

INORGANIC CHEMISTRY CALCULATIONS USING HETV - A VECTORIZED SOLVER FOR THE SO₄-NO₃-NH₄ SYSTEM BASED ON THE ISORROPIA ALGORITHMS

P.A. Makar (1), V.S. Bouchet (1) and A. Nenes (2)

(1) Air Quality Research Branch, Environment Canada, 4905 Dufferin Street, Toronto, Ontario, Canada M3H 5T4 (paul.makar@ec.gc.ca), (2) Department of Chemical Engineering, California Institute of Technology, Pasadena, Ca., USA 91125 (nenes@its.caltech.edu)

An essential component of the prediction of aerosol composition is the gas-particle partitioning described by inorganic equilibrium reactions, coupled with mass and charge balance equations. Despite the apparently simple nature of the governing equations, the added complexity associated with high concentration equilibrium chemistry, water content estimation, and deliquescence calculations, results in a highly nonlinear system, and a need for both simplifications and specialized solution methods.

The predictions of inorganic gas-aerosol partitioning on the regional scale requires the rapid solution of tens of thousands of individual equilibrium problems, with a separate iterative calculation being performed at each grid point in the regional model domain. By preference, these calculations should take into account the size distribution of the aerosol components at each gridpoint, further increasing the number of equilibrium calculations required. Highly efficient computational techniques are therefore required.

In this paper, a new heterogeneous chemistry code, HETV, will be described. The code is based on the SO₄-NO₃-NH₄ algorithms of the ISORROPIA solver of Nenes et al (1998), but was redesigned for maximum computational efficiency on a vector supercomputer, using the "vectorization by gridpoint" technique of Jacobson and Turco (1994). During the construction of the code, a number of important improvements were made to the original ISORROPIA algorithms, and these will be described.