

Editorial

60th Birthday of Jürgen Gmehling

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On January 13th, 2006, Jürgen Gmehling celebrated his 60th birthday. As a tribute to him, we would like to present this special issue of *Fluid Phase Equilibria*, where a large number of well-known authors have handed in their articles, representing many of Jürgen Gmehling's fields of activity.

Jürgen Gmehling started his career in 1962 as a laboratory assistant apprentice at the Duisburger Kupferhütte. After finishing his apprenticeship, he studied Chemical Engineering at the Essen School of Engineering (1965–1968) and Chemistry (1968–1970) at the Universities of Clausthal and Dortmund. In 1973, he finished his thesis at the University of Dortmund in Inorganic Chemistry.

He decided to work on the phase equilibrium topic for which Prof. Ulfert Onken was searching a scientist with considerable staying power. The idea was to develop a group contribution method for the prediction of vapor–liquid equilibria, similar to the ASOG method suggested by Derr and Deal in 1969. They recognized that the only way for a proper development was to gain complete access on the phase equilibrium data available, and they started to build up the Dortmund Data Bank. At the beginning, they had 174 components; meanwhile, there are more than 22,000. A lot of experimental work was done to systematically fill the gaps where no data for the determination of group interactions were available. They were supported by the beginning EDP technology, which made it possible to treat all the information electronically. From today's point of view, it is unbelievable how low the capacity of the first microcomputers was, and Jürgen Gmehling still loves it to tell stories about programming a phase equilibrium calculation with punched cards in the early 1970s. In 1977, it was a great success when Aage Fredenslund, Jürgen Gmehling and Peter Rasmussen published the first version of a comprehensive group interaction parameter matrix of the UNIQUAC Functional Group Activity Coefficients (UNIFAC) method in the well-known textbook “Vapor–liquid equilibria using UNIFAC”.

After a 2-year stay at the group of J.M. Prausnitz in Berkeley, California, from 1977 to 1978, he returned to the University of Dortmund and became an extraordinary professor.

In 1989 he became an ordinary professor for technical chemistry in Oldenburg, where he continued his work on phase equilibrium thermodynamics. In Oldenburg, he founded two companies, the DDBST GmbH with the focus on the further development of the Dortmund Data Bank and the LTP GmbH, which performs state-of-the-art measurements of thermodynamic properties. Jürgen Gmehling was awarded with the Arnold-Eucken prize in 1982.

Meanwhile, the Dortmund Data Bank comprises 3.2 million data points, and the original UNIFAC method has almost been replaced by Mod. UNIFAC (Dortmund), which provides temperature-dependent group interaction parameters and

an improved combinatorial contribution. Besides vapor–liquid equilibria, also activity coefficients at infinite dilution, excess enthalpies, and liquid–liquid equilibria can be predicted. An industrial consortium consisting of more than 40 companies is promoting the further development of this method. After 10 years, the numbers of groups has been increased to 85. Continuously, the whole parameter matrix is revised, and new group interaction parameters are added. The comparably inexpensive but accurate measurement of excess enthalpies ensures that the information necessary for the description of the temperature-dependence of activity coefficients can easily be made available. The UNIFAC consortium is an excellent example of Jürgen Gmehling’s way to perform research close to industrial application.

However, his favourite target is the development of a universal model which can also treat supercritical mixtures. The g^E mixing rules for cubic equations of state have been forcefully developed and tested for applicability. The Predictive Soave–Redlich–Kwong equation (PSRK) has already become a powerful tool in commercial process simulators, and professional circles are looking forward to the next improvement step, the Volume-Translated Peng–Robinson equation (VTPR), with great expectations.

Jürgen Gmehling has published approximately 340 articles in scientific journals, together with the monographs DECHEMA Chemistry Data Series (more than 40 volumes), the compilation “Azeotropic Data”, and the textbooks as the above-mentioned “Vapor–liquid equilibria using UNIFAC”, “Thermodynamics”, and “Thermodynamics of Phase Equilibria”. Beyond thermodynamics, he also authored a textbook called “Unit operations”, an introduction to process engineering, and a major contribution to the Winnacker–Küchler encyclopedia on “Thermal Process Technology”.



Thus, it is clear that Jürgen Gmehling is one of the most experienced authors in our scientific area, and everyone who has joined him in writing a publication knows his notorious sixth sense for errors and misprints, which, however, finally guarantees a high quality. We and the authors hope that we have maintained his standard with this small collection of papers and that he will enjoy reading it.

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