
    - view/edit component data and explore the pure component basic data display
    - compare the acentric factor to the results from Antoine constants and critical data
    - explore the other tabs in the "edit component data" dialog (salts, adsorbents, ...)
    - close the dialog "edit component data"
  - display structure
  - select component

Molecular Structure Database and ARTIST

ARTIST
- search (full structure, sub-structure)
- display and structure input
- fragment molecules into structural groups for ≈ 100 methods
- estimate properties using ≈ 100 methods
- ......
Demonstration

• Entering a structure in Artist.

Workshop

• Start Artist and open a new struct
• Enter the following structure:

   \[
   \begin{array}{c}
   \text{O} \\
   \text{N} \\
   \text{O} \\
   \text{O}
   \end{array}
   \]

• Search as sub-structure. Stop the search after the first 2000 components.
• Save the components matching the search structure as a list under the name “nitrobenzenes”

DDB Literature Management (Lear)

Lesson Objectives

• Open and search Lear data banks
• Linked documents
• Links to data banks
• Find data from a reference
Search in LEAR

quick and advanced search

Linked Documents

LEAR query results (list)

Document

LEAR query result (data set)

Linked document list (not in delivered Version)
How are Documents linked to LEAR References?

- Each user can individually specify a list of directories for each LEAR data bank.
- Lear will search these directories for files or folders that start with "'<LEAR Number>' or "'L<LEAR number>'".

Example: Valid links for LEAR dataset 1234:
- 1234 calculation.xls
- L01234 FPE 1983 p 33.pdf
- ....

Links are public or limited to groups or individual users through the operating system folder access rights.
Linked files can easily be moved without generating broken link errors.

Document Linking can
- make original (scanned) reports for your own in-house data available to a specific set of users.
- make documents with calculations, notes etc. concerning a document easily available to a defined set of users.

Workshop
- In the Mixture Properties Query dialog, select Reference/s Selection
- Search for papers where “Rarey” is among the authors:

(in LEAR, complex queries can be entered, saved and loaded)

Select reference number 32869 and click

A Mixture Properties query result dialog will show all the data from the references found. Select different data bank sheets and explore the tree-view for the system studied in the paper.
**Lesson Objectives**

- Draw molecular structures
- Retrieve structures from the DDB
- Fragment structures for group contribution methods
- Estimate different properties
- Judge method quality
- Optimize the 3D-structure
- Prepare an input file for Gaussian (σ-Profile calculation)
Selecting a property enables quality if available.

Selecting a single method for a T-dependent property allows to estimate over a range.
**Workshop**

- **Start Artist**, open a new document window and draw the structure of 1,4-butanediol (HO-CH₂-CH₂-CH₂-CH₂-OH) using ![structure](image)
- Use ![adddelete](image) to add and delete hydrogen atoms.
- Search the structure in the DDB (exact search).
- Accept the found component 614 ![accept](image). Now Artist has access to all properties stored in DDB for this component. 2 different structures are stored ![structures](image).
- Fragment the structure into the UNIFAC-groups (Calculate – Group Assignment, UNIFAC.ink).
- Go to Calculate – Calculate and mark the node Critical Temperature in the tree-view (Additional needed properties will offer the normal boiling point from the DDB).
- Compare the estimated values with the basic data value of 727 K.
- Retrieve the quality information for critical temperature estimation methods.
- Estimate the normal boiling point (experimental value approx. 503.15 K).
- Generate vapor pressure values between 273.15 and 393.15 K in 5 K steps (Rarey/Nannooolal with estimated Tᵦ) and regress Antoine constants.
Property Estimation Using Artist – Workshop 2

- Enter the following Structure into Artist:
- Add and remove hydrogen atoms

- Search this structure in the DDB as substructure
- Estimate important properties like critical data, normal boiling temperature and vapor pressure curve using different methods. Compare the results. (the experimental normal boiling point is 590.15 K)

- Examine the method quality estimation for a method ranking.
- Select some estimation results and export these to an Aspen inp file.

