# Statistical Mechanics of Solutions and Surfaces

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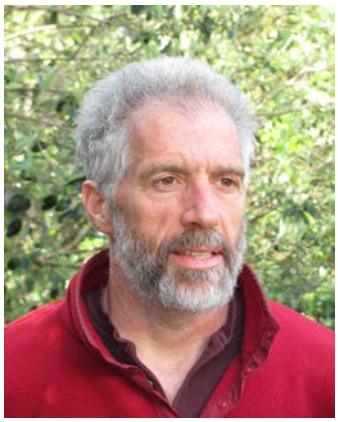


## Dr. Anthony S. Wexler

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**Abstract:**

An accurate and fundamental description of the bulk and surface composition and phase state of aerosol particles will help us understand how they interact with gas phase atmospheric compounds and radiation, and how they activate into clouds.

BET sorption isotherms are well known to describe surface sorption thermodynamics, but less well known is that BET also describes highly concentrated solutions where the "solvent," say water, sorbs to the "solute," say a water soluble organic, like glycerol. BET employs a single sorbed monolayer and a single "mulitlayer." In recent work we extended BET to an arbitrary number of monolayers, a mulitlayer, and a Debye-Huckel term. This new set of equations describes solution activity over the full concentration range from pure solvent to pure solute with remarkably few parameters. These parameters' values are related to the solute and solvent size and dipole moment. In 1998, Ally and Braunstein at ORNL extended BET to an arbitrary number of solutes. We have accomplished the same for our multiple monolayer model and have shown when it is equivalent to ZSR, the mixing model used in most aerosol thermodynamics models.

Since our extended BET isotherm is inherently surface-based and incredibly successful at modeling solutions, it should be able to model surface tension too. Applying similar sorption thermodynamics tools, we have derived the first equations that describe surface tension of solutions that contain electrolytes or organics and that are accurate over the full concentration range. Again, very few parameters are required for each solute.

In the talk, I will explain how we obtained both solution and surface isotherms and show comparisons between the model and predictions. Ultimately, these isotherms will be incorporated into our E-AIM thermodynamics website so that users worldwide can easily calculate the bulk and surface properties of the aqueous and organic phases of aerosol particles.


See http://mae.ucdavis.edu/wexler/

Please join us for a meet and greet opportunity
with Dr. Wexler after the seminar.
~Refreshments will be served~

Date: Tuesday, February 26

Location: EMSL Auditorium

Time: 11:00 am

*Host: Phil Rasch 372-4464 POC Sarah Fillmore 375-6315*