

Dortmund Data Bank (DDB)

Vapor-Liquid Equilibria (VLE) of Mixtures

DDBST

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Vapor-Liquid Equilibria

Vapor-liquid equilibria provide basic information for the most important separation process in the chemical industry: Distillation.

A deep understanding of the VLE allows to design a distillation column with its optimal size and lowest possible energy consumption to achieve the wanted purity.

Some Typical VLEs

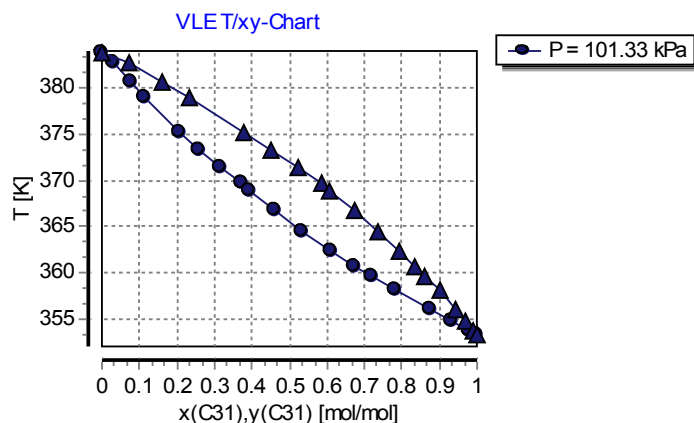


Figure 1: Benzene [31]/Toluene – A nearly ideal system

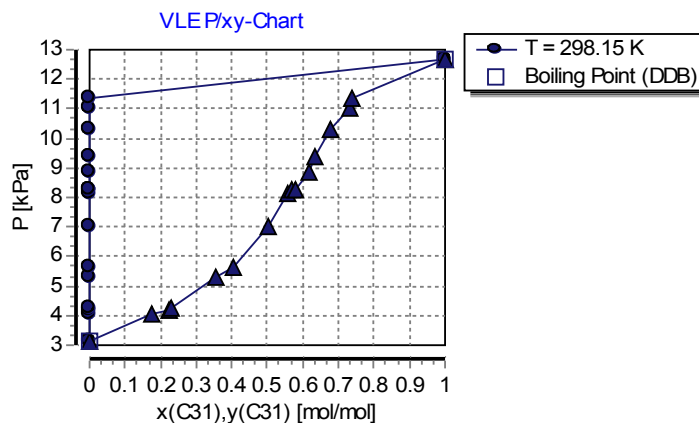


Figure 2: Benzene [31]/Water – Large mixing gap

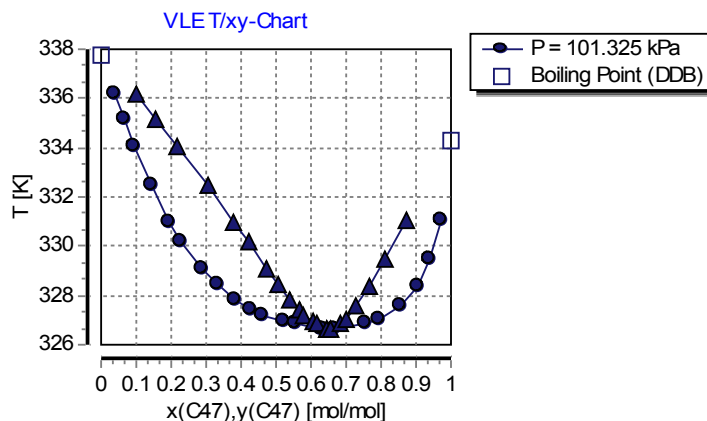


Figure 3: Chloroform [47]/Methanol – Azeotropy

The Data Banks

Overview

The Dortmund Data Bank (DDB) contains three separate data banks for vapor-liquid equilibria. These three data banks are

Data bank	Sets	Points	References	Description
VLE	26245	383319	5844	Vapor-liquid equilibria for systems containing components with a boiling point above 0 °C
HPV	24722	214988	2791	Vapor-liquid equilibria for systems containing components with a boiling point below 0 °C
ELE	5503	65836	706	Vapor-liquid equilibria for systems containing solved salts

Data Sources

The DDB only contains experimental data obtained from original sources (references) like

- published articles from around the world (also China, India, Brazil, Japan, Korea, Taiwan, etc.)
- theses
- private communications
- deposited documents (from Ukraine, Russia, Belarus, Kazakhstan etc.),
- data from industry (mainly, but not exclusively, from former GDR companies).

Data Types

VLE/HPV Data Banks

The VLE and HPV data bank contain the same kind of data:

- vapor composition
- liquid composition
- temperature
- pressure

If a data set is stored in one or the other data bank is decided by the normal boiling points of the components. If T_b is greater $0\text{ }^{\circ}\text{C}$ for all components the data set is stored in the VLE data bank, if any component in a measurement has a T_b below $0\text{ }^{\circ}\text{C}$ the data are stored in the HPV data bank. HPV stands for **H**igh-**P**ressure **V**LE.

