



# **Dortmund Data Bank (DDB)**

## **Status, Accessibility and Future Plans**

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# Short History of nearly 30 Years of DDB

- Started 1973 at the University of Dortmund for the development of a group contribution  $g^E$ -model (VLE)
- Extended to LLE,  $h^E$ ,  $\gamma^E$ , azeotropic data,  $c_p^E$  and SLE for the development of mod. UNIFAC
- Extended to VLE of low boiling components for the development of group contribution EOS (PSRK, VTPR)
- Extended to VLE, GLE of electrolyte systems and salt solubilities (ESLE) for the development of electrolyte models (LIQUAC, LIFAC)
- Extended to PURE for the development of estimation methods for pure component properties (in cooperation with groups in Prague, Tallinn, Berlin and Graz) (Cordes/Rarey, ...)
- .....

In 1989 DDBST GmbH took over the further development of the DDB. DDBST also supplies a software package for data handling, retrieval, correlation, estimation, and visualization as well as process synthesis tools.



## Status of DDB-MIX Phase Equilibria

Phase Equilibria		Abbreviation		
Vapor-Liquid Equilibria	normal boiling substances	VLE***	22 900	data sets
Vapor-Liquid Equilibria	low boiling substances	HPV***	19 400	data sets
Vapor-Liquid Equilibria	electrolyte systems	ELE	2 920	data sets
Liquid-Liquid Equilibria		LLE	12 950	data sets
Activity Coefficients	infinite dilution ( in pure solvents )	ACT	40 750	data points
Activity Coefficients	infinite dilution ( in mixtures)	ACM	885	data sets
Gas Solubilities	non-electrolytes	GLE***	13 875	data sets
Gas Solubilities	electrolyte systems	EGLE	310	data sets
Critical Data of Mixtures	critical lines	CRI	700	data sets
Solid-Liquid Equilibria	mainly organic compounds	SLE	10 770	data sets
Salt Solubilities	mainly in water	ESLE	3 520	data sets
Azeotropic Data		AZD	45 750	data points
Partition Coefficients	octanol-water partition coefficients	KOW	6 500	data points
Adsorption Equilibria	vapor phase	ADS	3 100	data sets

\*\*\* including unpublished data from chemical companies in the former German Democratic Republic.



## Status of DDB-MIX Excess Properties and Recommended Values / Parameters

<b>Excess Properties</b>		<b>Abbreviation</b>		
Excess Enthalpies		HE	16 420	data sets
Excess Heat Capacities		CPE	1 485	data sets
Excess Volumes		VE	15 900	data sets

<b>Recommended Values and Parameters</b>	
Critical Temperatures	for approx. 1260 components
Antoine Constants (Vapor Pressure)	for approx. 3360 components
Liquid Density Equation Parameters	for approx. 1080 components
Liquid Viscosity Equation Parameters	for approx. 1870 components
Surface Tension Equation Parameters	for approx. 1580 components
Thermal Conductivity Equation Parameters	for approx. 400 components
$g^E$ -model binary interaction parameters	for approx. 440 systems*
UNIFAC Structural Groups	for approx. 7000 components
Molecular Structures (Connection Tables)	for more than 15000 components
...	

