F0AM Model with ISORROPIA and CMAQ 5.3.2 Aerosol Module Integration

Development of a 0D box model framework to compare CMAQ to laboratory findings

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Motivation

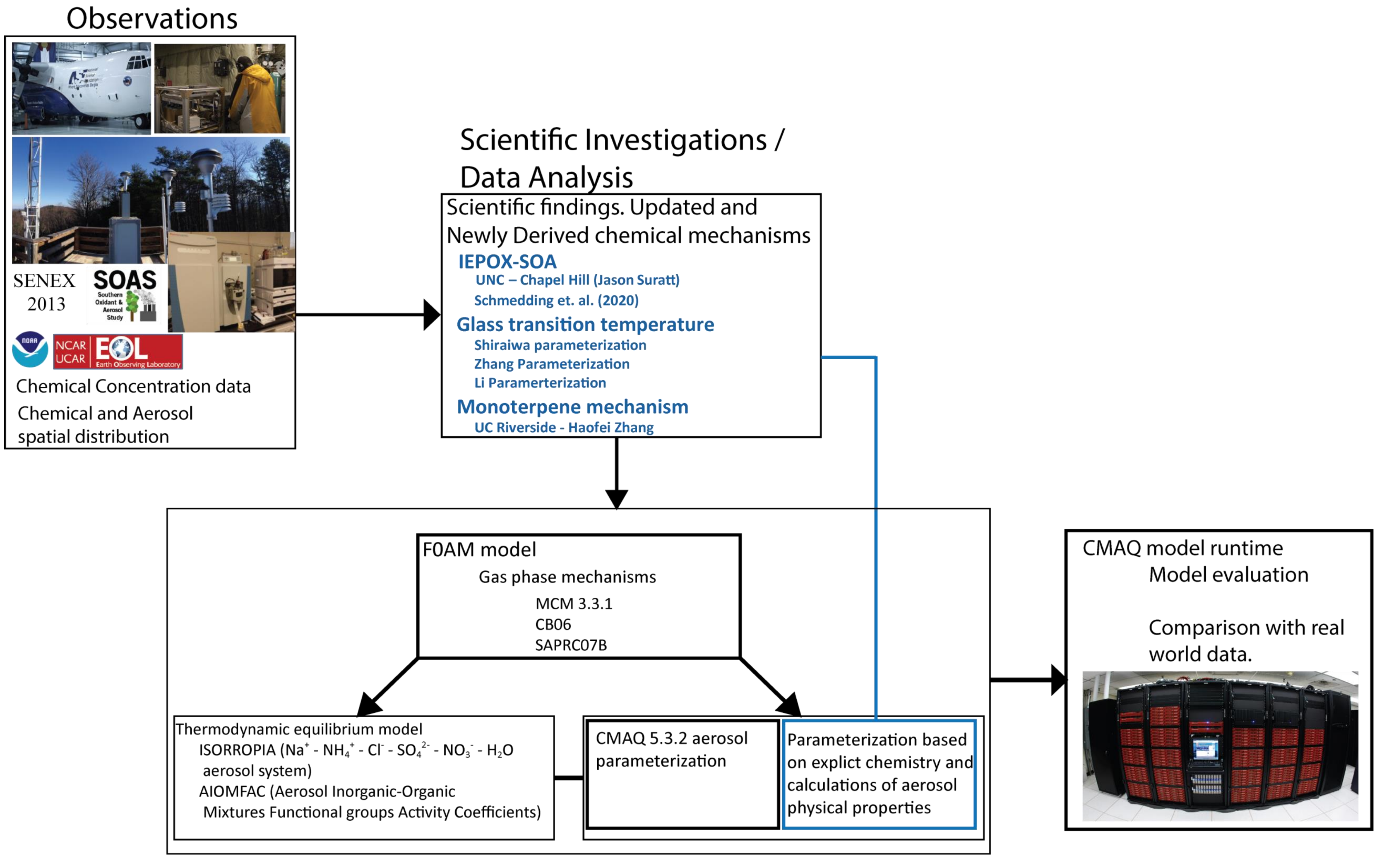
- To have a test 0D framework for adjustments or updates to the multiphase chemistry within regional models or global models
  - Reduce computational expense
  - Easier for other disciplines to add their input in the form of explicit mechanisms found from laboratory work.
- Design goals…
  - Integrate and validate the performance of ISORROPIA II
  - Equivalent performance of CMAQ, other explicit models