Property Estimation Using Artist – Workshop 3

- Load acetone and diacetone alcohol into 2 separate drawing windows in Artist.
- Calculate the heat of formation and reaction enthalpy using Domalski/Hearing.
The DDB structure data bank can store any number of different structures for each component. Typically a flat structure and a 3D-structure can be found. When adding hydrogen to a flat structure, a simple geometry optimization is performed automatically. More rigorous structure optimization can be performed using the free packages MOPAC and Tinker. ARTIST allows to save the current structure as a Gaussian input file with the commands for a COSMO-calculation as required by COSMO-RS and COSMO-RS(OI). 3D display is available via the free tool RasWin.

Load nicotine and add hydrogen atoms.

Calculate – MOPAC - run to optimize the molecular geometry, use coordinates. Rotate the structure.
Display the structure using RasWin:

![Structure Image]

```
shell]
$G09$ (E=0P-31G(dp,p)) OPTIMIZATION GAS PHASE
   C   CH2 (CH3)2
   H   CH2 (CH3)2

#M06-2X/6-31G(dp,p) optimization
$G09$ (E=0P-31G(dp,p)) OPTIMIZATION GAS PHASE
   C   CH2 (CH3)2
   H   CH2 (CH3)2
```


```
Pure Component and Mixture Data Retrieval and Output

Lesson Objectives

- learn to retrieve data of interest
- study the different specific tabular and graphical output options

The largest data bank in DDB is PURE

Access via "Dortmund Data Bank"

The programs contain a multitude of options, please explore the menu items.

- Data can be stored to files and loaded, exported as CAPE-Open files or Aspen inp-files, csv-files for Excel, ..... 
- Different units can be selected for plots and tables 
- Data can be shown graphically in 2D- or 3D-representations. 
- Data can be shown together with the results from correlation equations or group contribution methods 
- Data can be regressed using a multitude of equations.
- ....
DDB - Pure Component Data Bank - Workshop

Workshop

- Start "Dortmund Data Bank" and search for data for acetone (System (Exact Match))
- Select all vapor pressure data
  (use property list below tree on the left to display only vapor pressure data and then mark one set and enter ctrl-a to select all data points)
- Plot the vapor pressure data as ln(P) vs. 1/T using .
- Zoom, move the mouse to see the values and sources of individual data points.
- Plot the thermal conductivity. Explain the data.
- Plot the 2nd virial coefficient together with predictions using the RK, SRK and PR equations of state using .

It is also possible to select and view data for a group of components.

Workshop
- Plot the vapor pressure of nitrobenzenes as log(P) vs. 1000/T.

Use the component list file previously stored from ARTIST.
DDB - Dortmund Data Bank Software Package

DDB - Mixture Properties - Query

- Status of the DDB in your installation
- Special Selectivity Query
- Add components via selection dialog, component lists via file open dialog
- List of components or component lists
- Select data banks to search (usually all)
- Add components or component lists via code numbers

DDB - DDB Statistics
Workshop

In the „Dortmund Data Bank“ query dialog, select edit-options and explore the different option screens.

Search for a system

Once a list of components or component lists was entered, different search options are available.

It is possible to go back to the search dialog with or without closing the result dialog.

Data sets can be moved between the search result dialogs by drag’n drop.

Salts like sodium chloride appear both as normal components and as salts.
**Search for a System**

**System (exact match)**
Search for all data sets for the given system. If a list item is a component list, any one component in the list matches the query.

**Example:**
Component: ethanol
Component: water
List: benzene, cyclohexane

All data for the systems ethanol-water-benzene and ethanol-water-cyclohexane will be found.

**Example:**
Component: benzene
List: nitrobenzenes.stl

All binary mixtures of benzene with a nitrobenzene will be found.

**Search for a system**

**As Subsystem**
Search for all data sets for the given system and higher systems where this system is a subsystem.

**Example:**
Component: ethanol
Component: water
List: benzene, cyclohexane

All data for the systems ethanol-water-benzene and ethanol-water-cyclohexane will be found as well as quaternary and quinary systems with additional components, e.g.

ethanol – water – benzene – ethyl-3-methyl butyrate
