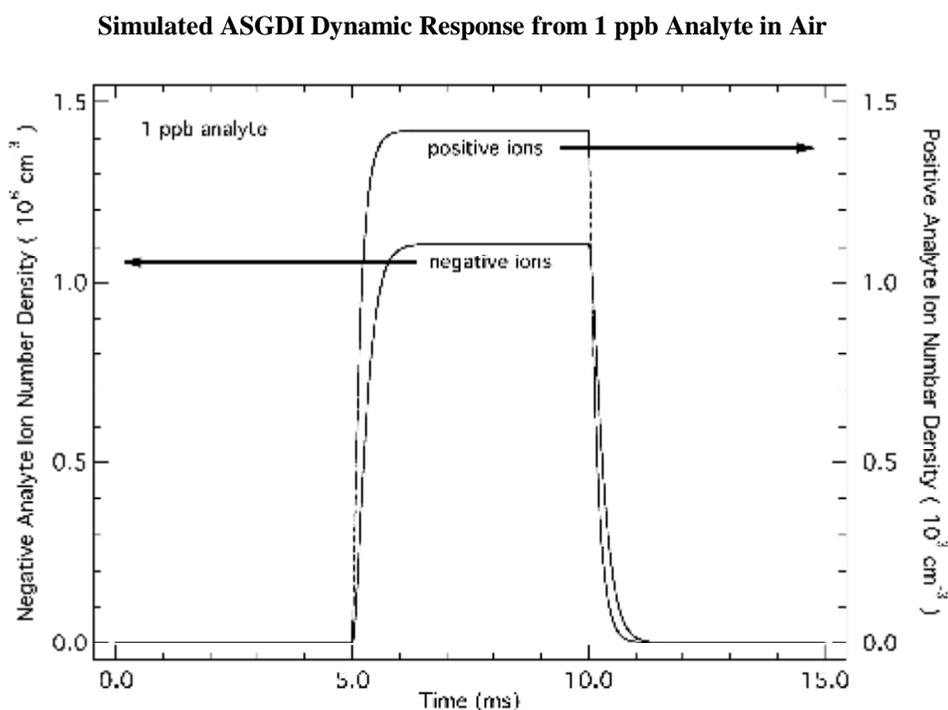


## Advanced Molecular Detection Dynamics Modeling

Basic research at the Oak Ridge National Laboratory has led to the first computer simulation of the atmospheric sampling glow discharge ionization (ASGDI) source, a device developed there for the direct trace-level detection of heteroatom-containing organic compounds in ambient air. The detailed ASGDI model incorporates secondary electron generation and thermalization, reagent and analyte ion formation via electron capture and ion-molecule reactions, ion loss via recombination processes, diffusion, and ion-molecule reactions with matrix components, and the physical operating parameters of the source. By using numerical methods to solve the differential equations for the above dynamic processes, the influences of fundamental ion processes and design parameters on its ultimate analytical sensitivity were revealed. Such understanding is necessary to achieve improvement in performance when the device is used in combination with mass spectrometry for important applications such as detection of explosives vapors, chemical warfare agents, and contraband.



This research was performed by Douglas E. Goeringer, Chemical Sciences Division, Oak Ridge National Laboratory. It was published in the *Journal of the American Society for Mass Spectrometry*, **2003**, 1315-1326.