What is the F0AM model: model capabilities as a framework

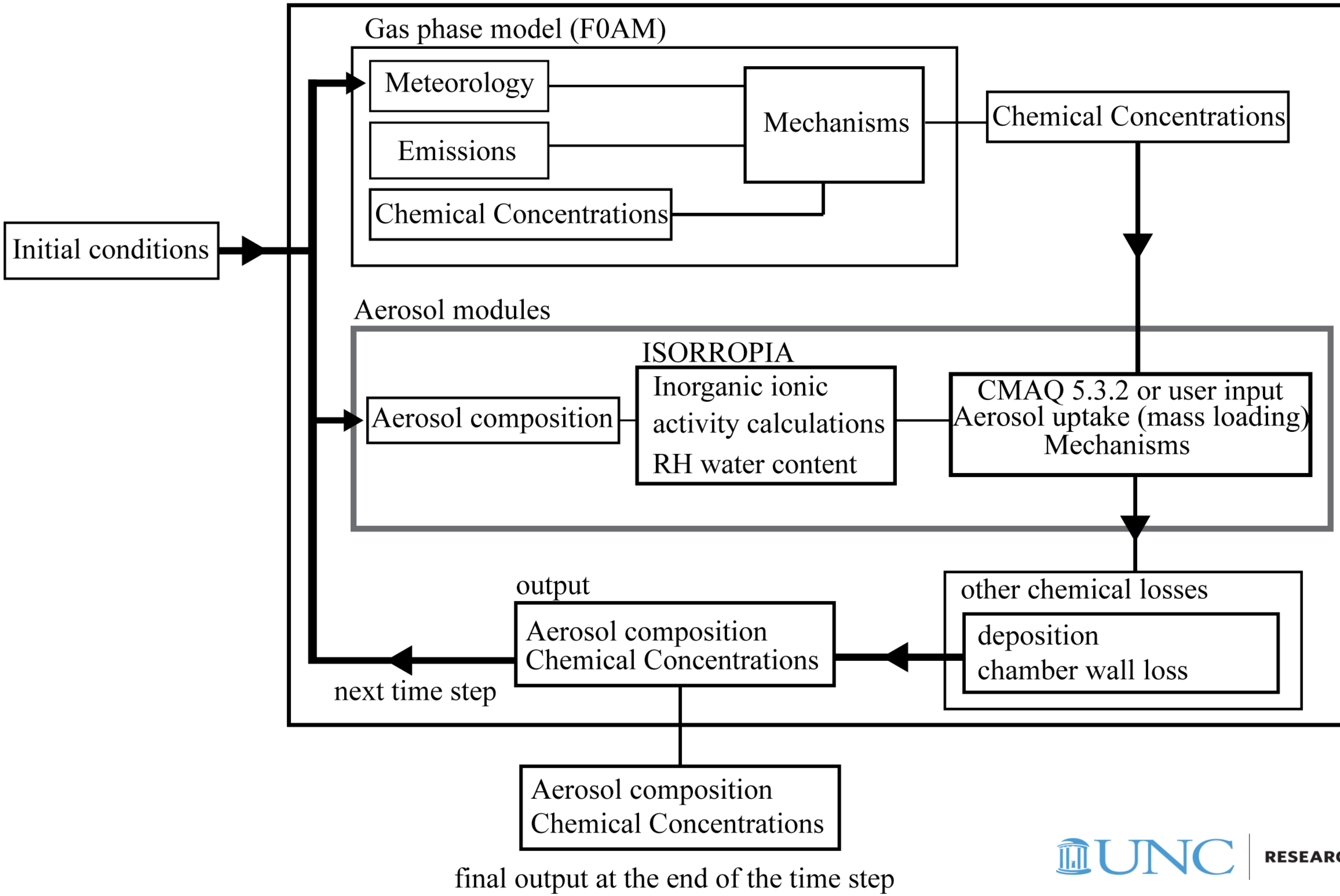
- Gas phase chemistry
  - The model simulates processes at a single point in space. You can think of this point as a uniform box, 0D (homogenously mixed)
  - It does NOT explicitly simulate transport or mixing processes.
  - User specifies a set of initial conditions and Chemical mechanism
    - **Chemical Concentrations** (ppmv)
    - **Meteorology** (j values (actinic flux vs. wavelength) or other photolysis related, solar azimuth, Pressure (mbar), Temperature (K), Water vapor number density (molec•cm^{-3}) or RH %)
    - Emissions/Deposition
    - Aerosol (organic / inorganic) number density (#/cm^3), **surface area density** (cm^2/cm^3)
    - Mechanisms

