SCHOOL OF CHEMICAL, BIOLOGICAL & MATERIALS ENGINEERING
And
UNIVERSITY OF OKLAHOMA BIOENGINEERING CENTER
100 E. Boyd, Sarkeys Energy Center, T-335
405-325-5811
The University of Oklahoma
Norman, Oklahoma

2010 – 2011 Seminar Series

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DIFFERENT DAY – MONDAY; DIFFERENT PLACE – FELGAR HALL 304; & DIFFERENT TIME – 3:45 !

DR. IRINA SMIRNOVA

PROFESSOR
INSTITUTE OF THERMAL SEPARATION PROCESSES
HAMBURG UNIVERSITY OF TECHNOLOGY
HAMBURG, GERMANY

Will present a seminar on

"PHASE EQUILIBRIA IN MULTICOMPONENT MICELLULAR SOLUTIONS: MODELLING AND EXPERIMENTAL STUDY"

This talk is related to the investigation of phase equilibria in multicomponent micellar solutions with the aim to optimize surfactant based separation processes, like micellar extraction and micellar chromatography. Both methods are well known for the separation and analysis of products from aqueous systems and are based on the formation of aggregates of different size and shape (micelles) in aqueous solutions. The partition of target molecules is mainly caused by hydrophobic and electrostatic interactions between the micelles and the solute. The most relevant factor is the partition coefficient of all related species, which defines the selectivity of the process. Efficient separation processes can be designed if an appropriate surfactant or surfactant combination is selected for a multi component system. The dominating factors influencing a micellar separation process are the surfactant itself, its concentration, the characteristics of the solute, the pH-value of the solution and the ionic strength. Effective processes need fully optimized systems, however the vast amount of parameters need a theoretical description and modeling of the present interactions.

In our institute the optimization of the separation processes is realized based on the predictive thermodynamically based modeling of the solute partitioning. Two models will be presented: the structure-interpolating UNIFAC model and the a-priori quantum chemistry based COSMO-RS model. The partitioning of a variety of solute classes in aqueous solutions of nonionic and ionic surfactants under different experimental conditions is investigated. It is demonstrated that the prediction can be achieved quantitatively based solely on the chemical structure of the substances. Furthermore, COSMO-RS model accounts for the concentration of each ingredient, ionic strength, and dissociation of the compounds at corresponding pH. Regarding the vast amount of different parameters like the influence of e. g. buffers, salts and alcohols in situ predictions using COSMO-RS is an effective tool to optimize surfactant based separation processes.

Further, the modeling is extended for other types of liquid-liquid equilibria, especially in the field of drug delivery and biotechnology. Modelling of the product isolation from the biotechnological production based on salt/sugar induced liquid-liquid phase split is discussed.

At the end, an overview of other research areas and the experimental facilities of the institute will be given.

MONDAY, DECEMBER 2, 2010
COOKIES AND COFFEE -- 3:35 P.M.
SEMINAR -- 3:45 P.M.
FELGAR HALL, ROOM 304

THIS IS A REQUIRED SEMINAR FOR CHE 5971

Accommodations on the basis of disability are available by contacting the office above three days before the event.