ethanol – water – cyclohexane – i-octane – xylene
Search for a system

**System and Subsystems**
Search the system of the components specified plus all subsystems. This is the typical search when compiling the available data for the description of a multicomponent mixture. Instead of single components also lists of components can be included.

Instead of only including m-xylene, it is a good idea to include a list of the 3 isomers plus "xylene (isomer not specified)". There is practically no difference in the activity coefficients when exchanging the isomers in a mixture.

**Example:**
Specifying the components ethanol – water – cyclohexane will retrieve data for the systems:
- ethanol – water
- water – cyclohexane
- ethanol – cyclohexane
- ethanol – water - cyclohexane

**Sets Containing only Components from Line**
Some companies have a limited range of compounds they are interested in. This option allows to retrieve e.g. all systems containing only silicon compounds or alkanes. A component list file containing all silicon compounds and alkanes has to be prepared before.

To prepare and modify component list, a "Compound List Editor" is available:
DDB - Mixture Properties - Query - Result

- **Data Bank Pages**: show data sets of only one data bank. Switch between the data banks by a single-click on the data bank pages.

- **Overview Line**: shows number of references, data points, and sets found in the selected data bank for the current view of the 'Dataset List'.

- **Tree View with Info Field**: shows list of references, systems, components, properties (only PCP), solutes and solvents (only AGT, ACM)

- **Dataset List**: shows the data sets for the current data bank with some elementary information.

- **Extended Hint Field**: shows background information when moving the mouse cursor over the Tree View, Info Field and Data Set List.

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Different options in the 'Query Result' dialog

- Selecting databanks, systems, references and properties
- Plot data sets
- Predict data sets
- Color Link options
- RecVal
- Fit data sets
- Composition Units
- Modify data sets
- Consistency tests

Select a Data Set (3 ways)

- With a left mouse button click a single line will be marked.
- With a Shift-left-mouse-button click a range of lines will be marked.
- With a Ctrl-left-mouse-button click several disjunct lines will be marked.

Context Menu (right mouse button)

- Most functions are duplications of the menu and the tool bar, except:
- Create New Query Result From Marked Sets.
- Remove Selected Sets From Query Results. This allows to delete unneeded data sets from a result list.
Workshop

In the query dialog, search for data for the system ethanol – water – acetone and its subsystems.

In the query result dialog, select VLE data for the binary acetone - ethanol.

The query result dialog should look like this:

![Query Result Dialog]

---

Workshop

Double-click data set 580 to display a data table. Close the data table.

Mark all VLE data sets for the system acetone – ethanol, generate a plot of the data. The plot windows should contain these and more plots:

![Data Table and Plots]

Zoom into an area in one of the 2D plots. Zoom full again.

Change the P-axis in the Px-diagram to logarithmic scaling.

Close all plot-windows ( `*` ).
**Workshop**

In the query dialog, look at the comment column. Mark all data sets. Now run Consistency-automatic tests (marked sets). The comment column will show the result of the test (area test, point-to-point test):

- `?` test not available
- `+` consistent
- `-` inconsistent

Consistency – Single Set with options will show detailed results of the tests.

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**Pure Component Data Regression**

*Lesson Objectives*

- Select and regress pure component property data
- Reduce the experimental data by removing unreliable data
- store the resulting parameters in the parameter data bank
"PCP Equation Fit" allows to regress nearly all types of pure component data to a multitude of equations.

Workshop

- In "Dortmund Databank", select the component methanol, then select the vapor pressure data and run "PCP Equation Fit", select the Antoine equation and click the fit-button.
- In the fit-dialog, select the uppermost objective function from the pull-down menu, where the error is divided by the probable error.
- Click Fit, after the regression is finished, click plot.
- Exclude data points with a larger deviation.