Wolfe, G. M., M. R. Marvin, S. J. Roberts, K. R. Travis, and J. Liao (2016), The Framework for 0-D Atmospheric Modeling (F0AM) v3.1, Geosci. Model Dev., 9, 3309-3319, doi:10.5194/gmd-9-3309-2016.

https://sites.google.com/site/wolfegm/models


Observations
SENEX 2013
SOAS Southern Oxidant & Aerosol Study
NCAR UCAR
EOL Earth Observing Laboratory
Chemical Concentration data
Chemical and Aerosol spatial distribution
Scientific Investigations / Data Analysis
Scientific findings. Updated and Newly Derived chemical mechanisms
IEPOX-SOA
UNC – Chapel Hill (Jason Suratt)
Schmedding et. al. (2020)
Glass transition temperature
Shiraiwa parameterization
Zhang Parameterization
Li Paramerterization
Monoterpene mechanism
UC Riverside - Haofei Zhang
F0AM model
Gas phase mechanisms
MCM 3.3.1
CB06
SAPRC07B
Thermodynamic equilibrium model
ISORROPIA (Na^+ - NH_4^+ - Cl^- - SO_4^{2-} - NO_3^- - H_2O aerosol system)
AIOMFAC (Aerosol Inorganic-Organic Mixtures Functional groups Activity Coefficients)
CMAQ 5.3.2 aerosol parameterization
Parameterization based on explict chemistry and calculations of aerosol physical properties
CMAQ model runtime
Model evaluation
Comparison with real world data.

F0AM 4.1.1 0D box model + ISORROPIA, CMAQ 5.3.2 aerosol mechanism



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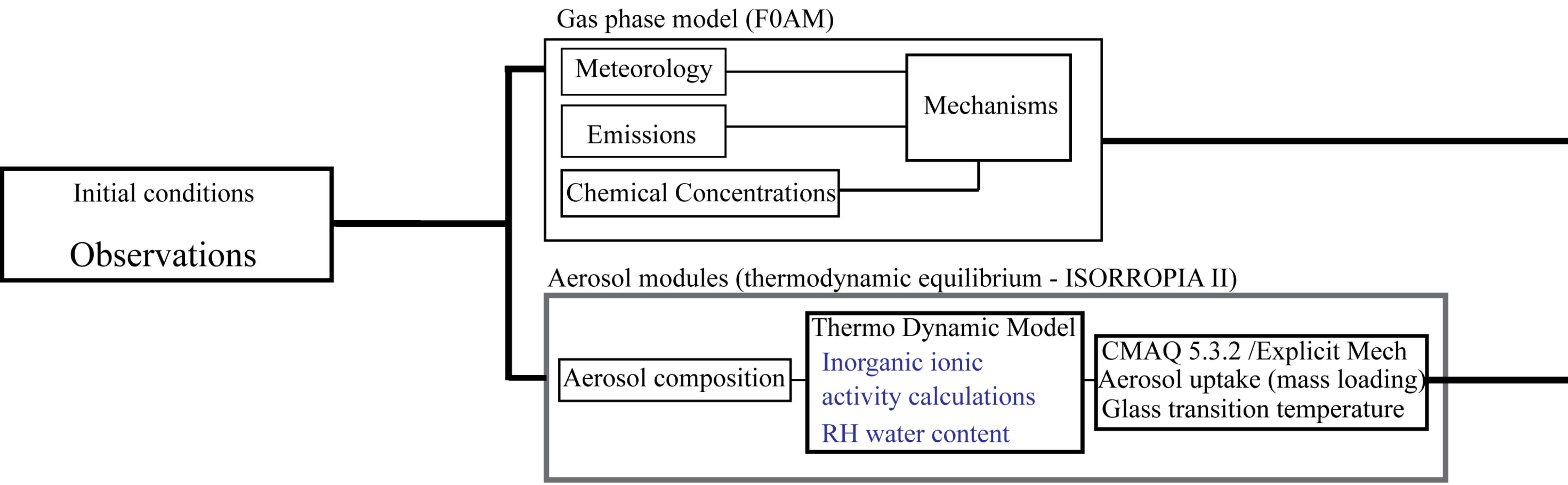
F0AM 4.1.1 0D box model + ISORROPIA (Thermodynamic Model), CMAQ aerosol mechanism



