

Modeling Indoor Aerosol Inorganic Thermodynamics with ISORROPIA

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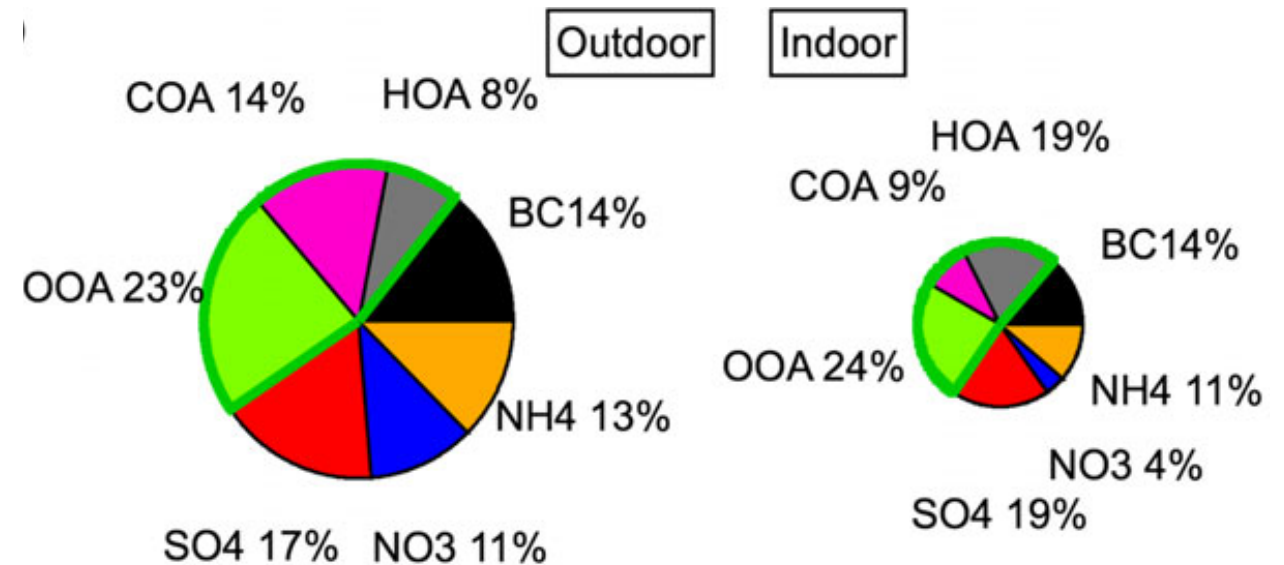
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Motivation

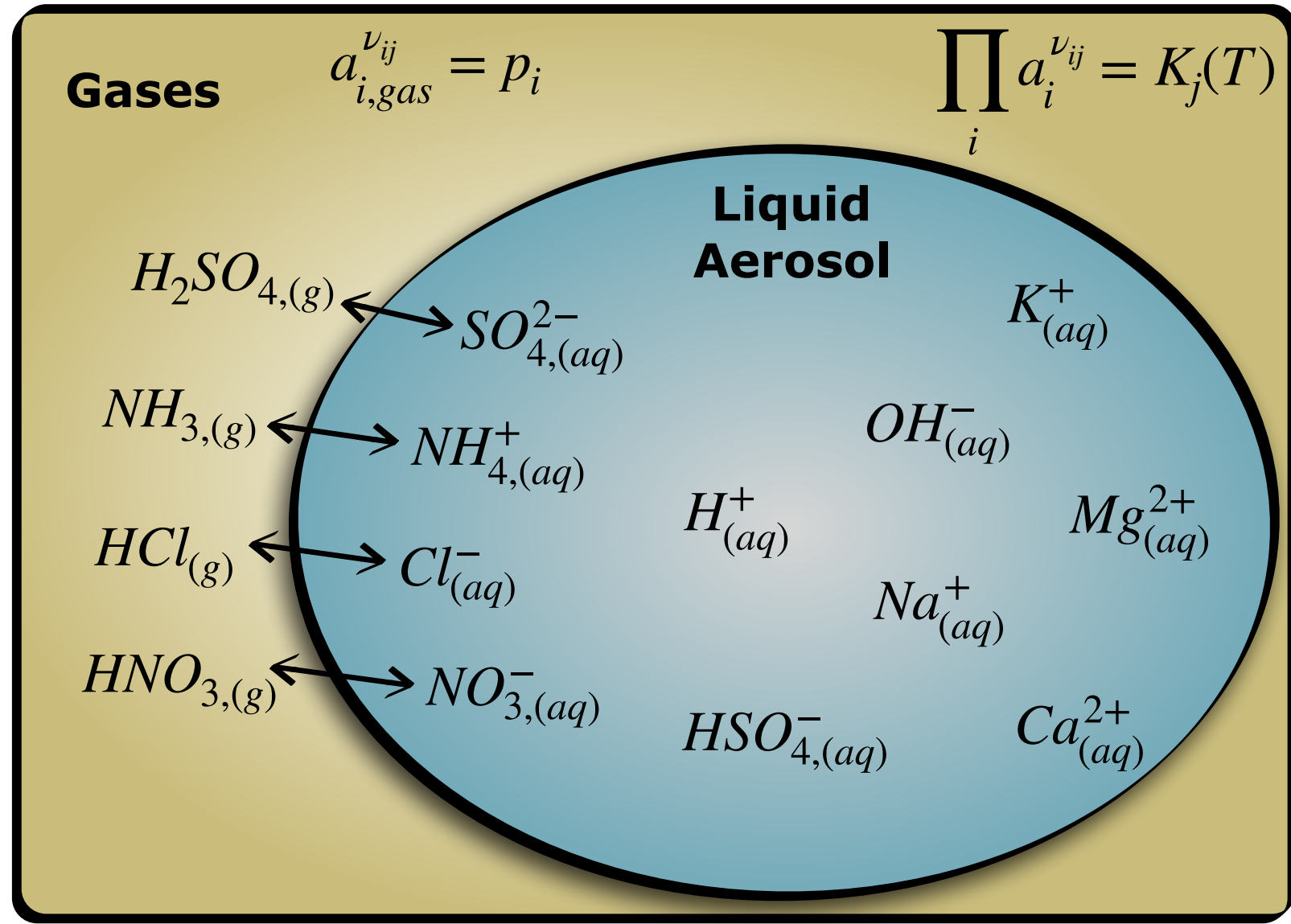
- High concentrations of ambient aerosols are linked to respiratory and cardiovascular conditions
- Citizens of developed countries spend most of their time indoors
- We want to better understand how HVAC systems with mechanical ventilation influence indoor aerosol composition and chemical processing
- This work demonstrates a proof of concept for addressing these gaps with a focus on indoor inorganic aerosols (IA) from outdoor origin by expanding Cummings & Waring (2019) indoor organic model