- Refit the selected data and examine the deviations in the plot.
- Store the parameters in the private DDB.
- In "PCP Equation Fit" plot the experimental data together with the curve from the newly fitted and saved parameters.
Mixture Data Regression

Lesson Objectives

- examine different possibilities for the regression of individual types of data or individual data types
- examine the regression results
- store regressed parameters in the parameter data bank

Workshop

In the query dialog, mark data set VLE18870. Click the fit button in the toolbar. In the regression dialog, click fit – table in the upper part.

A regression result output similar to the DEHEMA Chemistry Data Series – VLE Data Collection (DCDS) and a dialog offering to store the regressed parameters in the private parameter Data bank will be shown.

Close both windows.
Select fit – plot. The dialog on the right hand side will come up:

Display a plot of the separation factor ($\alpha_{12}=K_1/K_2$) as function of mass fraction of ethanol. Move the mouse cursor in the plot to display the numeric values.
Workshop
Search for data for the system ethanol – water - benzene.
Fit/Plot the LLE-data at 298 K using the NRTL-model.
Plot the partition coefficients of component 2.

Workshop (continued)
Store the regressed parameters in the parameter data bank
and use them to calculate the VLE ethanol-water at 1 atm.
Compare the results to experimental data.
Simultaneous Mixture Data Regression

Lesson Objectives

- inspect the different options required for simultaneous mixture property regression
- understand the interrelation between different kinds of mixture data
- regress reliable temperature dependent model parameters for a binary system
Starting Recpar/1 from the Data query Result dialog:

Recpar/1 allows to correlate simultaneously VLE, HPV, ACT, AZD, LLE, HE and CPE-data using different g²-models or compare the data to the results of UNIFAC or mod. UNIFAC

The different features of Recpar/1 are demonstrated before the workshop.

Workshop
Search for data for the system ethanol-ETBE (ethyl-tert.-butyl-ether) in Mixture Properties and start Recpar/1 using all available data.
Save the project as ethanol-ETBE
Examine the different options in the Edit-menu and regress temperature dependent NRTL-parameters to the data. Remove data sets that are obviously wrong or of low quality.
In the first step, use ideal vapor phase. Switch to real vapor phase for the final regression.
RecPar/1 Regression Dialog

RecPar/1 Results

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**Mixture Data Estimation**

**Lesson Objectives**

- predict mixture data using group contribution methods
- examine the parameter matrices of the different methods
- learn, how to modify existing parameters or add new parameters
If no experimental data are available for a system, pseudo-experimental data can be estimated or predicted from a variety of methods and then be processed in the same way as experimental data.

**Workshop**
Search for data for the system acetone - ethanol.
Now select predict from the Mixture Properties Query dialog and predict a VLE-data set at 1 atm using the mod. UNIFAC (Dortmund) group contribution method (use "Predict (Dataset/s returned to Mixview")
In the Query Result dialog, choose Predict and select the mod. UNIFAC (Lyngby) and COSMO-SAC model. Mark all sets and plot.

**Note concerning Prediction in the Query Result window:**
Selected data sets and predicted data sets will be shown in a new Query Result dialog but can be moved to the previous result table by drag and drop.

---

The program GC-Models Parameter gives full access to the group interaction parameters of the different methods for the prediction of the real mixture behavior.

In case a local copy of the parameters is used and mapped to via file replacement, the user could enter or modify group interaction parameters. Use this feature with great care!
Test Process Simulator Parameters Prior to Process Simulation

Lesson Objectives

- Check Aspen Plus calculation results against data from the DDB

Calculation using Simulator Thermodynamic to verify physical property issues prior to process simulation.

Example:

Aspen Plus:
VLE, HPV, LLE, $h^E$, $c_p^E$, $v^E$,
$P^s$, $c_p^s$, $c_p^v$

Next step:
- Additional properties
- Parameter regression
Import Project Components into Query

Open Aspen Project File

Search for Data

Search for System and Subsystems

