

Sulfuric acid and water models and atmospheric nucleation  
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Sulfuric acid plays a large role in atmospheric chemistry. The acid plays a major role in the nucleation of atmospheric particles, although the mechanism is not fully understood. The purpose of this research is to examine empirical sulfuric acid and water models via Monte Carlo simulations. It is hoped that these models can be used to screen a wide variety of cluster properties in order to isolate the most interesting properties for further examination with first principles simulations. The models evaluated were developed by Kathmann and Hale<sup>1</sup> and Ding et al.<sup>2</sup> These models utilized different features such as the deprotonation of an acid molecule, hydrogen bonding, and the magnitude of the partial charges within the molecules in the model (ionic v. neutral). Liquid phase densities and structures were evaluated for both the Kathmann and Ding models over a range of compositions (0 – 50 wt. % sulfuric acid) and the results were compared to experimental data. Additionally, simulations of a range of vapor phases were completed to examine the clustering. The initial data suggests that the force field plays a strong role in the extent of the cluster formation.

#### References

1. Change -Geng Ding, Tuulia Taskila, Kari Laasonen, Ari Laaksoen. *J. Chem. Phys.* **287** (2003) 7-9.
2. S. M. Kathman, B. N. Hale. *J. Phys. Chem. B.* **105** (2001) 11719-11728.