Johnson et al., Indoor Air, 2017

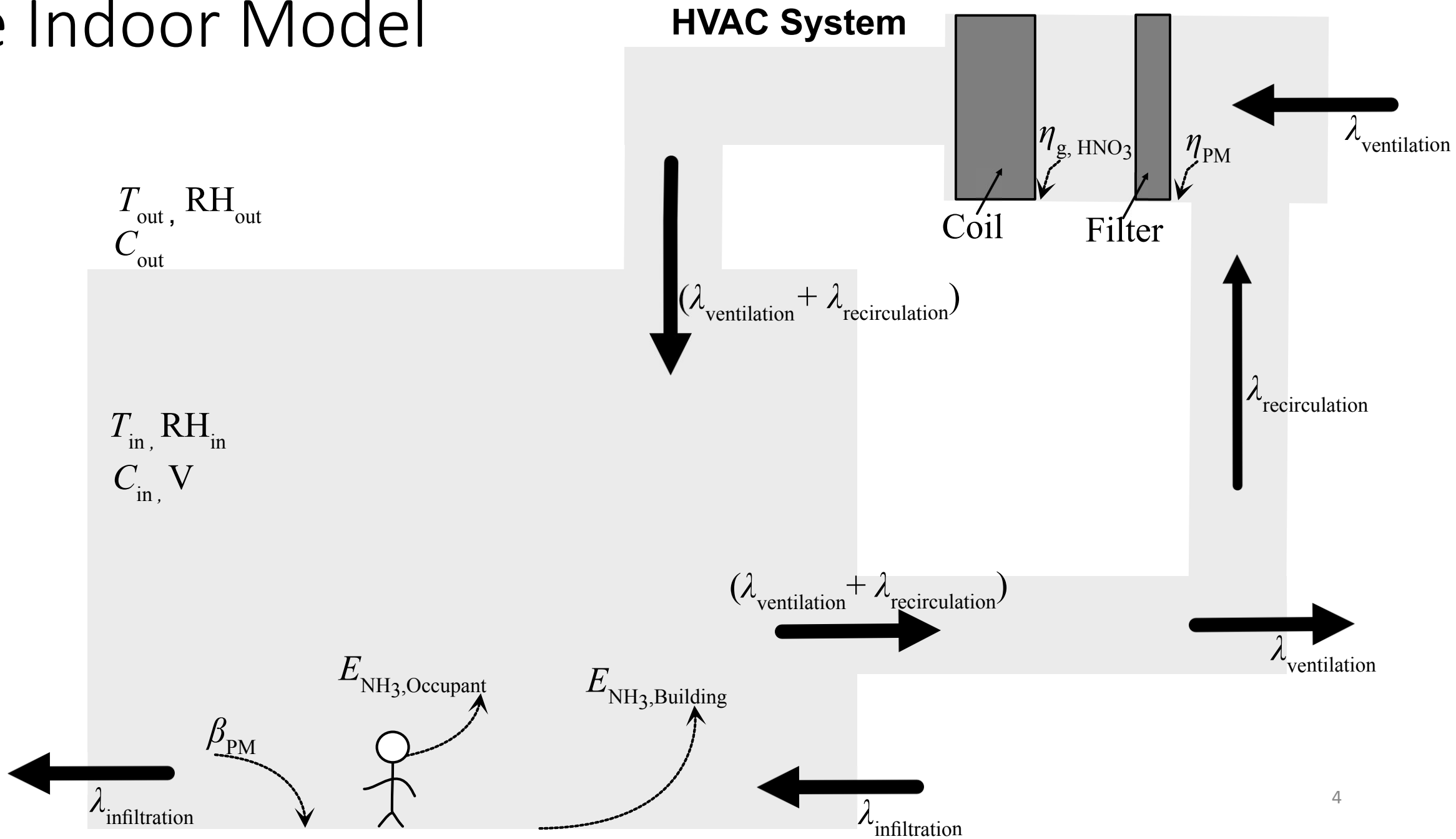
ISORROPIA

- Inorganic aerosol (IA) thermodynamic equilibrium model
- Widely used to predict gas/particle partitioning
- Inputs for forward mode are temperature (T), relative humidity (RH), and total concentration
- The stable mode can have both solid & liquid phase aerosol while the metastable mode only has liquid state aerosol
- First instance of applying ISORROPIA in an indoor model



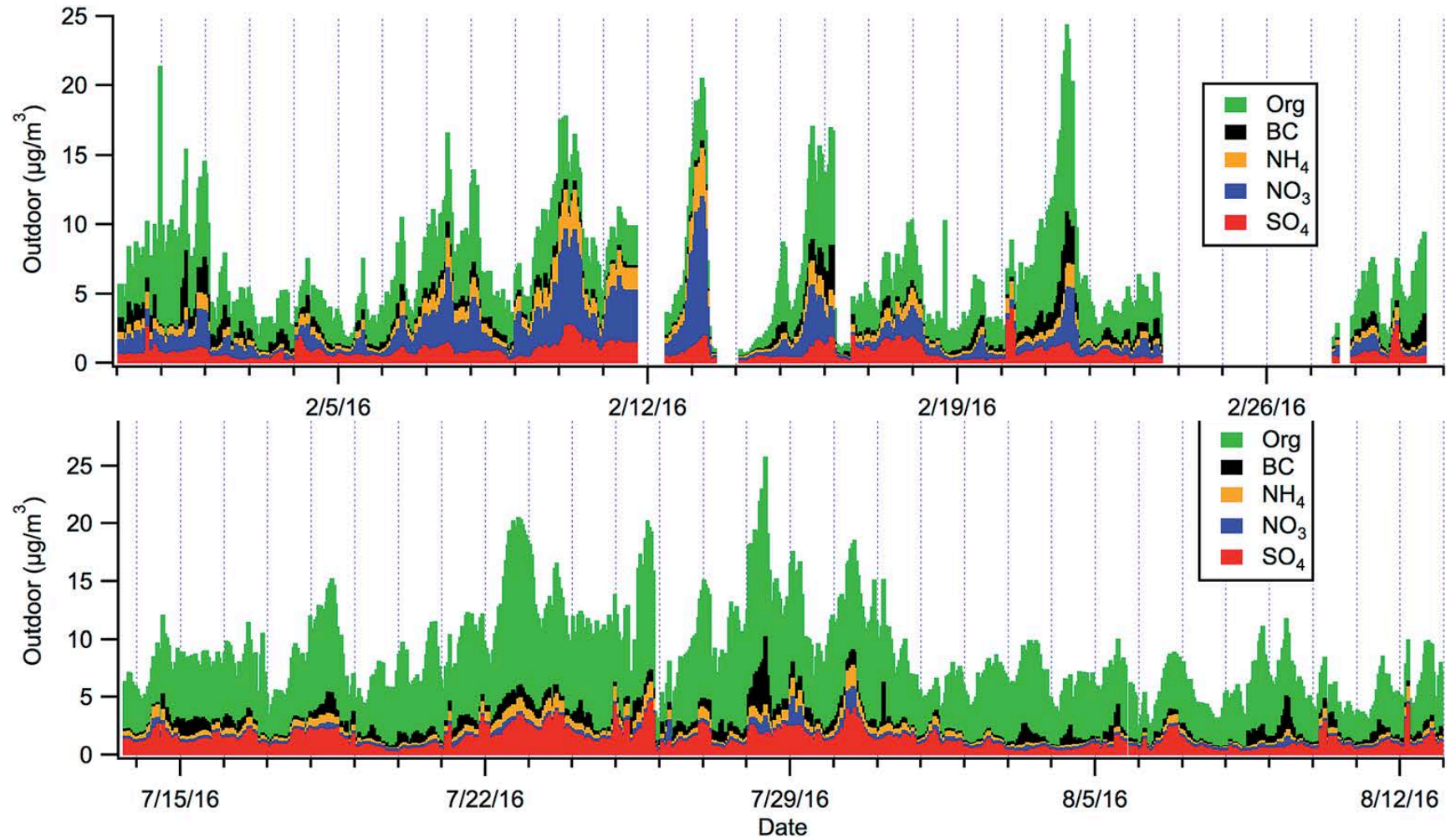
Nenes et al., *Aquatic Geochemistry*, 1998; Fountoukis et al., *Atmospheric Chemistry and Physics*, 2007