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Mark all VLE Data Sets Acetone-Water at 101 kPa - Select Prediction

In the prediction dialog, the last selected Aspen project file is already given as default.

Base method: UNIQUAC

Select one of the options, in this example: Predict and Plot
### DDB Parameter Data Bank

**Lesson Objectives**

- examine the DDB parameter data bank
- learn, how to search for parameters
- learn about the possibility to use the Parameter DB for your own in-house parameters

**Temperature as function of liquid and vapor phase composition**

Workshop: Carefully examine the different diagrams, repeat the procedure for a system of your choice.
The DDB parameter data bank can hold all types of pure component or mixture properties and parameters and can be accessed via Editors – Parameter DDB Organizer.

It is integrated into the software and is automatically accessed when values or parameters are required.

**Workshop**

Use the previous example but instead of Aspen Plus, use NRTL to predict the VLE data of acetone-water at 1 atm.

In the $g^E$-Model Interaction Parameters Manager, select a parameter set from the data bank. Examine the option to copy/paste Aspen Plus parameters.
Does your company have a set of recommended parameters for e.g. vapor pressure equations, $g^E$-models, equations of state, ...?

**Please ask us for an import tool** into the private part of Parameter-DB

<table>
<thead>
<tr>
<th>Recommended Values and Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Critical Temperatures</td>
</tr>
<tr>
<td>Antoine Constants (Vapor Pressure)</td>
</tr>
<tr>
<td>Liquid Density Equation Parameters</td>
</tr>
<tr>
<td>Liquid Viscosity Equation Parameters</td>
</tr>
<tr>
<td>Surface Tension Equation Parameters</td>
</tr>
<tr>
<td>Thermal Conductivity Equation Parameters</td>
</tr>
<tr>
<td>$g^E$-model binary interaction parameters</td>
</tr>
<tr>
<td>UNIFAC Structural Groups</td>
</tr>
<tr>
<td>Molecular Structures (Connection Tables)</td>
</tr>
</tbody>
</table>

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**Process Synthesis**

**Lesson Objectives**

- examine the different programs in the process synthesis package.
- select a selective solvent for extractive distillation and verify its performance
- select an entrainer for azeotropic distillation
When designing a simple 3 component distillation with feed, top and bottom product, feasible products are not always obvious.

In a ternary diagram, feed, bottom and top product must be on a straight line. Top and bottom product must be on the same distillation curve. Instead of distillation curves, often the qualitatively identical but easier to calculate residual curves are plotted.

In DDBSP, these plots can be generated using Synthesis – Residual Curves. The plot on the right shows feasible product regions for two different feed compositions in a complex 3 component system with miscibility gap.

**Workshop**

Plot the azeotropes, boundary curves and residual curves for the mixture acetone – chloroform – methanol using mod. UNIFAC (Do) at 300 K.

Examine and explain the result.

Add the temperature contour lines to the plot.

Generate the 3D plot.
Synthesis – Residual Curves Workshop

Temperature: 300.00 K
mod. UNIFAC (Do)
Vapor Phase Model: Ideal or Chemical Theory

Methanol/3
P = 18.41 kPa

Acetone/1
P = 23.05 kPa

Chloroform/2
P = 28.40 kPa

x1/2/3 = 0.2964/0.3651/0.3573
P = 33.35 kPa

x1/2/3 = 0.4980/0.0000/0.3984
P = 28.40 kPa

x1/2/3 = 0.3496/0.3963/0.2597
P = 28.00 kPa

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A typical task for process engineers is the selection of a suitable solvent for azeotropic or extractive distillation, extraction, ...

DDB and DDBSP can assist via Process Synthesis – Entrainer Selection.

The action of an entrainer for extractive distillation results from the different activity coefficients of the components to be separated using an entrainer. The greatest effect is usually observed when the components are infinitely diluted in the entrainer.

The effect of the entrainer on the activity coefficients can result in an azeotropic point of one of the components with the entrainer, which should be avoided.

Solvent Selection either uses the DDB or the results of predictive models (UNIFAC, ...) as a source for activity coefficients (ACT) or azeotropic data (AZD). The program is very powerful and has many important options, only a very simple example is shown here.

If the components are chemically very similar (as in case of isomeric compounds), usually no suitable entrainer can be found!
