

Software Demonstration of the Dortmund Databank (DDB) and its Application for Process Design

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With a history and continuous development of more than 25 years, the Dortmund Data Bank (DDB) grew to be the worldwide standard source for thermodynamic data. Starting with vapor liquid equilibria data for the development of group contribution models, the data bank was continuously extended for mixture and pure component properties of electrolytes, non-electrolytes, and ionic liquids. The data bank includes phase equilibrium data (such as VLE, SLE, and LLE), caloric properties (such as heat capacities and excess enthalpies), and transport properties (such as viscosities and thermal conductivities). It contains, in total, more than 40 properties for about 15,000 pure components and more than 15 mainly phase equilibrium and excess properties are stored for about 75,000 binary, ternary or multi component systems. The data bank contains experimental data retrieved from scientific literature all over the world including east European and Asian literature, e.g., unpublished Russian reports. More than 76,000 references have been collected and evaluated up till now.

Around the comprehensive data compilation a powerful software package was developed for the storing, handling, verifying and processing of data including correlation and calculation tools. To fill data gaps several properties can be estimated using integrated software tools like ARTIST. This tool allows the prediction of more than 30 different properties using various published estimation methods by only drawing a structure or loading it from a database of over 15,000 structures.

The combination of the Dortmund Data Bank and the software package allows the analysis of the real mixture behavior of a system of interest and the ability to fit reliable model parameters (GE-models, equations of state, group contribution methods) for the synthesis and design of chemical processes on the basis of the most actual experimental data and estimation methods.

In addition, the data banks for activity coefficients at infinite dilution, azeotropic data, LLE and VLE serve as ideal sources for, e.g., the selection of suitable solvents for azeotropic or extractive distillation, extraction, and absorption.