The Indoor Model



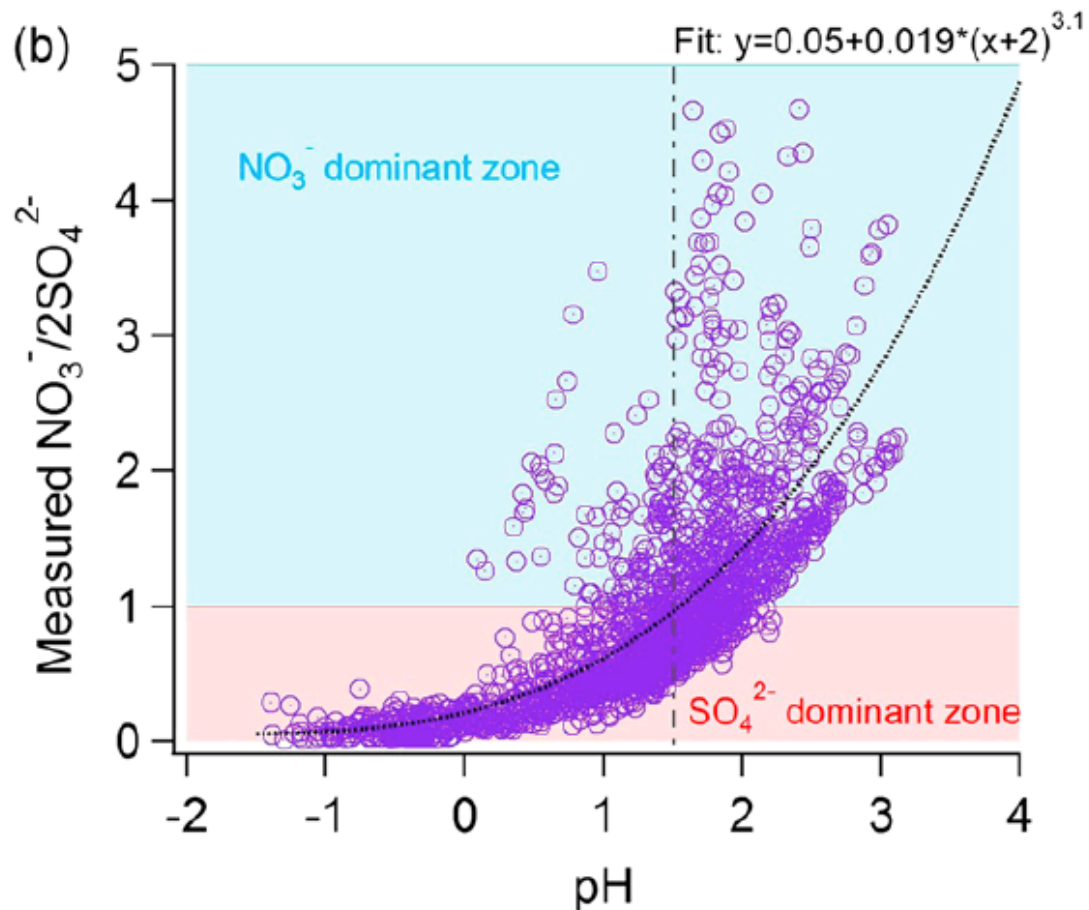
Model Input

- Measured indoor and outdoor T , RH , and CO_2 , as well as outdoor IA concentration data from Avery et al (2019) was used as input for this model
- Assumed the same air flow rates as Avery et al. (2019)
- Occupant NH_3 was derived from CO_2 data using methods from Li et al. (2020)
- Background NH_3 was estimated using a correlation published by Ampollini et al. (2019)