\* under construction

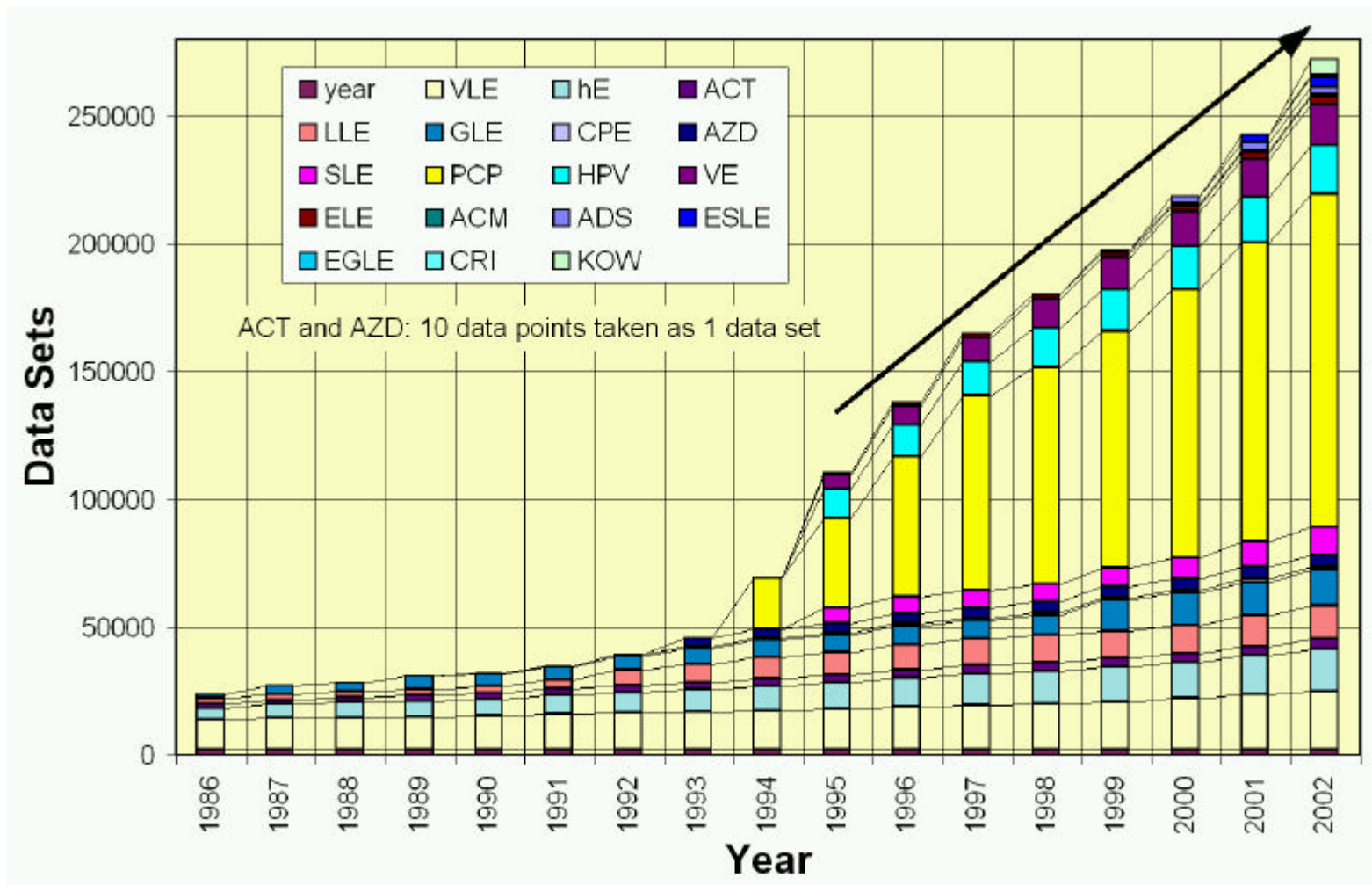


## Status of DDB-PURE Pure Component Properties

<b>Property</b>	<b>Compounds</b>	<b>References</b>	<b>Sets</b>	<b>Points</b>
Vapor Pressure	4993	5490	19708	140896
Critical Data	884	835	3070	3072
Viscosity	2084	2171	15183	91846
Kinematic Viscosity	505	201	1242	5445
Density	6859	5190	35370	258704
Melting Point	4471	2578	11275	11995
Molar Heat Capacity	1872	1391	7645	120276
Enthalpy of Vaporization	2149	965	4375	9541
Heat of Fusion	1653	990	2769	2808
Thermal Conductivity	761	876	8365	76285
Surface Tension	1992	569	4363	18987
Entropy	1434	876	2563	7550
Std. Heat of Combustion	1105	327	1284	1284
Std. Enthalpy of Formation	2576	1093	3634	3641
Transition Temperature	343	291	655	661
Heat of Transition	303	257	519	528
Ideal Gas Heat Capacity	1267	693	2239	30839
.....	.....	.....	.....	.....
<b>Total</b>	<b>13295</b>	<b>16855</b>	<b>130222</b>	<b>841290</b>



## Regular Update of the DDB - The Big Picture



**90 data sets per working day!**



## Regular Update of the DDB

Performed by:

- scientific and non-scientific coworkers at DDBST
- I. Adamczyk and his group at FIZ CHEMIE, Berlin
- Prof. Siimer and coworkers in Tallinn, Estonia
- Prof. Huemer and his group at TU Graz, Austria
- contributors in Brazil, China, Korea, Japan,...