Workshop
Start Process Synthesis – Entrainer Selection
Go to the Process sheet, select the Extractive Distillation sheet
Select the components benzene - cyclohexane
Run entrainer selection by DDB access. After a short time the result dialog on the next slide will be shown.
The green hyperlink in front of the solvent names leads to the thermophysical properties and mixture data the selection is based on.
Examine further options in the dialog.
Search for selective solvents using the predictive method UNIFAC.

This option tests all components in the DDB for their mixture properties with the system to be separated provided the behavior can be predicted with the selected model.

The list will contain many components, which are not suitable regarding their chemical stability, price, ...

- When using DDB-access, only solvents can be found, for which data are available (Often the measurements were performed to show the effect as selective solvent). Solvent selection via DDB access can offer components, which are not available via predictive methods.
- Selection via predictive methods can lead to solvents never before considered for the separation. The results can suggest, what types of components could be promising.

Both ways complement each other and are of similar importance.
Instead of using a selective solvent for extractive distillation, it is also possible to add an entrainer that forms a binary azeotrope with one of the components or a ternary heterogeneous azeotrope. Components of industrial use for the aliphatics – aromatics separation in case of aromatic-rich mixtures like acetone or 2-butanone are found when searching for an entrainer for azeotropic distillation:

Search for an entrainer introducing at least one further binary azeotrope with DDB-access leads to the output on the right:

Addition of e.g. acetone will send the binary azeotrope with cyclohexane to the top of the column.
Another possibility is the introduction of a heterogeneous ternary azeotrope. Look for an entrainer for the separation of the system ethanol – water. The program will first display the following message:

"Continue Evaluation" as we do not consider a vacuum distillation with unfavorable separation factor.

The following list of entrainers is shown:

The list contains components like benzene and cyclohexane used in large scale ethanol dehydration.
Using mod. UNIFAC, the following residual curve plot can be calculated:

The actual implementation of the process is shown here using benzene as entrainer:
Data Input

Lesson Objectives
- enter a new pure component into the private basic data file
- Estimate and enter the most important properties required for calculations
- Enter a mixture property data set
- Test the data and append the data set to the private DDB

Users can store references, new components, pure component and mixture data, model parameters, molecular structures, ... in their own data bank.

Files and formats are identical to the DDB but files reside on a separate directory. Currently only one private data bank can be active at a time.

For data input, easy to use data editors are available.

Data input is described in detail in the manuals

  Edit Mixture Data Tutorial
  Edit Pure Data Tutorial
  Component Management Tutorial
  Lear Tutorial

in the documentation folder.
For data input, easy to use data editors are available.

For the following workshops, start with an empty private folder.

First we introduce a new private component and enter the structure and basic properties to be used as defaults for further calculations in the structure database and the component definition file.

For these entries, no links to data sources etc. are stored and the user should document his input separately.

Workshop

Task: Enter the component on the right as a new component into the private DDB.

Start the program Stoff Editor

Using the Open-button, select the private STOFF-file. The file does not exist and will be generated. The editor shows the first empty component entry (component 1)

Enter the english name 2,3-dimethyl-pentanal.
Enter the empirical formula.
Enter the CAS-number 32749-94-3

Click % to change the upper/lower case in the name to conform to the new DDB-standard.

* Stoff, the German word for substance was introduced as the name for the pure component definition file in the early days of DDB and has been kept ever since.