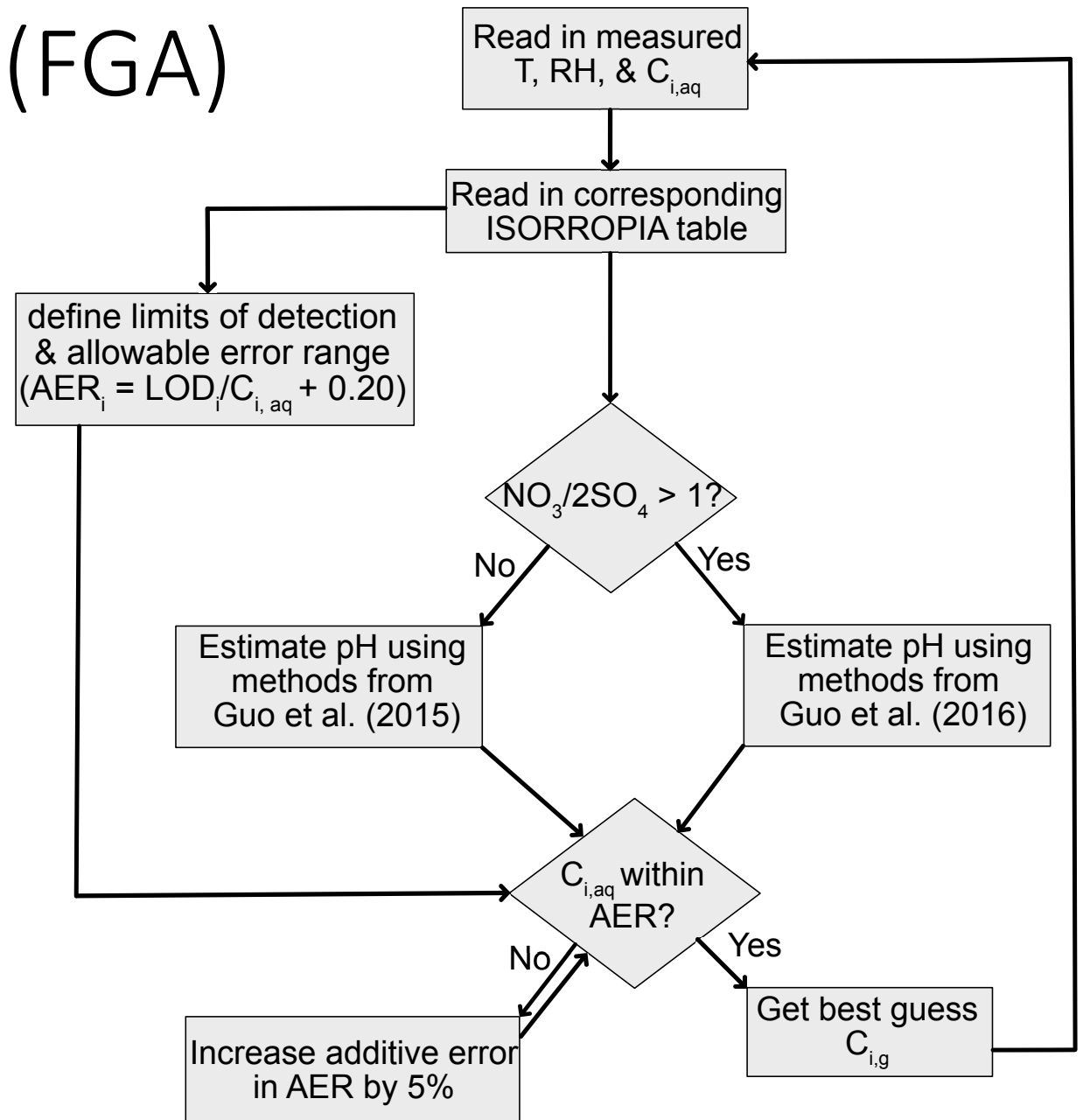


Avery et al. *Environmental Science: Processes & Impacts*, 2019

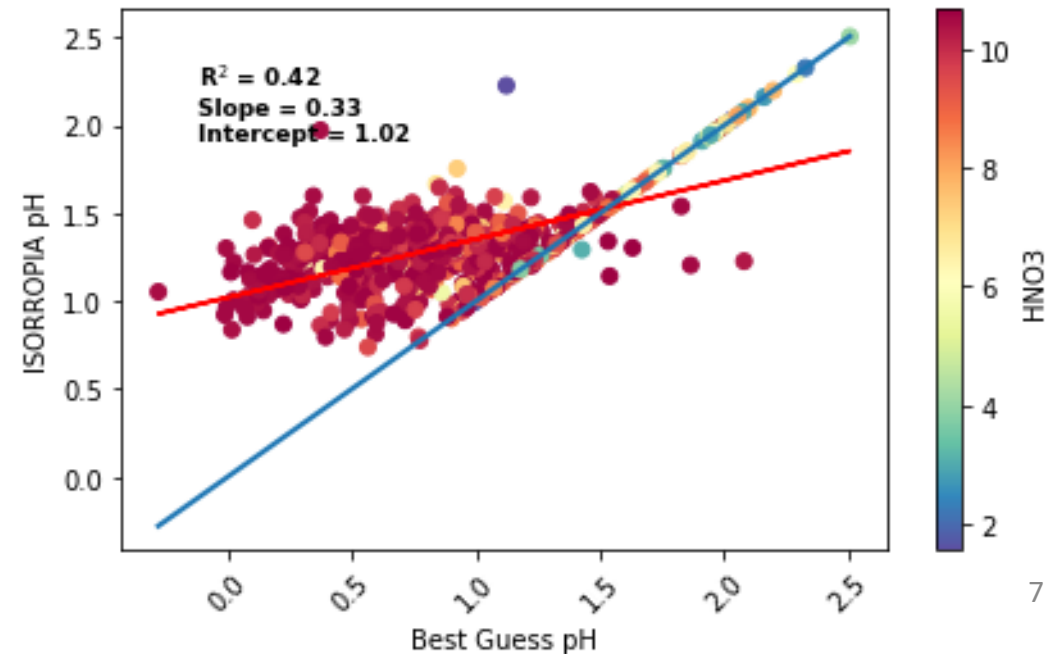
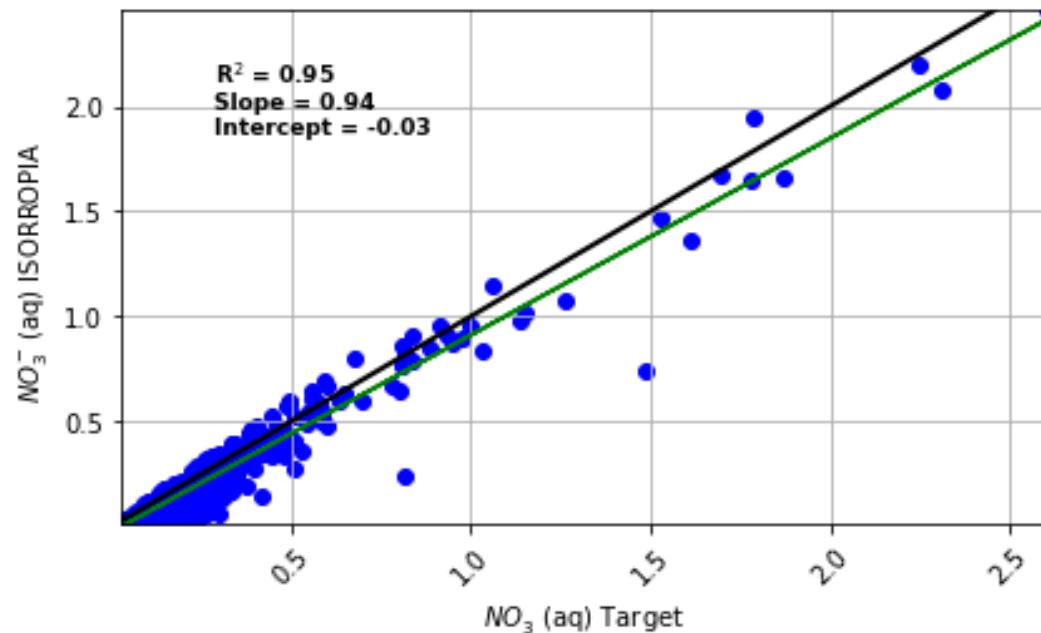
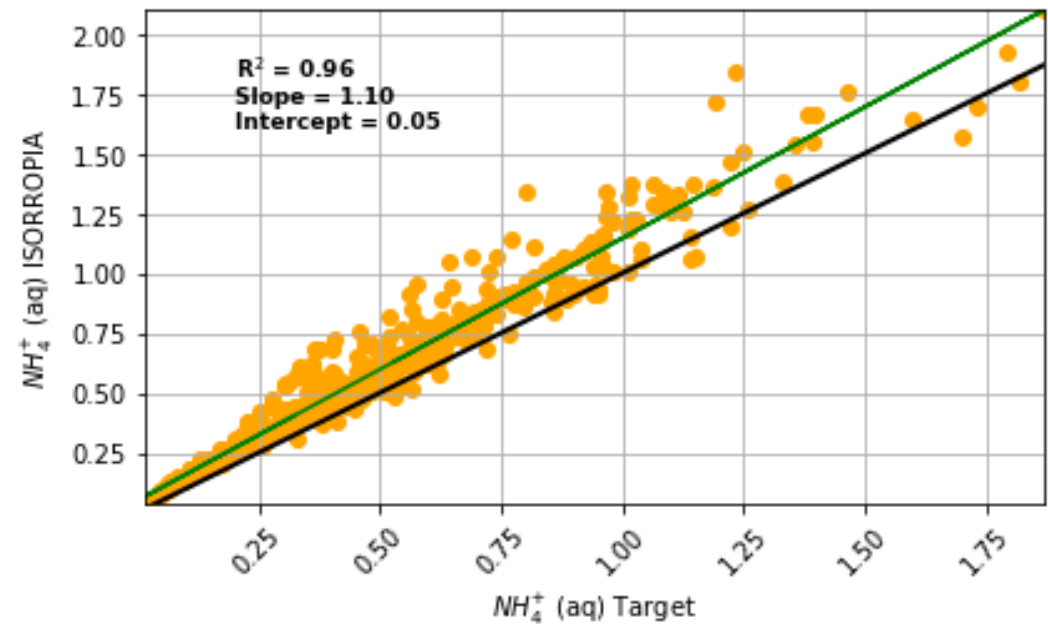
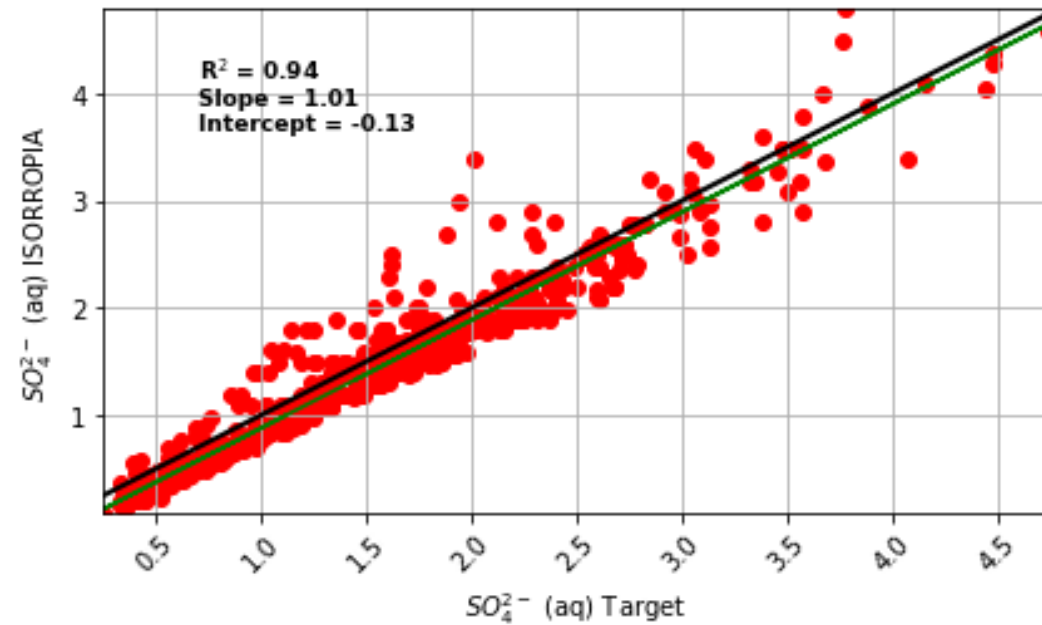
Find Gas Phase Algorithm (FGA)