## How to Access DDB - The Problem of Data Books



Phase Equilibria - Excess Properties - Pure Component Properties - Software Packages for Property Estimation - Process Synthesis

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# How to Access the DDB

- **Inhouse**

- by DDBST (DDB, DDBSP)
- by DECHEMA (DETERM)

- **Printed**

- by DECHEMA (Chemistry Data Series)
- by VCH (Azeotropic Data)

- **Online**

- DECHEMA, Aspen Tech
- STN, FIZ Karlsruhe

- **Data Service**

- DDBST, DECHEMA, FIZ CHEMIE

**Formats:**

data table

propr. DDBST (DDBST)

PPDX (DDBST,  
DECHEMA)

Aspen INP (DDBST)

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**Free Search:**

Internet (DETERM)

DDB Data Directory



## DDB - Research Discount - Experimental Data for Research

Phase Equilibria		Abbreviation			Yearly License Fee (€)	update volume 1999	update volume 2000	update volume 2001
Vapor-Liquid Equilibria	normal boiling substances	VLE***	22 900	data sets	3000	1300	1800	1100
Vapor-Liquid Equilibria	low boiling substances	HPV***	19 400	data sets	1950	500	1100	1300
Vapor-Liquid Equilibria	electrolyte systems	ELE	2 920	data sets	525	300	300	320
Liquid-Liquid Equilibria		LLE	12 950	data sets	1600	400	1050	900
Activity Coefficients	infinite dilution ( in pure solvents )	ACT	40 750	data points	1050	160	40	435
Gas Solubilities	non-electrolytes	GLE***	13 875	data sets	1375	500	500	875
Gas Solubilities	electrolyte systems	EGLE	310	data sets	165	-	-	310
Critical Data of Mixtures	critical lines	CRI	700	data sets	165	-	-	700
Solid-Liquid Equilibria	mainly organic compounds	SLE	10 770	data sets	925	700	1800	770
Salt Solubilities	mainly in water	ESLE	3 520	data sets	550	-	-	320
Azeotropic Data		AZD	45 750	data points	1500	500	1500	750
Excess Properties		Abbreviation			Yearly License Fee (€)	update volume 1999	update volume 2000	update volume 2001
Excess Enthalpies		HE	16 420	data sets	1800	550	800	1420
Excess Heat Capacities		CPE	1 485	data sets	225	100	200	135
Excess Volumes		VE	15 900	data sets	500	1000	1300	1100
Pure Component Properties		Abbreviation			Yearly License Fee (€)	update volume 1999	update volume 2000	update volume 2001
PURE		PURE	130 200	data sets	4425	12500	12000	13200



# Educational Version of DDB/DDBSP

## Pure Component and Mixture Data for 30 Components

Acetone, Ethanol, Ethyl Acetate, Benzene, Trichloromethane, Cyclohexane, n-Hexane, Methanol, Water, Carbon Dioxide, Methane, Sodium Chloride, 1-Butanol, NMP, iso-Propanol, CH<sub>3</sub>CN, Nitrogen, KCl, Naphthalene, Sulfolane, Hexen-1, Hexadecane, p-Xylene, m-Xylene, Diethylether, Acetic Acid, Glycol, Butadiene, Butyl Acetate, THF

## Data Bank Retrieval Programs Pure and MIX

Data Retrieval, Calculation, Estimation (UNIFAC, mod. UNIFAC, PSRK, ...), Graphical and Tabular Representation, Correlation, ...