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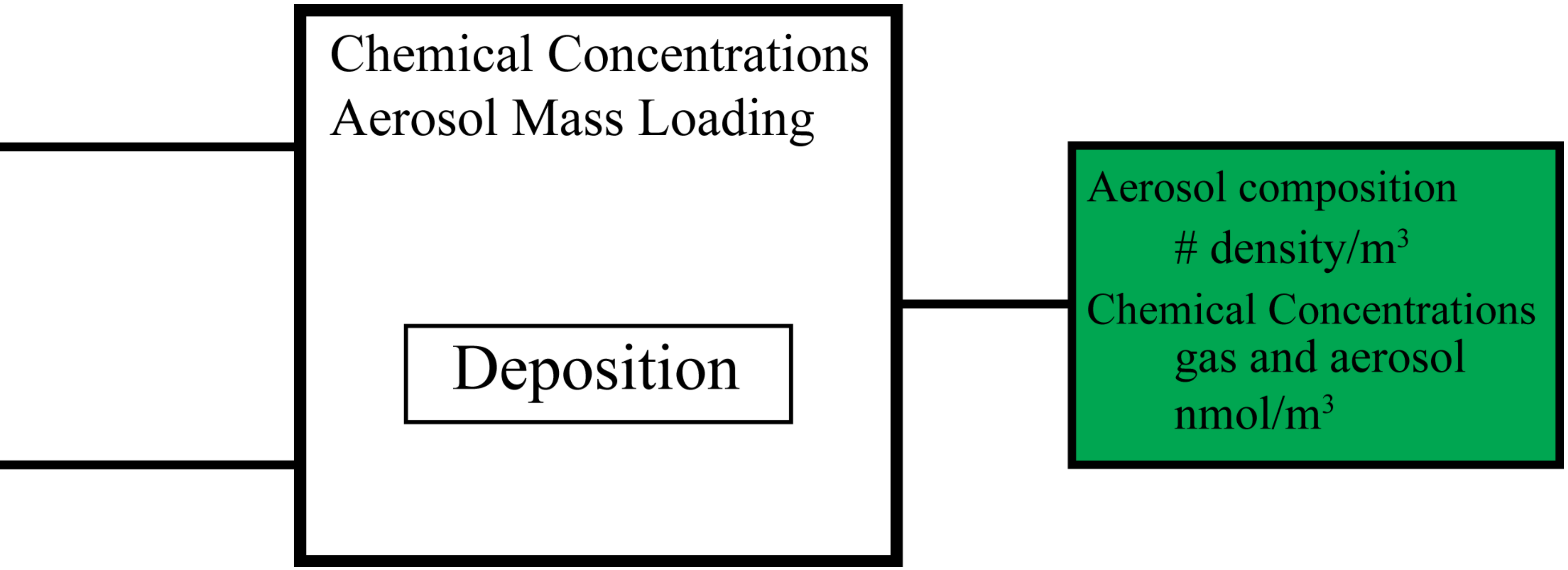
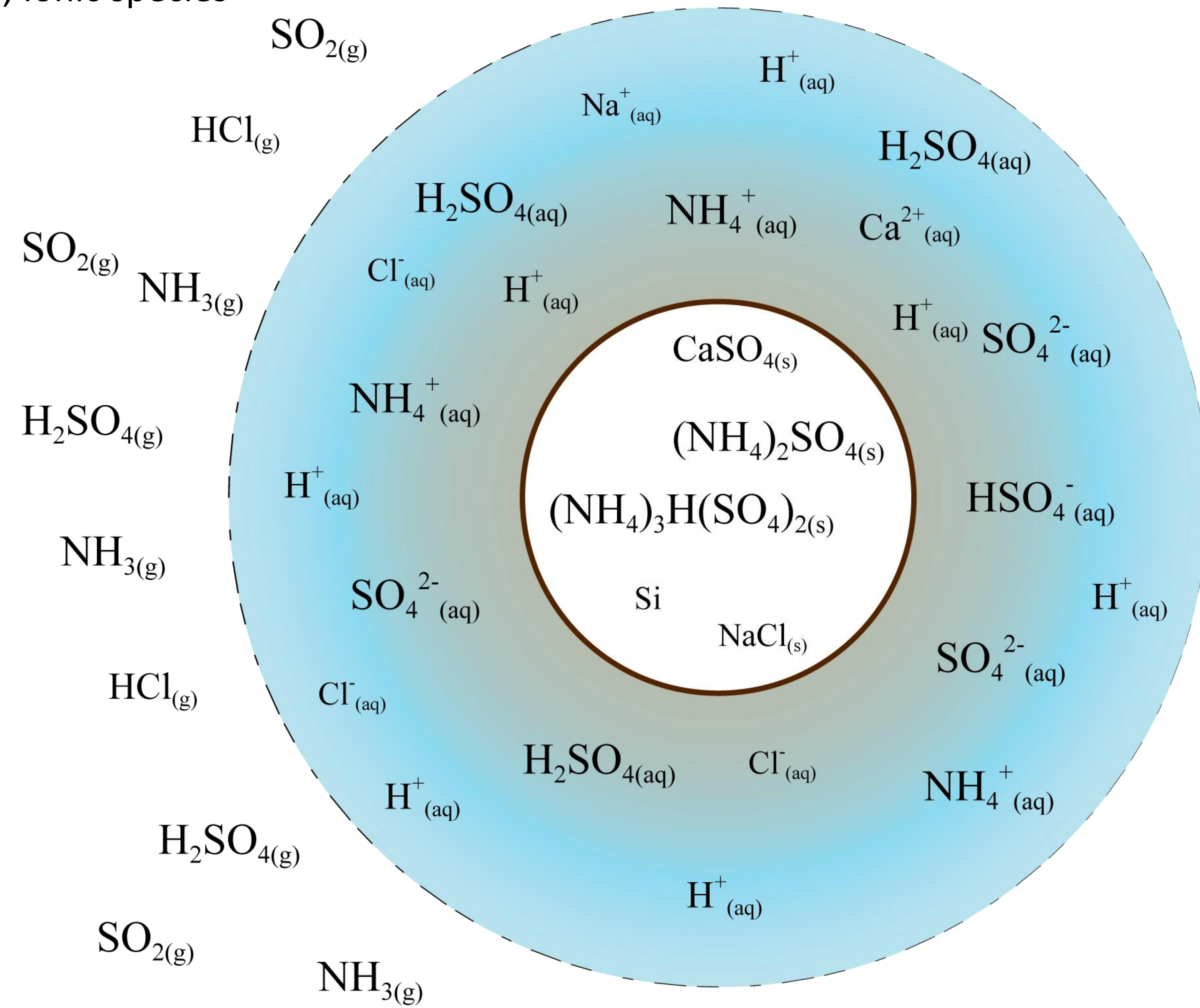
F0AM 4.1.1 0D box model + ISORROPIA (Thermodynamic Model), CMAQ aerosol mechanism



