The Dortmund Data Bank and its Integrated Software Package - A Comprehensive Tool for Process Development

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With a view to the synthesis and design of separation processes, fitting and critical examination of model parameters used for process simulation and the development reliable predictive models (UNIFAC, mod. UNIFAC Dortmund, PSRK, VTPR, …) with a large range of applicability, a computerized data bank for phase equilibrium data was started 50 years ago by J. Gmehling and U. Onken at the University of Dortmund. While at the beginning, mainly VLE data for non-electrolyte mixtures (T_b > 0 °C) were considered, later on also VLE including compounds with T_b < 0°C, LLE, h^E, γ^∞, azeotropic, $c_P{}^E$, SLE, v^E, adsorption equilibrium, polymer data, transport properties, ... for non-electrolyte and electrolyte systems as well as pure component properties were stored. The DDB currently (November 2023) contains more than 10.1 million data tuples for 94,400 components from 92,000 references (206,900 evaluated).

At the same time, a large number of software tools have been developed to search, retrieve, export, visualize and regress the data. The DDB software package features a wide variety of functionalities to optimally employ the vast amount of knowledge stored in the DDB and a variety of modern property estimation and regression techniques. Special data mining tools for process synthesis potentially lead to new solutions for engineering and environmental problems.

The selection of entrainer for extractive and azeotropic distillation, extraction and absorption which will be the focus of our demonstrations.