

Adsorptive-Adsorbents Equilibrium Data Bank (AAE)

Part of the Dortmund Data Bank (DDB)

DDBST

Software & Separation Technology GmbH

Marie-Curie-Straße 10

D-26129 Oldenburg

Tel.: +49 (0) 441 361819 0

Fax: +49 (0) 441 361819 10

E-Mail: support@ddbst.de

Web: www.ddbst.de

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Introduction

The knowledge of the adsorption equilibrium is needed for the design, the calculation, and the simulation of adsorption processes. With the help of this adsorption data bank and the related software it is possible

- to find available literature data for a definite equilibrium of pure component or mixed component adsorption
- to manage own experimental data in a private data bank
- to display, plot, print, and export data sets
- to correlate pure component adsorption data sets and to predict and correlate data sets for binary mixture adsorption
- to export the calculation results in an unformatted data file

The Dortmund Data Bank

The AAE data bank is part of the Dortmund Data Bank which contains several other properties like phase equilibria (vapor-liquid, liquid-liquid, solid-liquid), caloric and transport properties, P-v-T data, and many more properties for mixtures and pure components.

The AAE data bank has been built up initially in the years from 1990 to 1995 in a project funded by the German federal government (see papers ⁱ, ⁱⁱ, ⁱⁱⁱ) and is now maintained and updated by **DDBST** GmbH.

Data Bank Content

The data sets always contain data for a single adsorbent and a list of adsorptives.

The overview shows that the AAE data bank currently contains 3513 data sets from 188 different sources.

	Sets	Points	References (Articles, Theses, Private Communications, Deposited Documents, etc.)
AAE	3513	42226	188

The following table shows the amount of available data separated by the number of adsorptives.

				Mixed Adsorption		
	Components	Systems Summary	Pure Adsorptive	Binary Adsorptives	Ternary Adsorptives	Higher Systems
AAE	128	496 systems 3513 sets 42226 points	342 systems 2701 sets 36553 points	127 systems 690 sets 4754 points	23 systems 113 sets 819 points	4 systems 9 sets 100 points

The 128 components can be separated in exactly 100 adsorptives and 28 adsorbents. The adsorbents are

- Activated carbon (1271 Sets)
- Carbon black
- Graphitized carbon black
- Aluminophosphate - 5
- Activated aluminum oxide
- Metal oxide
- Molecular sieve carbon (143 Sets)
- Mordenite (152 Sets)
- Organic polymer
- Silica
- Silica gel (272 Sets)
- Silicoaluminophosphate
- Zeolite beta
- Zeolite A (409 Sets)
- Zeolite X (488 Sets)
- Zeolite Y (229 Sets)
- Zeolite ZSM – 5 (227)
- Zeolite ETS
- Zeotypes
- Charcoal
- Clinoptiolite
- Zeocarbon
- MCM-41
- MCM-48
- SBA-1
- SBA-15
- KIT-1
- Multi-Walled Carbon Nanotube

The list of adsorbents doesn't reflect the vast amount of different adsorbents in the data bank because this list only contains rather rough classifications of the adsorbents by their molecular structure but it doesn't describe the actual form of the adsorbent used in the concrete measurement. These details are given in every single data set.

Supported Data Types

Pure component adsorption

- isothermal data (constant temperature)
- isosteric data (constant amount of adsorptives)
- isobaric data (constant pressure)

Binary mixture adsorption

- isobar data (pressure, constant temperature)
- isotherm data (vapor phase mole fraction, constant temperature)
- isotherm data (relative saturation with water, constant temperature)
- isotherm data (volume ratio at the beginning, constant temperature)
- isotherm data (pressure is nearly constant, constant temperature)