VLE Data Bank Overview

Table Entries	Constant	Data Sets	Data Points
x y P	T	4910	67973
x y T	P	7586	131267
x P	T	7805	111635
x T	P	2352	26829
x y	T	798	10655
x y	P	538	8370
y P	T	135	794
y T	P	38	508
x y P T	-	2083	25288

HPV Data Bank Overview

Table Entries	Constant	Data Sets	Data Points
x y P	T	7370	70088
x y T	P	407	4086
x P	T	7258	55381
x T	P	766	4472
x y	T	18	86
x y	P	7	43
y P	T	4599	34698
y T	P	350	2518
x y P T	-	3947	43661

Incomplete data are a result of the used measurement methods. P-x-T data (e. g. missing vapor compositions) are typically a result of a static or dynamic apparatus. A short list of measurement methods for VLE is given in the appendix.

ELE Data Bank

The ELE data bank contains besides x, y, P, T data also some other data like

- salt concentration
- osmotic coefficients
- γ^+

There are also many data sets that are not complete. This is typically a result of measurement methods where e. g. vapor compositions are not easily available.

ELE Data Bank Overview

Table Entries	Constant	Data Sets	Data Points
x_s y P	T Conc.	55	446
x_s y T	P Conc.	436	4509
x_s P	T Conc.	24	240
x_s T	P Conc.	13	137
x_s y	T Conc.	242	2131
x_s y	P Conc.	24	210
x_s y T P	Conc.	12	95
x_s y Conc. P	T	156	1302
x_s y Conc. T	P	416	5430
x_s Conc. P	T	153	1539
x_s Conc. T	P	21	136
x_s y Conc.	T	127	936
x_s y Conc.	P	22	233
x_s y Conc. T P	-	38	507
Conc. P	T	1140	10727
Conc. T	P	71	944
Conc. Osm.Coeff.	T	1177	17561
Conc. Osm.Coeff.	P	6	54
Conc. γ^{+-}	T	820	12142
Conc. T P	-	278	2719
x_s y T	P sat.	66	828
x_s T	P sat.	4	64
x_s y	T sat.	7	54

Table Entries	Constant	Data Sets	Data Points
x_s γ	P sat.	5	39
x_s γ T P	sat.	2	26
T Osm.Coeff.	sat.	5	50
T γ^{+-}	sat.	1	14
T P	sat.	112	1738
Conc. P Osm.Coeff.	T	1	24
Conc. T Osm.Coeff.	P	24	432
Conc. P γ^{+-}	T	21	137
Conc. T γ^{+-}	P	24	432

x_s : salt-free composition of solvents

Conc: salt concentration

γ^{+-} : activity coefficient

sat.: saturation (saturated vapor pressure)

Osm.Coeff.: osmotic coefficient

Systems

The amount of data sets not sufficient to describe the comprehensiveness of a factual data bank since this doesn't show the diversity of the data.

The number of components and systems however directly shows how many *different* data a data bank contains.

DDB	Components	Systems summary	Binary systems	Ternary systems	Quaternary systems
ELE	447	1032 systems 5503 sets 65836 points	487 systems 2735 sets 37488 points	505 systems 2637 sets 26892 points	40 systems 131 sets 1456 points
HPV	1137	3839 systems 24722 sets 214988 points	2953 systems 21464 sets 179535 points	786 systems 2961 sets 32920 points	100 systems 297 sets 2533 points
VLE	1573	8577 systems 26245 sets 383319 points	7102 systems 23785 sets 322288 points	1272 systems 2173 sets 55328 points	131 systems 188 sets 4440 points

Appendix

Selected Measurement Methods for Vapor-Liquid Equilibrium Data

Measurement Method	Pressure Range	Temperature Range	Obtained Data
Static Apparatus, High Pressure	< 400 bar	25 - 400 °C	x, y, T, P
Static Synthetic Apparatus, High Pressure	< 200 bar	-60 - 200 °C	x, T, P
Computer Driven Static Synthetic Apparatus	< 3 bar	-10 - 90 °C	x, T, P
Computer Driven Static Synthetic Apparatus	< 30 bar	-10 - 160 °C	x, T, P
Flow Apparatus for the Determination of Critical Points	< 400 bar	25 - 400 °C	z, T, P
Headspace Gaschromatograph	< 3 bar	0 - 150 °C	x, y, T
Static Analytic Apparatus, High Pressure	< 250 bar	0 - 200 °C	x, y, T, P
Dynamic Still (NORMAG)	< 1 atm	25 - 160 °C	x, y, T, P
Dynamic Still (Swietoslawski)	< 1 atm	-20 - 220 °C	x, y, T, P
Flow Apparatus for Reactive Systems	< 1 atm	20 - 200 °C	x, y, T, P
Scott-Ebulliometer	< 1 atm	-20 - 300 °C	x, T, P
Static Synthetic or Analytic Apparatus with Variable Volume	< 150 atm	-20 - 150 °C	x, y, T, P, V
Flow or Circulation Apparatus with FTIR-Spectrometer	< 30 atm	80 - 350 °C	x, y, T, P

(List of methods made available by LTP GmbH, <http://ltp-oldenburg.de/>)