2.055 Simulation of the ionization efficiency of evolved gas molecules from aerosol particles in a thermal desorption aerosol mass spectrometer.

Early Career Scientist

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Abstract:

Thermal desorption aerosol mass spectrometers (TDAMSs) with electron ionization have been widely used to quantitatively measure chemical composition of aerosol particles. We have conducted laboratory experiments to investigate physical and chemical mechanisms affecting the ionization efficiency of evolved gas using a custom-made TDAMS. Sodium oxalate was selected as a test compound because the thermal decomposition products are expected to be simple (dominated by carbon monoxide (CO) and carbon dioxide (CO_2)). A numerical model for simulating the molecular dynamics in evolved gas plumes has been newly developed to interpret the experimental results. The simulation model consists of two main sections. The first section simulates elastic collisions of evolved gas molecules in a small region near the vaporization point where the mean free paths of molecules are much shorter than those in a surrounding high vacuum environment. The second section simulates the free-molecular dynamics from the vaporization to the ionization regions. The ionization efficiencies of CO and CO_2 are calculated by counting the number of CO and CO_2 molecules passing through the ionization region. Preliminary results suggest that the molecular collisions near the vaporization region could be an important mechanism affecting variability in the ionization efficiency. Details of the experiments and simulations are presented and discussed.