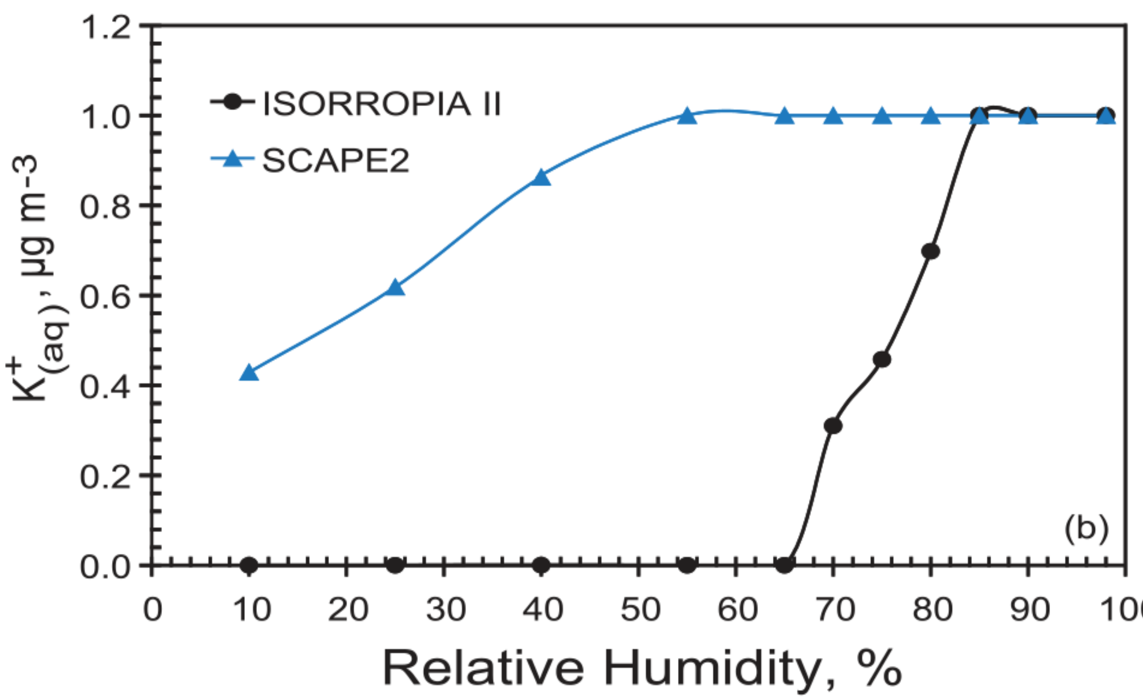
ISORROPIA II (K^{+} - Ca^{2+} - Mg^{2+} -Na^{+} - NH_4^{+} - Cl^{-} - SO_4^{2-} - NO_3^{-} - H_2O aerosol system)

