Thermodynamics for Process Simulation: Need of a Bridge from Research to Industry

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A major problem encountered in chemical engineering lies in the calculation of phase equilibria and thermodynamic properties. Fluid phase equilibria can be calculated using "heterogeneous" methods (use of an equation of state for gas phase fugacities and non-ideality in liquid phase taken into account using a model of free excess enthalpy) or "homogeneous" methods (which apply the same model to both phases present, generally an equation of state, ensuring continuity at the critical point). "Heterogeneous" application covers rather the domain of low pressures, but they do not satisfy the continuity existing in the critical zone between the vapor state and the liquid state. Also, the domain of application of equations of state with their classic mixing rules is limited to non-polar or few polar systems. By integrating the excess enthalpy models into the mixing rules of the equations of state, the authors managed to combine these two approaches. Moreover, some specific models were also developed for some domains of application: electrolytes, carboxylic acids, formaldehyde… . Even if industries want fewer (even single) models which could do more, new models have appeared these two last decades, like SAFT and COSMO. Several versions of these two families of models are published every year, but most of these publications don't deal with real industrial use cases. To be really useable for industrial purposes, there should be a "virtuous triangle" between academic researchers, industries, and software providers. So, an open thermodynamic server which can be embedded in any software used by chemical engineers and which can easily be enriched by any thermodynamic specialist (i.e. possibility to develop fugacity or activity coefficient calculation codes, which can be linked with native routines of the embedding software, like flash algorithms or derivative properties calculations) are required. Such a server which bridges the gap between research and industry will be presented.