Aalto University
School of Chemical Technology

School of Chemical Technology
http://chem.aalto.fi/fi/
Tel. +358 50 5222 381, Kati Sumu

Dissertation release 4.8.2014

Thermodynamic data and predictive methods for new fuel additives

Title of the dissertation	Measurements and modeling of physical properties for oil and biomaterial refining
Contents of the dissertation	New challenges related to the shortage of fossil fuels and the development of renewable sources of energy require new experimental thermodynamic data or reliable prediction models for data estimation. The availability of reliable thermodynamic data is of major importance for the estimation of the feasibility of an industrial process and the optimization of process costs. Experimental data are more reliable, but obtaining them is time consuming. Predictive models, however, can produce unexpected errors. A reasonable combination of experiments and models can optimize time and costs, while providing sufficient information for the optimization of new and existing processes for the production of oil additives and bio-based fuel components. In this work, experimental vapour-liquid equilibria data for 40 industrially relevant binary systems were obtained. The measured data complement each other and can be used for the prediction of physical properties of a variety of chemicals in a wide range of conditions. The data were used for the development of semi-empirical thermodynamic models (Wison, NRTL and UNIQUAC). Additionally, the experimental data were utilized for the critical evaluation of the UNIFAC and the COSMO-RS predictive models. A novel technique intensifying the use of available experimental data was suggested in this work for the prediction of pure compound thermodynamic properties. The investigated mixtures, predictive model validation and proposed physical property calculation technique contribute to a better knowledge of the chemical thermodynamic properties. Using the new technique as well as the obtained thermodynamic data allows accurate calculations of the phase equilibria in industrial processes and the optimization of process conditions.
Field of the dissertation	Chemical technology
Doctoral candidate	M.Sc. Anna Zaitseva
Time of the defence	15.8.2014 at 12 noon
Place of the defence	Aalto University School of Chemical Technology, Department of Biotechnology and Chemical Technology, Auditorium Ke 2, Kemistintie 1, (entrance from Biologinkuja), Espoo
Opponent	Professor Wolfgang Arlt, Friedrich Alexander University, Germany
Supervisor	Professor Ville Alopaeus, Aalto University School of Chemical Technology, Department of Biotechnology and Chemical Technology
Web address of the dissertation	https://aaltodoc.aalto.fi/handle/123456789/51
Doctoral candidate's contact information	M.Sc. Anna Zaitseva anna.zaytseva@aalto.fi 040 588 4482

A doctoral dissertation is a public document and shall be available at Aalto University School of Chemical Technology noticeboard (Kemistintie 1, Espoo, PL 16100, 00076 Aalto) and at the Department of Forest Products Technology.