Ternary and higher mixture adsorption

- variation of the total pressure and fixed vapor composition (Y_i , constant temperature)
- constant total pressure and constant vapor composition ratio (pressure, temperature, one constant Y_i)
- constant total pressure and constant vapor composition ratio (pressure, temperature, all Y_i constant)
- constant total pressure (pressure, constant temperature)
- variation of total pressure at constant partial pressure of water as component (temperature, constant Y_{H_2O})
- constant volume ratio of adsorptives at the beginning of the measurement (temperature, constant beginning volume ratio)
- only constant temperature (constant temperature)

Data Set Display

A typical output (AAE data set no. 1) is shown here:

```

data set number: 1 (Public DDB)  number of data points: 18 AAEDDB

      adsorptive 1:   Carbon dioxide           ( code no.: C1050 )
      adsorbent:     Mordenite                 ( code no.: A12 )
      adsorbent-info ( code no.: 15 )
                    TYPE Z - 900H, NORTON CO.
                    PS=1.588 MM, SA=450 M2/G, K=8H, SI/AL=4.7,
                    PR=0.59x0.70/0.39x0.47, PV=0.2E-6 M3/G
      experimental method: [4] static volumetric
      reference number:    21

ref.:
[22865] Talu O., Zwiebel I., AIChE J., 32(8), p1263-1276, 1986

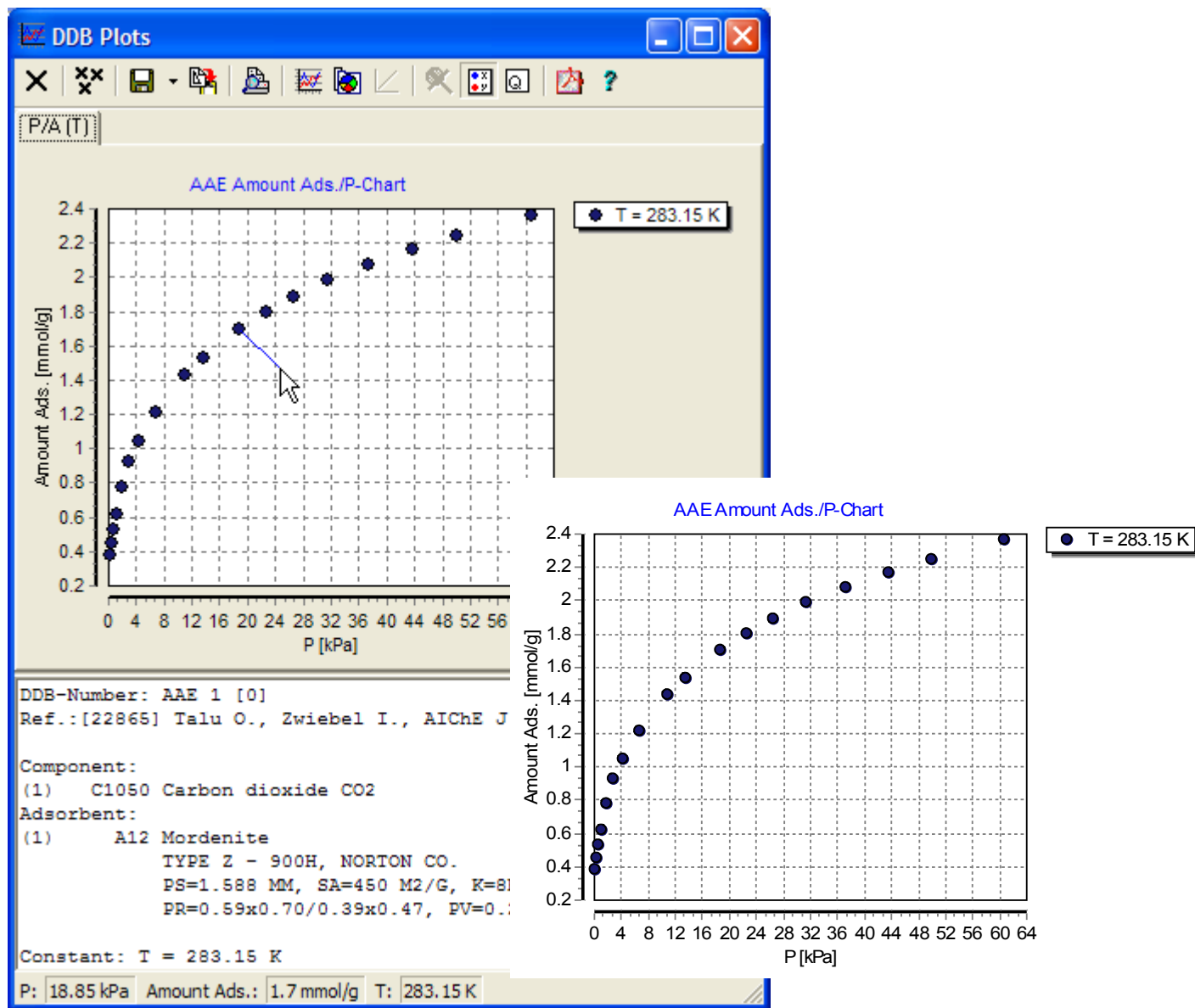
      data presentation:  TABULAR
      experimental range of
      - pressure, kPa      0.320      ....60.760

Constant value/s:
      T      283.15   [K]

      P      Amount Ads.
      [kPa]   [mmol/g]
      -----
      0.320   0.3800
      0.470   0.4500
      0.750   0.5300
      .....
      60.760  2.3600
  