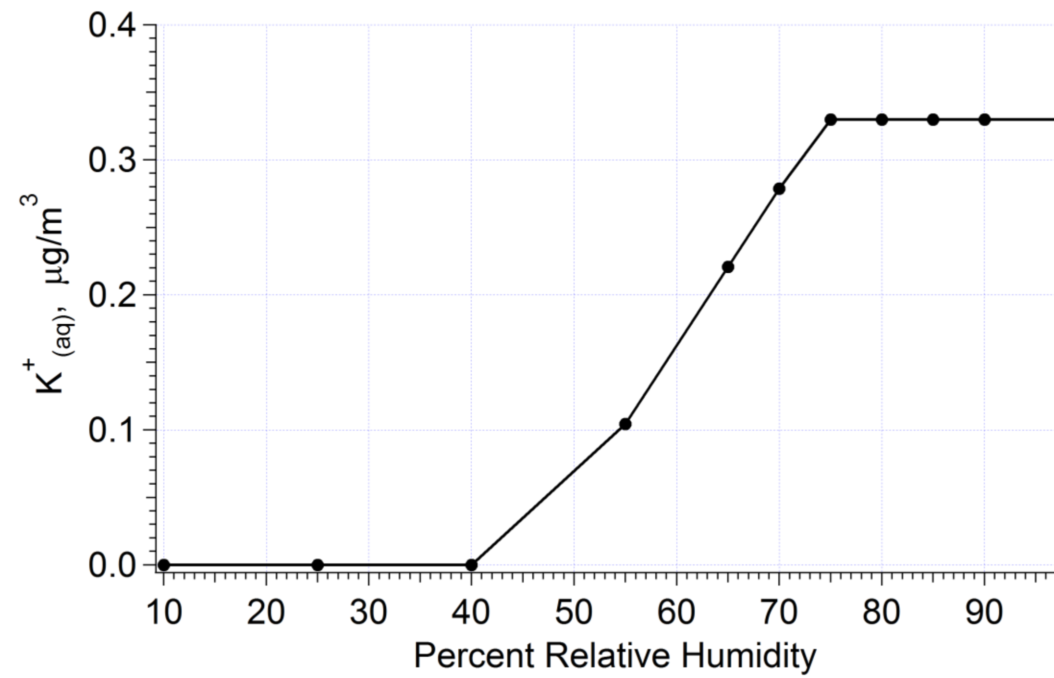
- Resulting Output for inorganic chemical species
- Mass loading onto aerosol (nmol/m^3), Ionic species
- Remainder solid and gas phase

The multiphase equilibrium for more than 45 ionic chemical species is determined by the thermodynamic model based on v 2.2 translated to MATLAB script



Preliminary Tests and Validation





Fountoukis, C., and A. Nenes (2007), ISORROPIA II: a computationally efficient thermodynamic equilibrium model for aerosols, *Atmospheric Chemistry and Physics, 7(17), 4639-4659.*

