EFCE Spotlight Talks

Working Party on Thermodynamics and Transport Properties

19 May

13:30 • 15:00 CET

Electrolyte Thermodynamics challenges from industrial needs to academic research

Many applications in the process industry deal with fluids that contain electrolytic species. While thermodynamic models for neutral molecules are now well established, there are still many unanswered issues related to the presence of ions in a fluid mixture. This webinar aims at informing the community about important initiatives that have been taken in order to further the understanding of these systems, both from a fundamental point of view, as applied to typical applications.

PROGRAM

A workflow for setting up an adequate thermodynamic model for process simulation
Jean-Charles de Hemptinne - IFP Energies Nouvelles, France

The EleTher Joint Industrial Project was initiated in order to set up an industrial community for promoting research on electrolyte thermodynamics. Best Practices are being identified based on some case studies that have been submitted by participating members. In this presentation, these best practices are detailed using a three-step workflow: (i) The first step is data analysis. It appears that even for simple systems, significant regions (temperature-composition) remain unexplored experimentally. (ii) The second step consists in extrapolating the data in the range of industrial interest. An example will be given using a simple graphical approach. (iii) In a the third step the parameters of a process simulator model must be regressed. The Aspen e-NRTL equation is used as a benchmark to investigate this part.
The presentation will summarize the achievements so far and lay some perspectives for future work. The final objective is to promote collaboration in view of a second version of the JIP.

Thermodynamic modeling of electrolyte solutions using the Debye-Hückel theory
Georgios Kontogeorgis - Center for Energy Resources Engineering (CERE), Technical University of Denmark

Electrolyte solutions are present almost everywhere, in numerous applications in chemical, biochemical, geochemical, petroleum engineering as well as in diverse disciplines such as geology, biology and medicine.
Almost 100 years ago (1923), Peter Debye and Erich Hückel published a 20-page long paper entitled "On the theory of electrolytes. I. Freezing point depression and related phenomena". This single manuscript, adopting the (then) pioneering concept (by Bjerrum) of complete dissociation of strong electrolytes, has revolutionized the field of electrolyte thermodynamics. Debye received the Nobel prize in 1936.
The Debye-Hückel theory has since 1923 been cited thousands of times, and mentioned even more without citation, derived and interpreted in numerous ways, approximated, extended, generalized, incorporated in other "more general" electrolyte models, compared to more "modern" approaches (like the mean-spherical approximation), called various things and re-baptized in many names (e.g. Debye-Hückel limiting law, extended law, etc), used (and misused) in many ways and many times. McQuarie wrote in 1976 in his famous book about Statistical Mechanics "*in spite of the great success of the Debye-Hückel theory, when it was originally proposed its range of validity was not at all clear*". Is it today?
The story of the Debye-Hückel theory was and is under extreme debate with many controversial aspects. In this lecture, I will try to present a modern status of the Debye-Hückel theory and outline both capabilities and limitations, from fundamental and engineering points of view. Future directions will also be briefly outlined.

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Registration

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