## Simultaneous Regression of Mixture Data (Recval/3 s-light)

## Program Package ARTIST

Property Estimation from Molecular Structure, Except Additional Methods Add-On

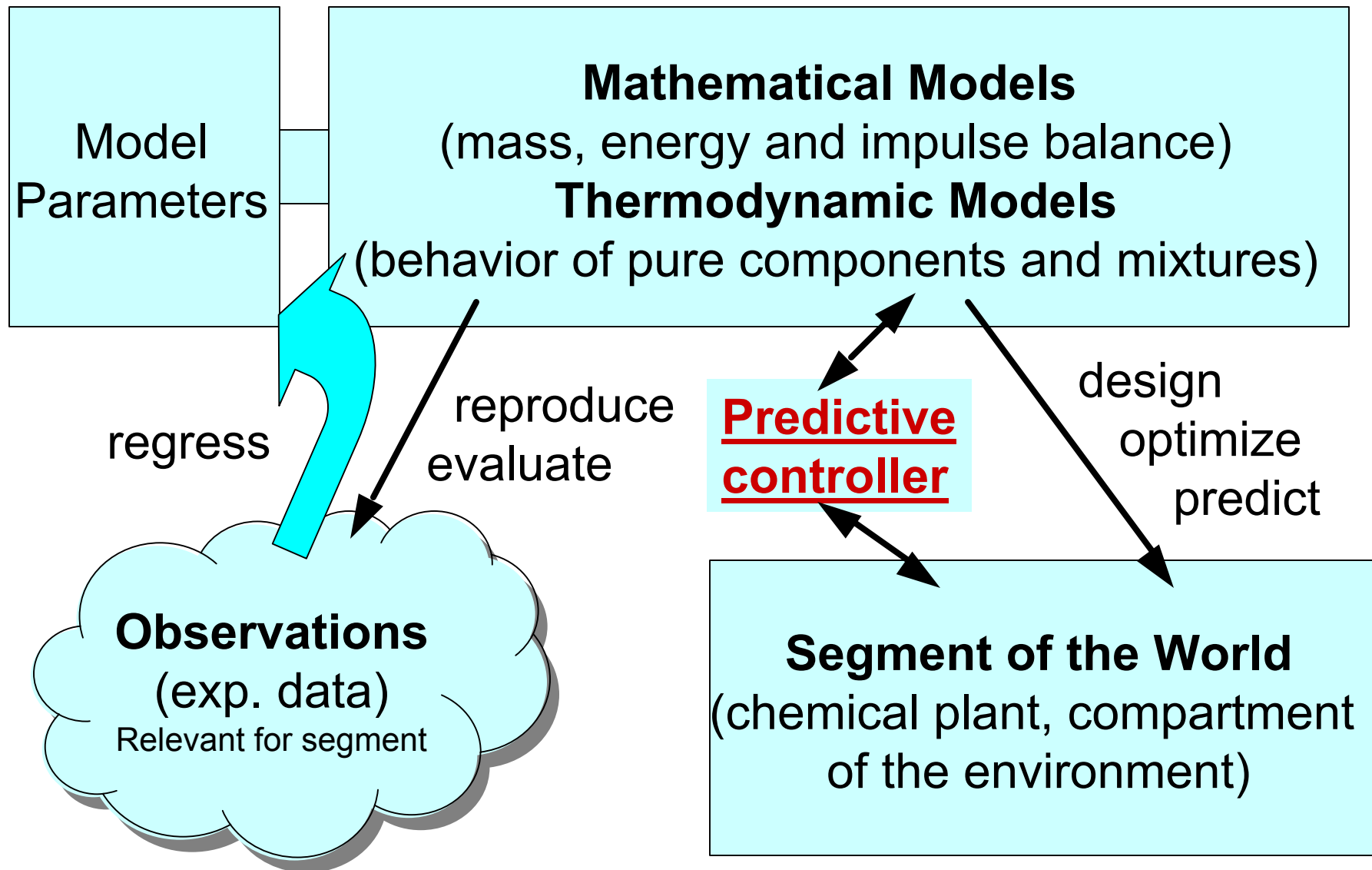
## Additional Properties

Component Names, Empirical Formula, CAS# (13 550 Components)  
Recommended Values and Parameters, Group Contribution Parameters, Structure Data Bank, ...  
(30 Components)

