Meeting: 998, Houston, Texas, SS 14A, Special Session on Space and Time Decomposition Methods in Computational and Applied Mathematics

998-49-228 **Jiwen He*** (jiwenhe@math.uh.edu), University of Houston, Department of Mathematics, 651 PGH, Houston, TX 77204-3008. *Computational Methods for Multi-phase Multi-reaction Equilibrium Problem - Modeling Urban and Regional Aerosols.*

Atmospheric particulate matter (PM) models are effective tools to quantify the relationship between sources of air pollutants and their health and environmental impacts. An ubiquitous component of the PM models is the thermodynamic module that simulates the partitioning of chemical species among the gas, aqueous, and solid phases and predicts the total mass and chemical composition of PM. When the temperature and pressure are both constant, the number of phases and the amount and composition of each phase which occurs at equilibrium in nature corresponds to the global minimum of the Gibbs free energy of the system. In this talk, we present a new avenue to appropriately predict the phase transition between the aqueous and solid PM phases, based on the reformulation of the optimality system as a nonlinear system of variational inequality type. Consequently, active set based Newton method is developed to obtain robust and stably convergent numerical solutions of multi-phase multi-reaction equilibrium problem. We conclude with numerical experiments, showing that the method is efficient, computationally suitable for its use in 3D Eulerian urban air-shed models. (Received February 27, 2004)