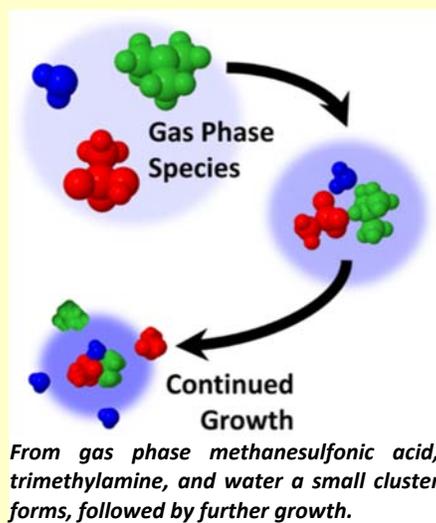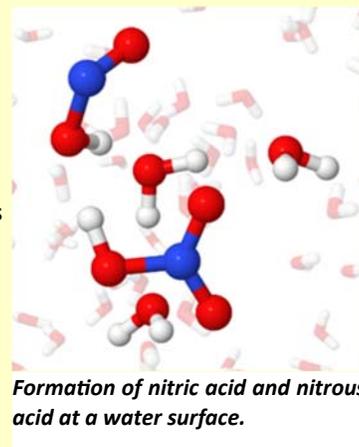# FACULTY-UNDERGRADUATE RESEARCH
PROFESSOR MYCHEL VARNER
COMPUTATIONAL ATMOSPHERIC CHEMISTRY

Atmospheric chemistry models describe relationships between chemical species to predict the concentrations of those species that are hazardous or otherwise of interest. To do so, these models rely on rates of reaction, photolysis rates, and relative energies, among other data. For many known gas-phase reactions this data can be very accurately determined through laboratory experiments. However, the model description can be insufficient in many ways. For example, these models may not account for unexpected side products, particularly weakly-bound molecules that can dissociate to yield the reactants and may be difficult to detect in laboratory experiments. Also, though the gas phase process may be well understood, the various surfaces that are present in the troposphere, the portion of the Earth's atmosphere that extends to ground level, may significantly alter the rate.

Formation of nitric acid and nitrous acid at a water surface.

From gas phase methanesulfonic acid, trimethylamine, and water a small cluster forms, followed by further growth.

In investigating incompletely understood atmospheric processes, computational approaches may be used as independent confirmation of laboratory experiments or in conjunction with experimental data. In the case of particle formation from gas phase species such as sulfuric acid and ammonia, it is not yet possible to probe the initial steps of complex formation that eventually lead to the nanometer-sized particles studied experimentally. Prediction of binding energies of various acid-base species that are found in the atmosphere bridges the gap in experimental data. An understanding of these processes can help determine which species may be relevant for formation of particles that negatively impact human health through inhalation, as well as influence the warming of the planet through radiative forcing.

The same factors that lead to unexpected atmospheric processes can also complicate the computational description. High-level methods may be required to accurately determine binding energies of weakly-bound species. And for reactions that happen at surfaces, the local environment must be taken into account. In some cases the nature of the interacting species themselves may present challenges, as when dealing with radicals and ions. In addition to the prediction of the stability of a species and probability of formation, the simulation of molecular spectra may aid in the assignment of laboratory spectra of atmospheric species.

If you would like to have more information and/or discuss the possibility of working in my group please feel free to reach me at: mvarner@iona.edu

Representative Publications

M.E. Varner, B.J. Finlayson-Pitts and R.B. Gerber, "Reaction of the $(NO^+)(NO_3^-)$ ion pair with water in the formation of atmospheric HONO: an ab initio Molecular Dynamics study", PCCP (2014) 16, 4483-4487.

M.A. Kebede, M.E. Varner, N.K. Scharko, R.B. Gerber and J.D. Raff, "Photooxidation of Ammonia on TiO2 as a Source of NO and NO_2 under Atmospheric Conditions", JACS (2013) 135, 8606-8615.

M.L. Dawson, M.E. Varner, V. Perraud, M.J. Ezell, R.B. Gerber and B.J. Finlayson-Pitts, "Simplified mechanism for new particle formation from methanesulfonic acid, amines, and water via experiments and ab initio calculations", PNAS (2012) 109, 18719-18724.