## Data Directory of the Dortmund Data Bank

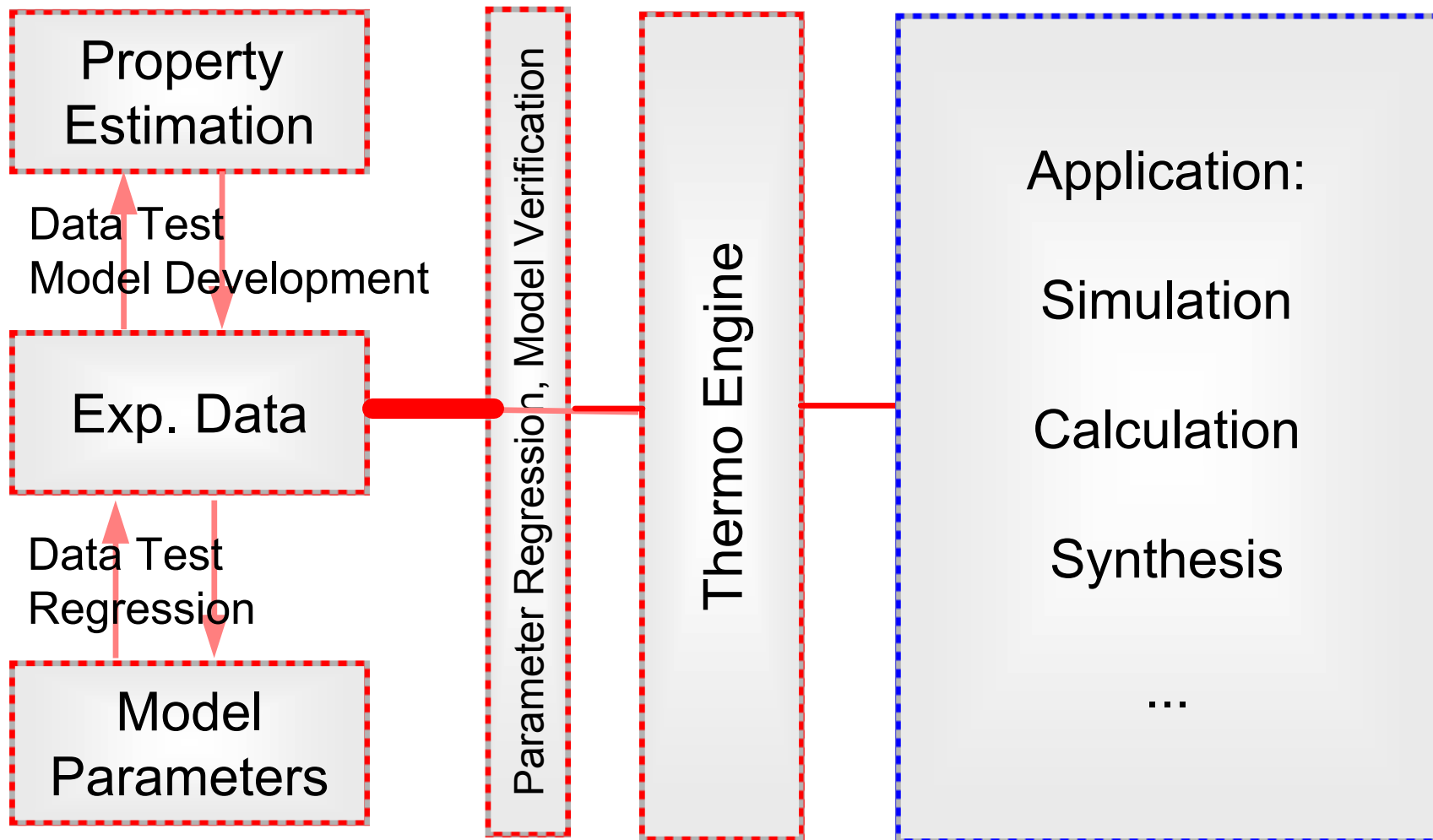


## What are Data Used for ?



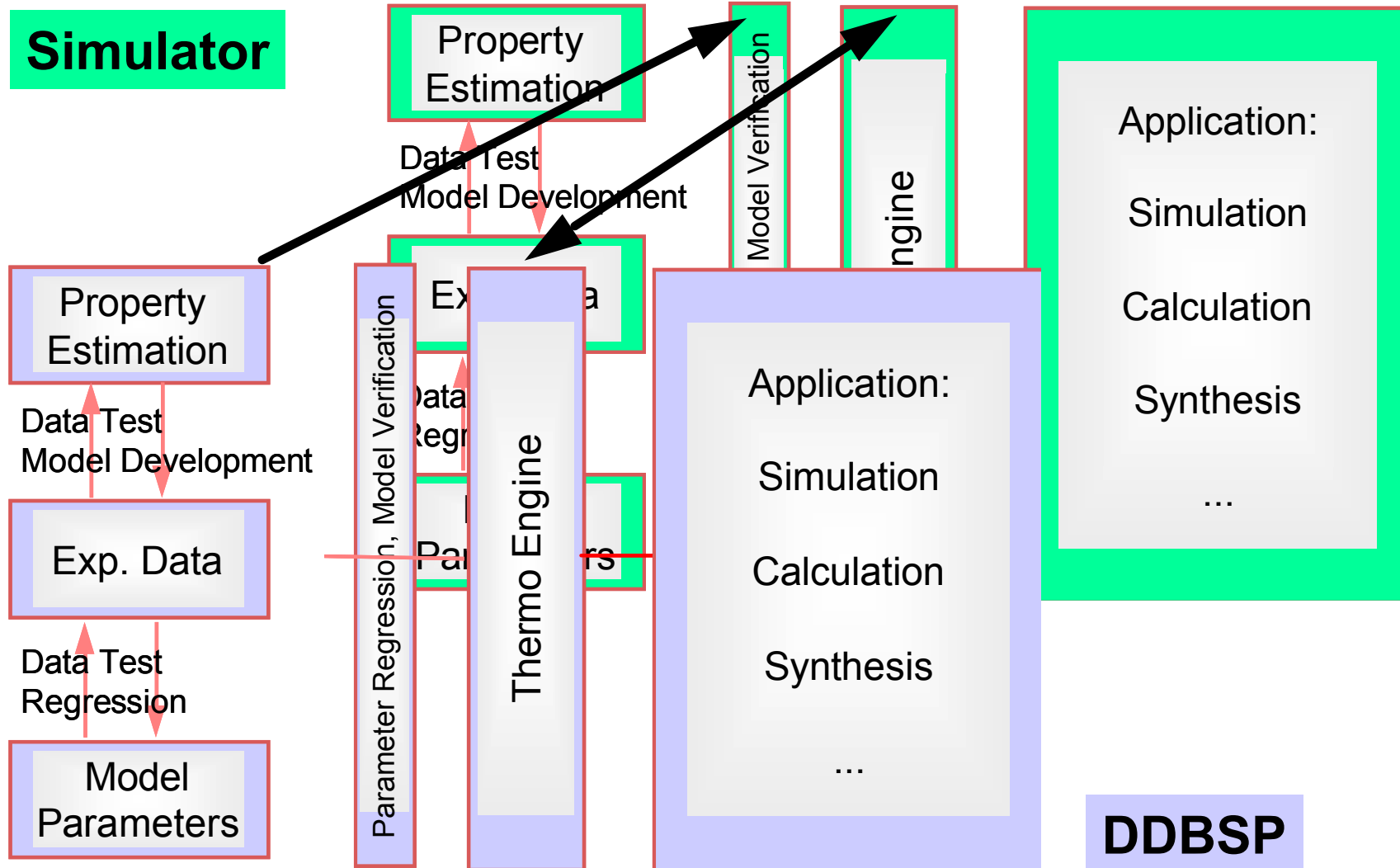


## General Application Structure





## Data and Parameter Exchange



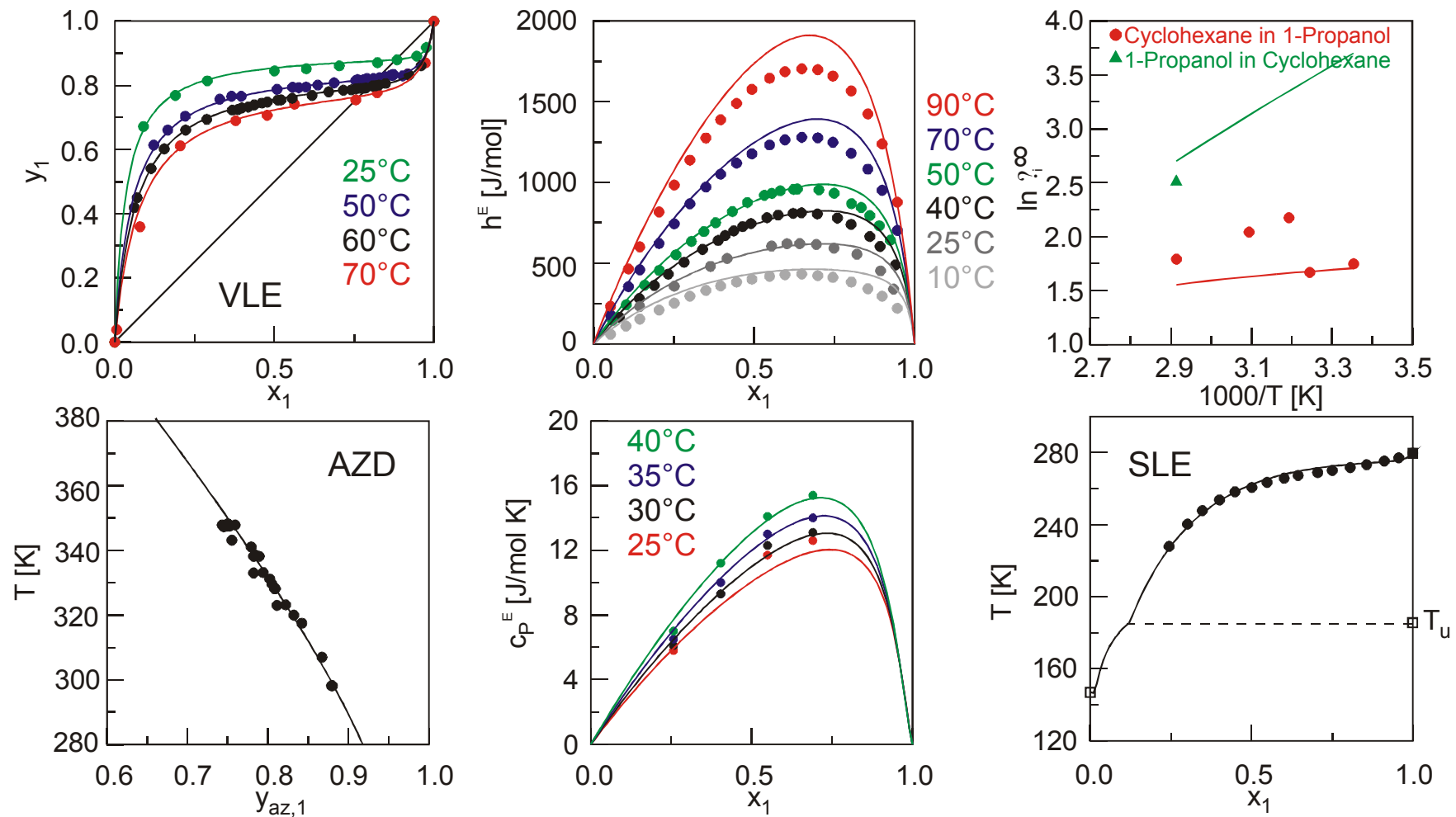


## Export of DDB Mixture Data to Aspen 11.1 via PPDx

Data Type	Subtype	Abbrev.	Comments
Vapor-Liquid Equilibria	normal boiling substances	VLE	export bin. tern. quart. import works for xyPT-and xPT-data
Vapor-Liquid Equilibria	low boiling substances	HPV	export bin. tern. import works for xyPT-and xPT-data
Vapor-Liquid Equilibria	electrolyte systems	ELE	no export