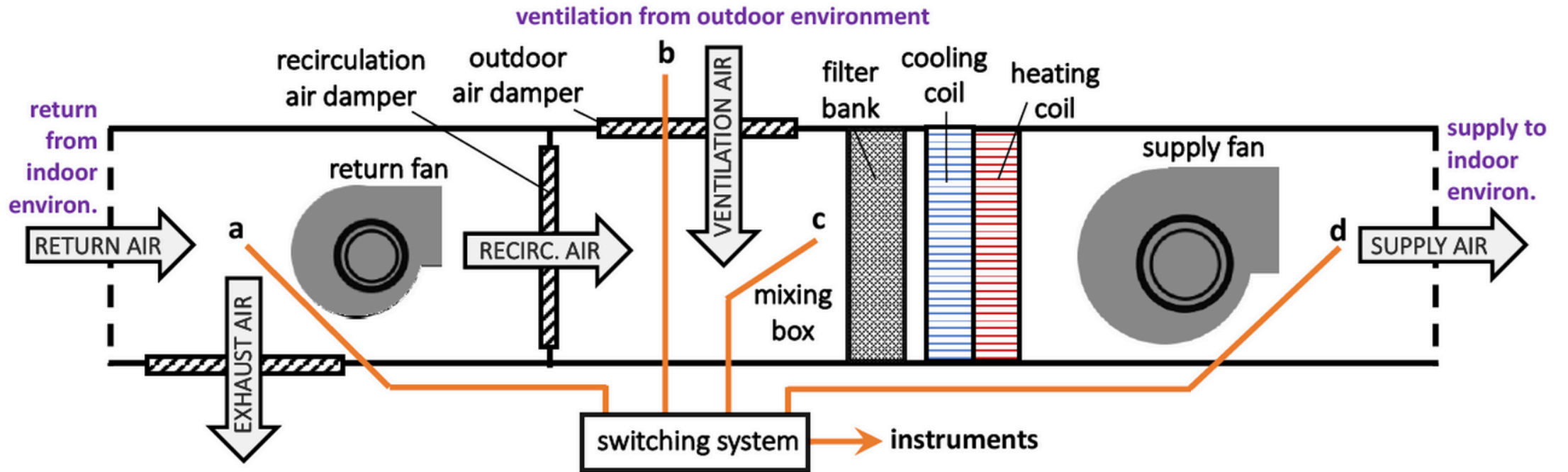
Guo et al., *Journal of Geophysical Research: Atmospheres*, 2016



