Modeling Investigation on Amines and Sea-salt Aerosol Interactions to Assess Their Potential Climate Impacts

Aerosols are solid or liquid particles suspended in air. Sea salt aerosols (which form from sea spray) serve as cloud condensation nuclei, assisting in the formation of clouds. Such atmospheric aerosols serve an important role in light scattering as a result, influencing the global radiation balance and possibly climate change. Amines are derivatives of ammonium with a hydrogen replaced by an organic group, emitted to the atmosphere from both natural and industrial anthropogenic sources such as carbon scrubbing in power plants, biomass burning, and animal husbandry.They typically are found in coastal areas, and they contribute to new particle formation (NPF), which has been shown to be a globally dominant mechanism of aerosols. One pathway for this particle formation with amines is acid neutralization, for example reacting with sulfuric acid. It's also known that sea salt aerosol can form hydrochloric acid with sodium chloride reacting with ammonium salts. Since hydrochloric acid (HCL) is more volatile than sulfuric acid and is closely related to sea salt aerosols, the purpose is to find out if amines will react with HCL to form amine chloride salt through acid neutralization, and if so will it be able to condense? This is important as it might show a new mechanism for particle formation through acid neutralization, in particular with an unexpected composition of condensation with HCl and amine chloride salts. It'll also provide more knowledge on how emission of industrial amines change the properties of sea salt aerosols while improving current atmospheric models. Finally, it'll further general knowledge on amines, aerosols, and their roles in light scattering, climate change, and indirectly human health as these aerosols might carry toxic components of the industrial amines. The hypothesis is that amines will react with HCL, the amine chloride will most likely be volatile at room temperature, and will be able to condense on sea salt aerosols at low temperatures. The independent variable is the temperature, and the dependent variable is the amount of amine chlorides as well as resultant properties (condensation, volatility). The control group will have sea salt aerosol not exposed to any amine in the same temperature range, and the constants are the concentration of inorganic and organic compounds. To model these interactions, the Extended AIM Thermodynamic Model (E-AIM) will be used, which simulates a chemical system with several phases including a gas phase, inorganic/organic solids, and hydrophobic and aqueous phases. For this project, Model IV will be used as it's the only one containing the necessary compounds and parametric temperature varying capability. Multiple trials are to be done under multiple scenarios. These are a base case with just ammonia and other inorganic compounds, one with methylamine, monoethanolamine, a case combining both amines and ammonia, and others with additional amines. Methylamines and monoethanolamine were chosen for their prevalence in atmosphere and likelihood for particle formation, respectively. In these, the water will be fixed at an amount of 0.07848 and 0.11189 moles for a respective RH of 60 and 85%. The inorganic ions are sodium (Na+), chlorine (Cl-), ammonium (NH4+), sulfate (SO^{2-}_{4}), and ammonia (NH3) which will be added as stated above, while organic compounds like amines can be added through an external library. In each case, the temperature will be evenly varied across 50 data points between 263.15K and 330K. Then, the data can be analyzed from the output of the model, as it can be outputted in the form of graphs as well as tables to then be directly interpreted. Since this is primarily a modeling project, there are no risks or hazards present. The student will be performing most of the experimentation with guidance from the mentor for model usage and data analysis.

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