Liquid-Liquid Equilibria		LLE	export bin. tern, import works for bin. and tern.
Activity Coefficients	infinite dilution ( in pure solvents )	ACT	exported import: Aspen dies with severe application error (same with ACT-files from DETHERM Internet)
Activity Coefficients	infinite dilution ( in mixtures)	ACM	no export
Gas Solubilities		GLE	no export
Solid-Liquid Equilibria	mainly organic compounds	SLE	export bin. tern. import: correct but additional steps required to use in Regression
Salt solubilities	mainly in water	ESLE	no export
Azeotropic Data		AZD	no export
Adsorption Equilibria	vapor phase	ADS	no export
Excess Enthalpies		HE	export bin. tern. import: components ok but no data sets (identical with DETHERM Internet)
Excess Heat Capacities		CPE	no export
Excess Volumes		VE	export bin. tern. import: not possible
Critical Data of Mixtures		CRI	no export



## Simultaneous Correlation of DDB-Data With the Help of DDBSP (Recval/3)

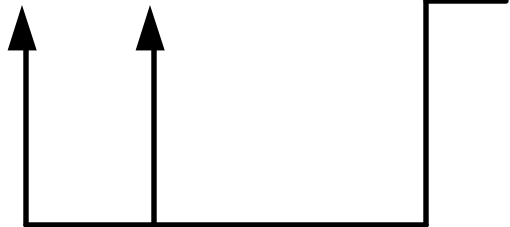


Simultaneous correlation of data for the system cyclohexane (1) – 1-propanol (2) with the help of the Wilson equation





Thank you for attending this Presentation!



You are welcome to a demonstration of the DDB and the DDB software package and a discussion about your special interests!