



CEE Seminar Speaker

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Professor

Distinguished Chair in Sustainable Energy at the College of Engineering
Texas Tech University

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INDUSTRIAL CHALLENGES WITH ELECTROLYTE THERMODYNAMICS

Process simulation is a crucial enabling technology for industrial process development, design, debottlenecking, and optimization. Success in process simulation is ultimately dependent upon advances in molecular thermodynamics for accurate descriptions of thermodynamic properties and phase behavior of concerned multicomponent chemical systems. As chemical engineers address societal issues such as sustainability and climate changes, advances in molecular thermodynamics for electrolyte solutions are urgently needed.

This presentation summarizes the industrial challenges with electrolyte thermodynamics and highlights the successes and limitations of state-of-the-art thermodynamic models for electrolyte solutions. It further presents the newly developed association electrolyte NRTL model aimed to address explicitly the solution nonideality due to ion hydration and ion-pairing, phenomena ignored in the existing electrolyte thermodynamic models that consider only long-range ion-ion electrostatic interactions and short-range ion-ion, ion-molecule, and molecule-molecule interactions. The association electrolyte model allows accurate correlations and reliable extrapolations of all thermodynamic properties of aqueous single and multicomponent electrolyte solutions including those with high charge density ions such as proton ion, hydroxide ion, lithium ion, rare earth element ions, and many others. Our on-going investigation has shown that the association electrolyte model has the real potential to address the industrial challenges with electrolyte thermodynamics in support of accurate process simulation of industrial processes with electrolyte solutions.

BIOGRAPHY

Chau-Chyun Chen is a Horn Distinguished professor at Texas Tech University and the Jack Maddox Distinguished Chair in Sustainable Energy at the College of Engineering, Texas Tech University. A co-founder of Aspen Technology, Inc., he is the inventor of the Aspen process simulation software for electrolyte systems, polymerization processes, small molecule drug solubility, CO₂ capture with chemical absorption, and molecular characterization for petroleum assays. He joined Texas Tech University in 2013 to further research in electrolyte thermodynamics, adsorption thermodynamics, membrane separation, among others. He holds over 160 scientific publications and book chapters, and more than 20 US and international patents.

Dr. Chen received BS degree in chemistry from National Taiwan University and MS and ScD degrees in chemical engineering from the Massachusetts Institute of Technology. He is a fellow of American Institute of Chemical Engineers, American Association for the Advancement of Science, and the National Academy of Engineering.