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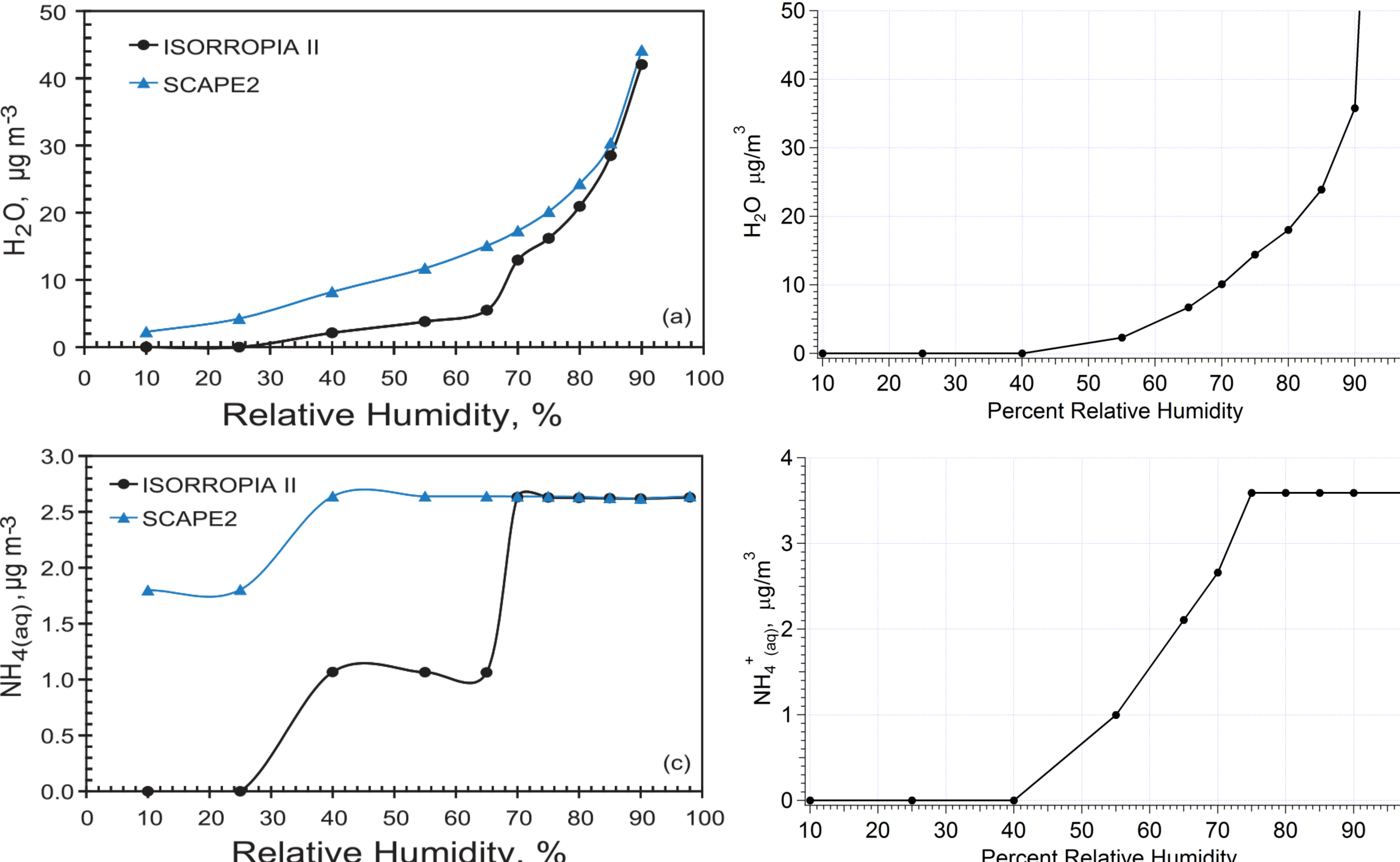

ISORROPIA II
SCAPE2
H2O, µg m-3
Relative Humidity, %
(a)
H2O µg/m3
Percent Relative Humidity
NH4(aq), µg m-3
(c)
NH4+(aq), µg/m3