Select the alias-button right of the name fields and enter the DDB-synonym "Test component for course"

Select the Artist-button in the toolbar and enter the molecular structure into the Artist document and save the structure in ChemDB under the first component. Click the small calculator close to the molecular weight field. The calculated values from the empirical formula input and the structure input will both be shown. They should be identical. Accept one of them.

We will now fill up some fields with the help of group contribution methods.

The only available information is the normal boiling point

**CAS:**

138-42°C

(2,3-Dimethylpentanal, (Institut Franco Tosi & p.A.), (1964), 7 pp., FR 1377741

**Beilstein:**

<table>
<thead>
<tr>
<th>Ref</th>
<th>185</th>
<th>142</th>
</tr>
</thead>
<tbody>
<tr>
<td>171</td>
<td>131</td>
<td>760</td>
</tr>
<tr>
<td>172</td>
<td>142</td>
<td>750</td>
</tr>
<tr>
<td>173</td>
<td>192</td>
<td>740</td>
</tr>
<tr>
<td>174</td>
<td>192</td>
<td>690</td>
</tr>
<tr>
<td>175</td>
<td>192</td>
<td>640</td>
</tr>
<tr>
<td>176</td>
<td>192</td>
<td>620</td>
</tr>
</tbody>
</table>


Use a value of 141°C (414K). Click the Artist button in the toolbar and calculate the normal boiling point using the different group contribution methods.
Now estimate the critical data and the density at 20°C in Artist.

Probable values are

\[ T_c = 602 \, \text{K} \]
\[ P_c = 3100 \, \text{kPa} \]
\[ v_c = 420 \, \text{cm}^3/\text{mol} \]
\[ \rho = 830 \, \text{kg/m}^3 \]

Ab-initio calculation gives a dipole moment of approx. 2.65 Debye.

The last required input now is at least one set of Antoine constants. Heat of fusion and melting point are only required for SLE calculations.

Start PCPEquationFit and select component 1 from the private DDB:

Select Fit and data source Hand to bring up the following dialog:

Enter the following data:

<table>
<thead>
<tr>
<th>T / °C</th>
<th>P / mmHg</th>
<th>T / K</th>
<th>P / kPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>59.5</td>
<td>26</td>
<td>332.65</td>
<td>3.47</td>
</tr>
<tr>
<td>91</td>
<td>152</td>
<td>364.15</td>
<td>20.26</td>
</tr>
<tr>
<td>130</td>
<td>740</td>
<td>403.15</td>
<td>98.63</td>
</tr>
<tr>
<td>141</td>
<td>760</td>
<td>414.15</td>
<td>101.30</td>
</tr>
</tbody>
</table>
After the fit the left plot can be shown. The vapor pressure curve shows a strong curvature, which is the combined result of the low quality of the data and the ability of the Antoine equation to describe this non-linear behavior. Nevertheless, it is very unlikely that the component of interest has such a vapor pressure curve. Select Refit and fit only A and B of the Antoine equation. This will result in the more realistic vapor pressure curve shown on the right:

With the critical data and parameters for a vapor pressure equation available it is now possible to calculate the acentric factor:
DDB - Private Component - Pure Component Data Input

Instead of entering the vapor pressure data into PCP Equation Fit by hand, it would have been better to store them in the PCP data bank. All data points could be stored in 2 data sets with the references CAS and Beilstein or each value could be stored separately with its primary source.

**Important Notice:** In the DDB, data are only extracted from the primary source, which is nearly always available at DDBST GmbH.

Experimental pure component or mixture data sets in DDB are linked to the component(s) in the component definition file STOFF and the source reference in the literature data bank LEAR.

When data sets are added, the component and reference entries must be available.

As we already entered 2,3-Dimethyl-Pentanal as a new component in the private data pure component definition file, we now must enter the reference for the first data set (the patent found via CAS).

DDB - Private Data - Reference Input

Start the program Lear. The following dialog will be shown:

As there currently is no private reference database, we need to create it. Select New – New Library. In the next dialog, select Create.
Double-click DDBST/p to open the data view dialog and select Edit – New Data Set:

Now enter the reference information as shown on the next slide.

You must also enter links to all data banks, to which data from this reference should be added!!!
DDB - Private Data - Reference Input

Let us enter the data with their primary source using Edit Pure Data:

Select New Set

DDB - Pure Component Data Input

In the dialog below, select vapor pressure as property, select the component 2,3-dimethyl-pentanal from the private DDB, select vapor-liquid as state.