FGA Evaluation | summer episode

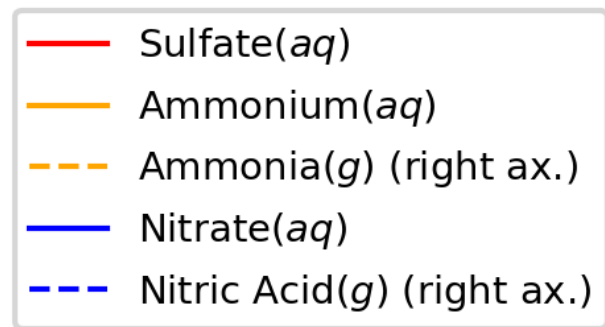


HVAC Thermodynamics

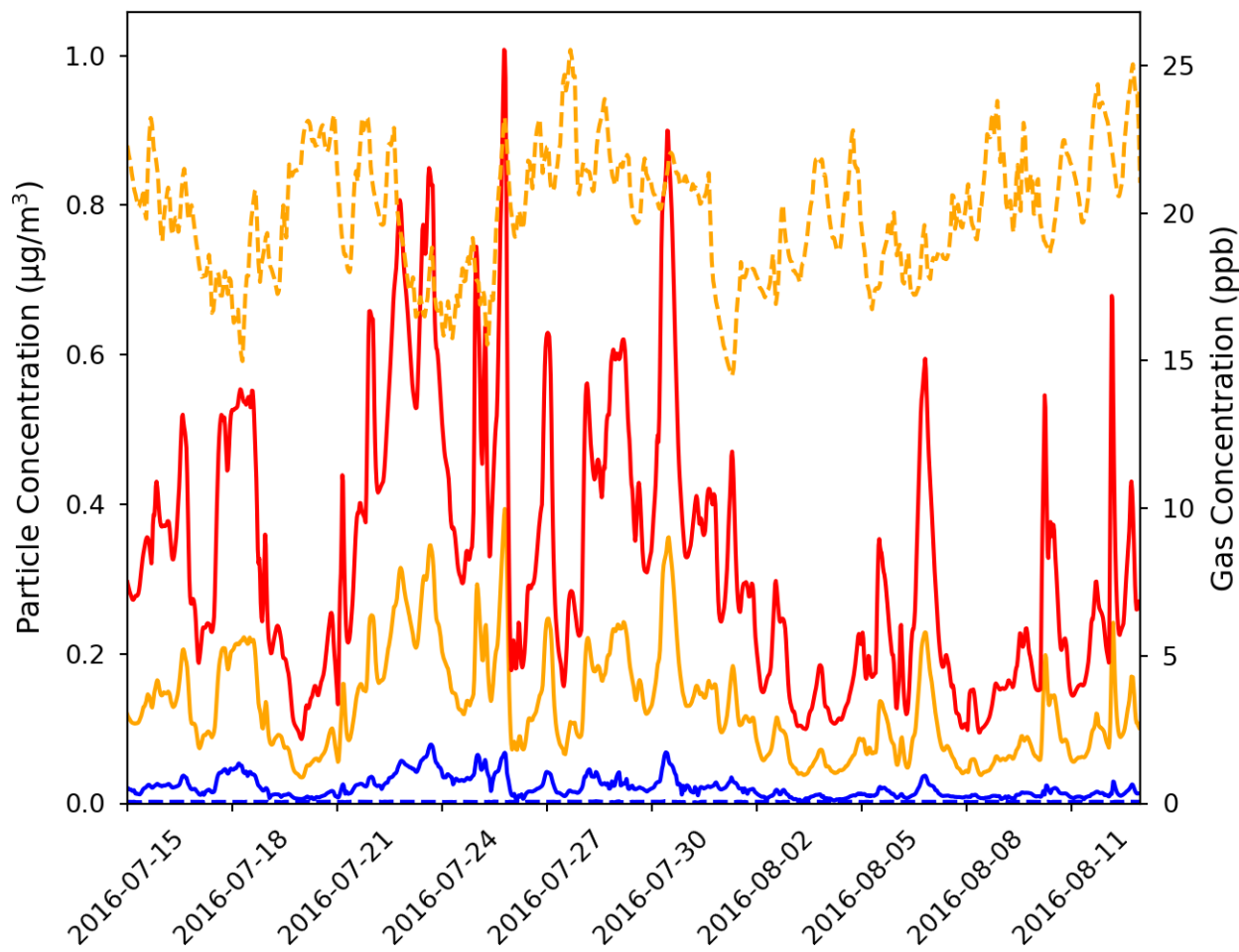


- Indoor aerosol will maintain an aqueous phase in the summer, but not in the winter
- Deliquescence is encouraged by warm air and particles being cooled down
- Efflorescence is encouraged by cold air and particles being warmed up
- A 75% HNO_3 loss to the cooling coil was used and based on a parametric test
- A filter efficiency of 10% and 30% for the summer and winter respectively was used