```

The adsorbent details are directly given below its classification name (“Mordenite”). Further information on data set details are given in the tutorial for the data editor (see “Other Documentation” chapter).

Data Set Plot



This plot can be copied to the Windows clipboard and used for documentation.

Available Fitting Functions

This chapter summarizes the list of models implemented in the old FORTRAN programs and the status of the recompiled but otherwise unchanged Windows-based programs.

Pure Component Isotherms

<i>Isotherm</i>	<i>Fully Implemented in Current Windows Programs?</i>
Freundlich	Yes
Langmuir	Yes
Brunauer-Emmett-Teller (BET)	Yes
Mixed Langmuir-Freundlich	Yes
Toth	Yes
Statistical Combined Langmuir	Yes
Modified Langmuir for SSTM	Yes
Virial-Isotherm-Equation (SPD)	No
Vacancy Solution Model	Partly
Dubinin-Astakhov-Isotherm for MI/RAST	No

Mixture Isotherms

The available models are

1. Ideal Adsorbed Solution Theory (I.A.S.T.)
2. Real Adsorbed Solution Theory (R.A.S.T.)
3. Wilson - Vacancy Solution Model
4. Flory-Huggins - Vacancy Solution Model
5. Multiphase I.A.S.T.
6. Multiphase R.A.S.T.
7. Predictive R.A.S.T.
8. Modified Statistical Thermodynamic Model
9. Simplified Binary Model

The implementation of these models must be updated since they are currently only usable under the DOS operating system. This update will be done in the near future.

Other Documentation

Editing AAE data sets and adsorbent information

EditMixtureData.pdf

ComponentManagement.pdf

Searching AAE data bank, displaying AAE data sets, plotting, and predicting

DortmundDataBank.pdf

Editing/Searching Literature

LEAR.pdf

These files and more information can be found on the DDBST web server at

<http://www.ddbst.de/new/Documentation.htm>

- i Sakuth M., Schweer A., Sander S., Meyer J., Gmehling J., "Databank and Software Package for Adsorption Equilibria of Gases and Vapors", Chem.Eng.Technol., 21, p866-869, 1998
- ii Sakuth M., "Messung und Modellierung Binärer Adsorptionsgleichgewichte an Dealuminierten Y-Zeolithen", Thesis, Oldenburg, 1993
- iii Sakuth M., Meyer J., Gmehling J., "Eine neue Methode zur Vorausberechnung von Gleichgewichten der Mehrkomponentenadsorption", Chem.Ing.Tech., 66(7), p940-945, 1994