The next step is to define the table entries in the small floating dialog. Let us enter the normal boiling point found via CAS. The columns should be temperature in °C, pressure in atm and temperature error in °C.

Factor is always 1 in our example. It is used in case the authors present a table in which all column values have to be multiplied with a common factor (e.g. 10¹⁰).

There are 2 ways to specify errors:

A in the column definition, an absolute or relative error can be specified for all data in the column
B an explicit error column can be introduced for absolute or relative errors of each property in each table line

In case of data sets with one data point, both choices are equally valid. Normally one would use option A and save the additional column.

Now that the data columns are available, enter the data and select the reference from the private reference file via F1 (search private file with "Lear Number is equal 1"):  

Now save the file and select Add to PCP, open the DHP-file just saved.
The following dialog will be shown:

Enter your initials under "Input by"
And select "Add to PCP Database"

Remark on Private Databanks:

Out of historical reasons, private data set numbers, reference numbers and component numbers are stored as negative numbers. This allows for exactly two databanks, one public and one private.

Newer developed programs use 3 integer numbers to identify the number and the data bank plus additional information, which will allow to handle the public and a large number of private data banks (company, group, individual user, ...) simultaneously.

Editor programs show the actually used negative numbers in the dialogs.
The input of mixture data works in a similar way as the pure component data input shown before.

**Workshop**

Enter the following h^E-data set into the private mixture data bank:

| Table III: Mixture Enthalpy of Formation \(\Delta H_f^E\) for Cyclic Ether + Cyclohexane and for Cyclic Ether + Cyclohexane at 298.15 K^* |
|---|---|---|---|
| \(x\) | \(\Delta H_f^E\) (kJ mol\(^{-1}\)) | \(\Delta H_f^E\) (kJ mol\(^{-1}\)) |
| 0.050 | 23.6 | 4.931 | 32.0 |
| 0.150 | 18.0 | 4.597 | 27.0 |
| 0.250 | 12.6 | 4.341 | 22.6 |
| 0.350 | 8.6 | 4.046 | 18.0 |
| 0.450 | 5.0 | 3.803 | 14.0 |

**Workshop**

After storing the data in the private data bank, use the different possibilities to plot and regress the data and to compare them to results of predictive models.

Various editor programs are available for the input and test of new components, references as well as pure component and mixture data.

In case a larger number of data is to be included from in-house data banks, please inquire about our batch import tools.
Data Import and Export

Lesson Objectives

- get an overview on the different possibilities of data export from DDB/DDBSP to
  - the Aspen simulator
  - Spreadsheets like Microsoft Excel

DDB-data and Parameters can be exported in a variety of ways:

- Cut/copy and paste
- DDB-format data files
- Aspen inp-files
- PPDX-files (Physical Property Data Exchange (ICCAPE))

Workshop

- In Mixture Properties, search for data for the system ethanol-ETBE.
- Export the data to an inp-file (Aspen inp export, show form, all possible data sets, Aspen inp export)
- Start the Aspen User interface and open the inp-file

As shown on the right all data sets and further specifications are set in the Aspen project.
DDBSP - Dortmund Data Bank Software Package

The data can directly be visualized using the Aspen plot wizard:

The regression case defined in the inp-file specifies ideal, evaluation and includes only the first data set. Change these settings as desired:

Complete Table Creation

For Spreadsheets

Collecting data sets by drag and drop

Table creation and copying to Windows clipboard
Only a rather rough walkthrough could have been presented in this part of the course.

This course did not cover any of the important aspects of mixture thermodynamic basics and applications. For this subject, special courses are available in German as well as English language.

When applying DDB and DDBSP to your own problems, please consult the manual or the hotline (support@ddbst.de).

In case of problems or special requirements, help including software patches can usually supplied quickly.

We are very busy improving and extending DDB and DDBSP. Please check wwwddbst.de for updates and patches.

Thank you very much for your interest.