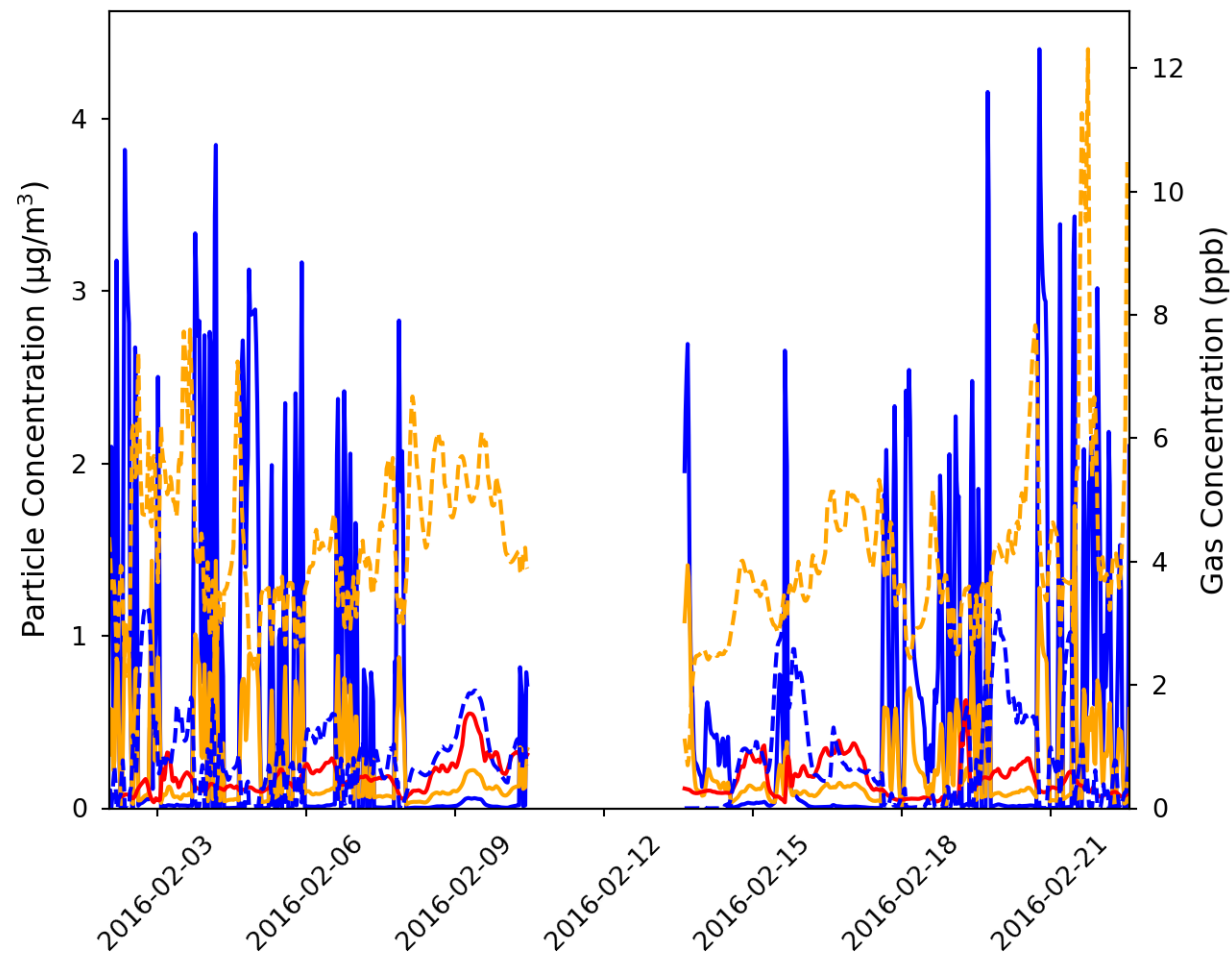
Indoor Modeled Concentrations



summer episode

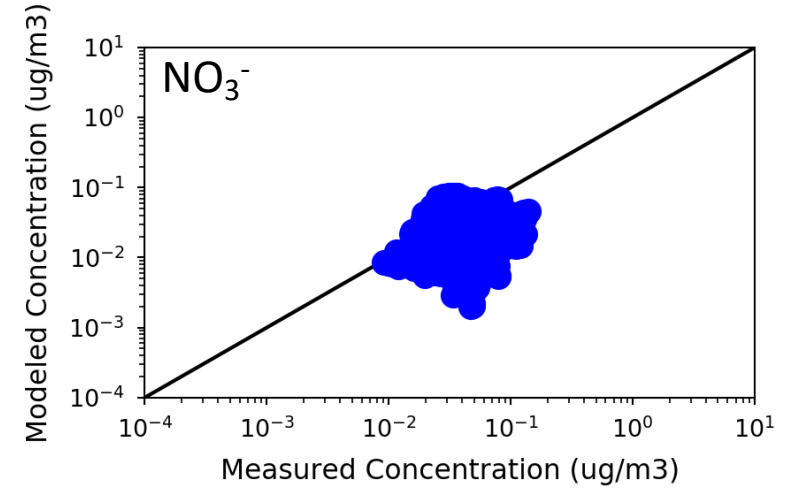
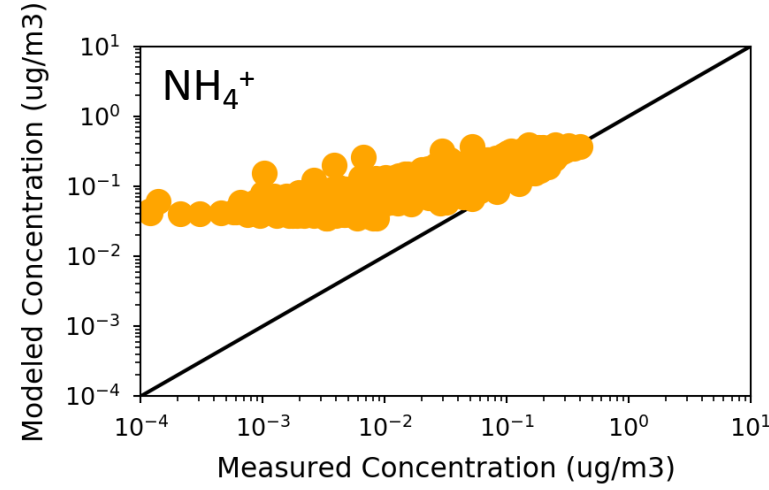
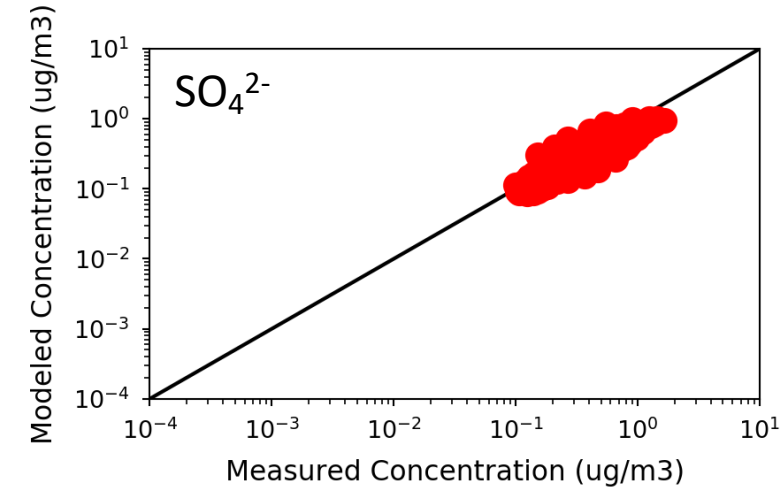


winter episode

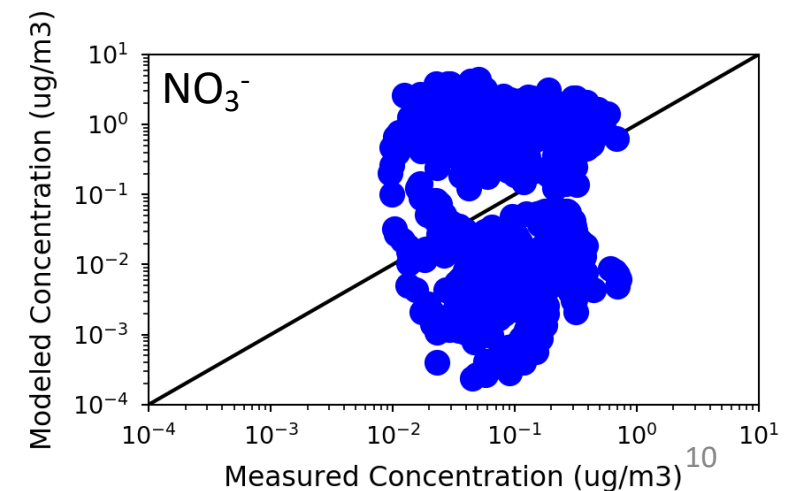
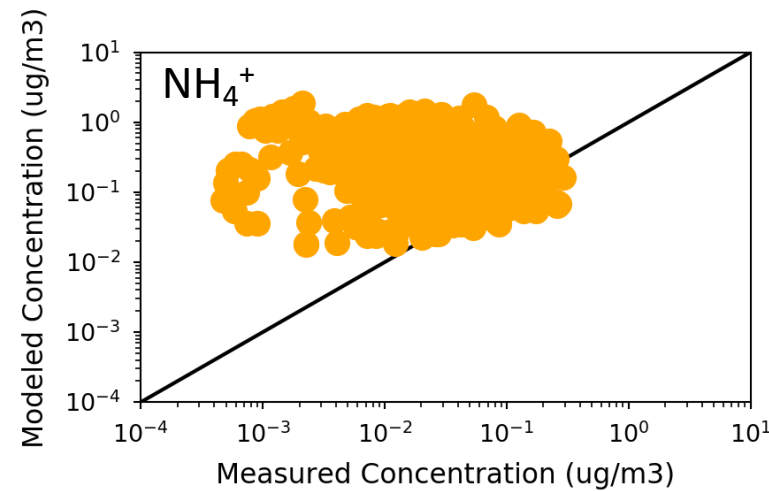
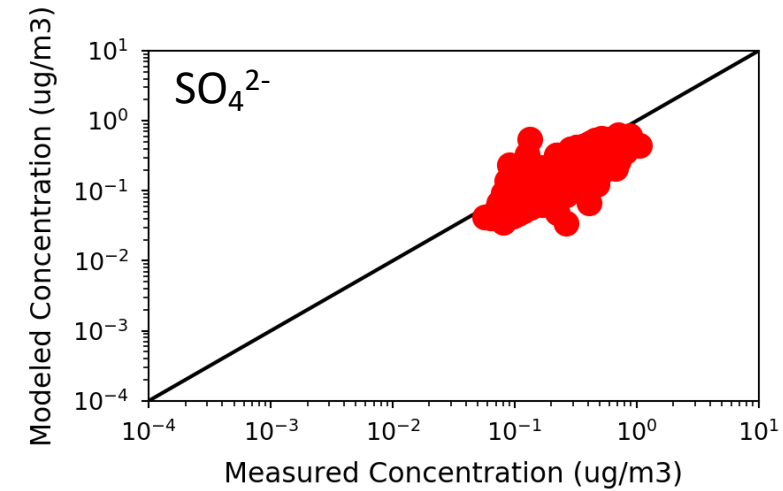


Comparison of Modeled & Measured Concentrations

summer episode



winter episode



Indoor-outdoor Ratio Behavior

$$[I/O]_{i/SO_4} = \frac{[I/O]_i}{[I/O]_{SO_4}}$$

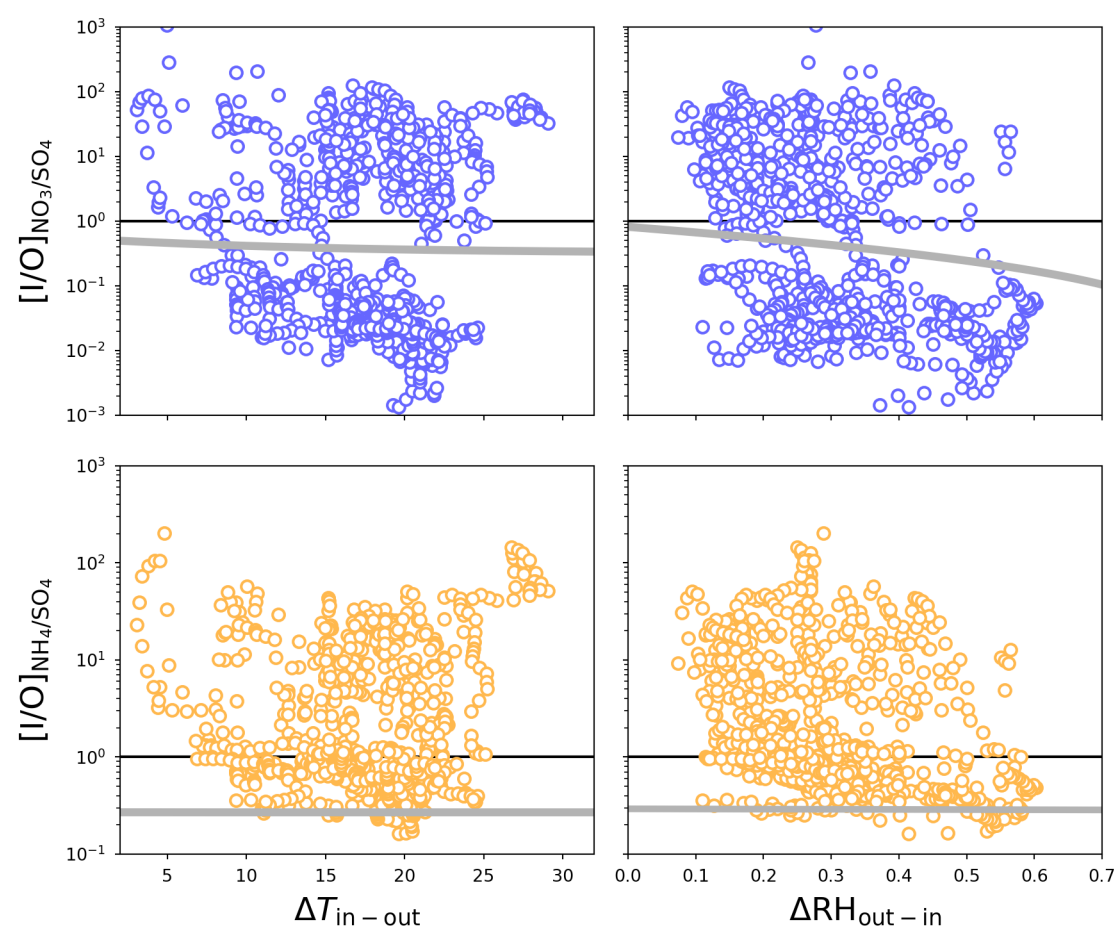
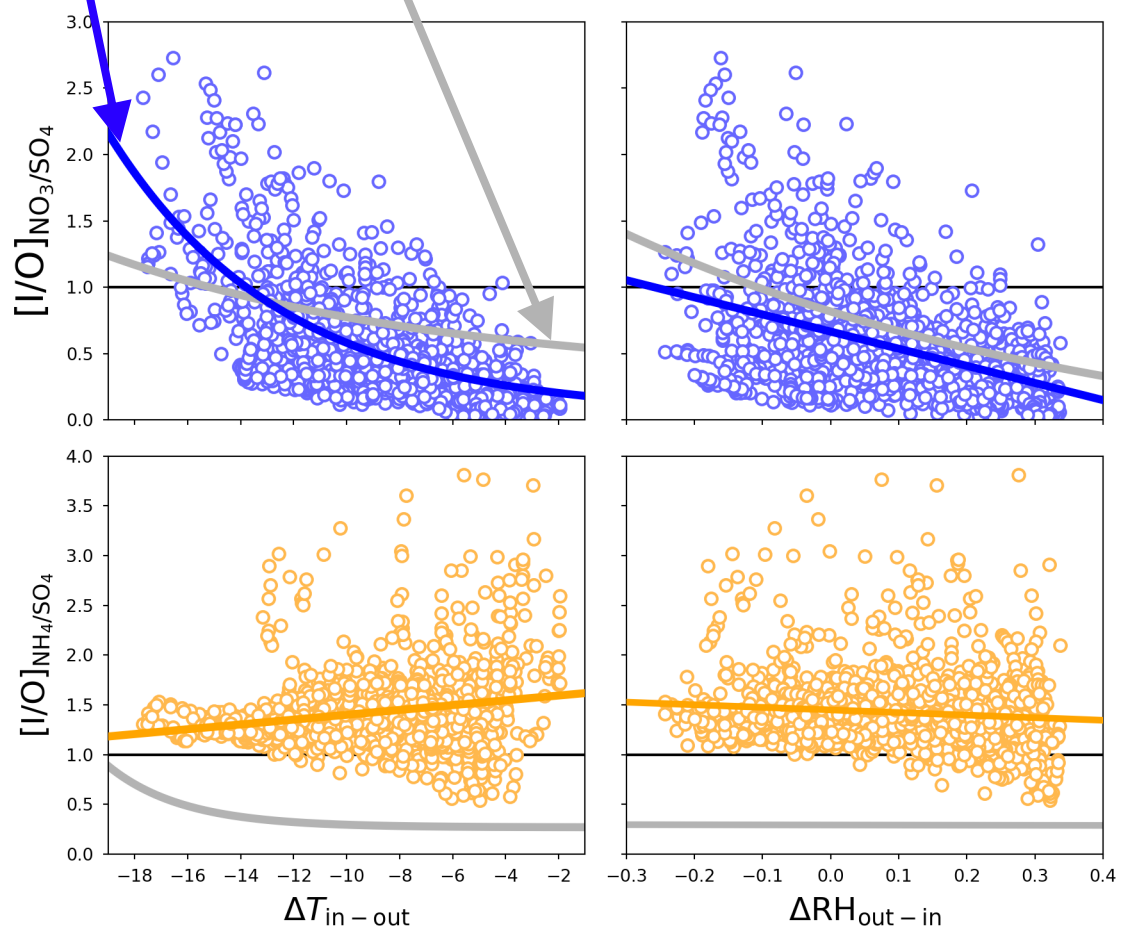
Johnson et al., Indoor Air, 2017

modeled
best fit

measured
best fit

Summer

Winter



Future Work & Summary

- Assessing model sensitivity to indoor ammonia sources (such as from third hand smoke) is ongoing
- ISORROPIA was integrated into an indoor aerosol model to predict IA partitioning for the first time
- Modeling IA partitioning in the winter could be more complicated or the FGA is only applicable to the summer set
- Serves as proof of concept towards exploring how heating, ventilating, and air-conditioning (HVAC) systems influence indoor aerosol composition and chemical processing, with a focus on indoor aerosols of outdoor origin, using ISORROPIA

Thank you!

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**ALFRED P. SLOAN
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