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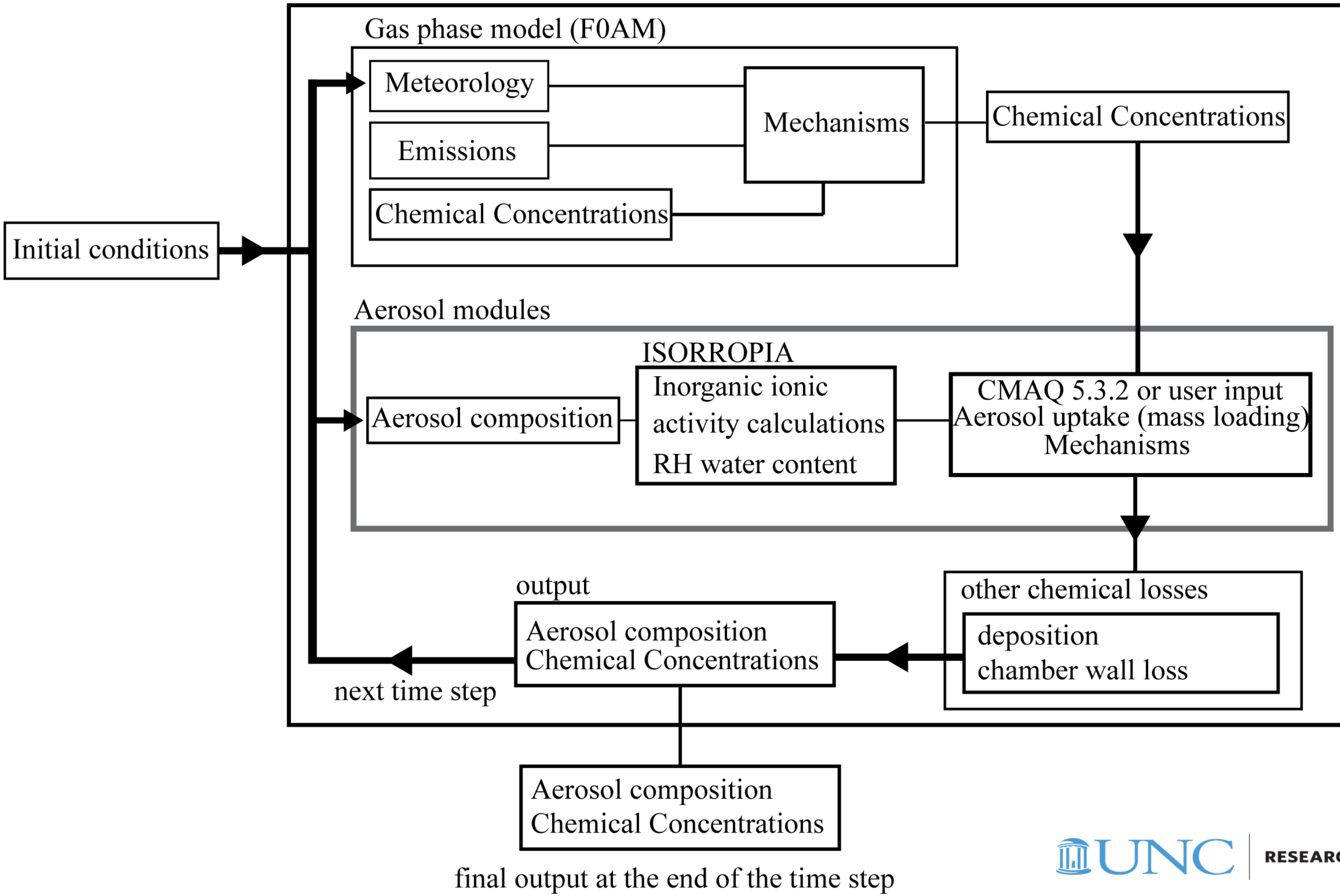

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Motivation : Performing an explicit determination of IEPOX SOA formation to compare to CMAQ

Reaction Probability or reactive uptake coefficient (γ_{IEPOX}) – **model relevant parameter**

$$IEPOX_{(g)} \xrightarrow{k_{het}}$$

$$k_{het} = \gamma_{IEPOX} S_a \omega / 4$$

$$IEPOX_{(aq)} + H^+ + H_2O \longrightarrow 2\text{-}MT + H^+ \quad k_1$$

$$IEPOX_{(aq)} + H^+ + SO_4^{2-} \longrightarrow MTS^- \quad k_2$$

$$IEPOX_{(aq)} + H^+ + 2\text{-}MT \longrightarrow 2\text{-}MT\ dimer + H^+ \quad k_3$$

$$IEPOX_{(aq)} + H^+ + MTS^- \longrightarrow MT\text{-}OS\ dimer^- + H^+ \quad k_4$$

$$IEPOX_{(aq)} + H^+ + MTS^- \longrightarrow other\ oligomers^- + H^+ \quad k_5$$

$$IEPOX_{(aq)} \longrightarrow Volatiles \quad k_6$$

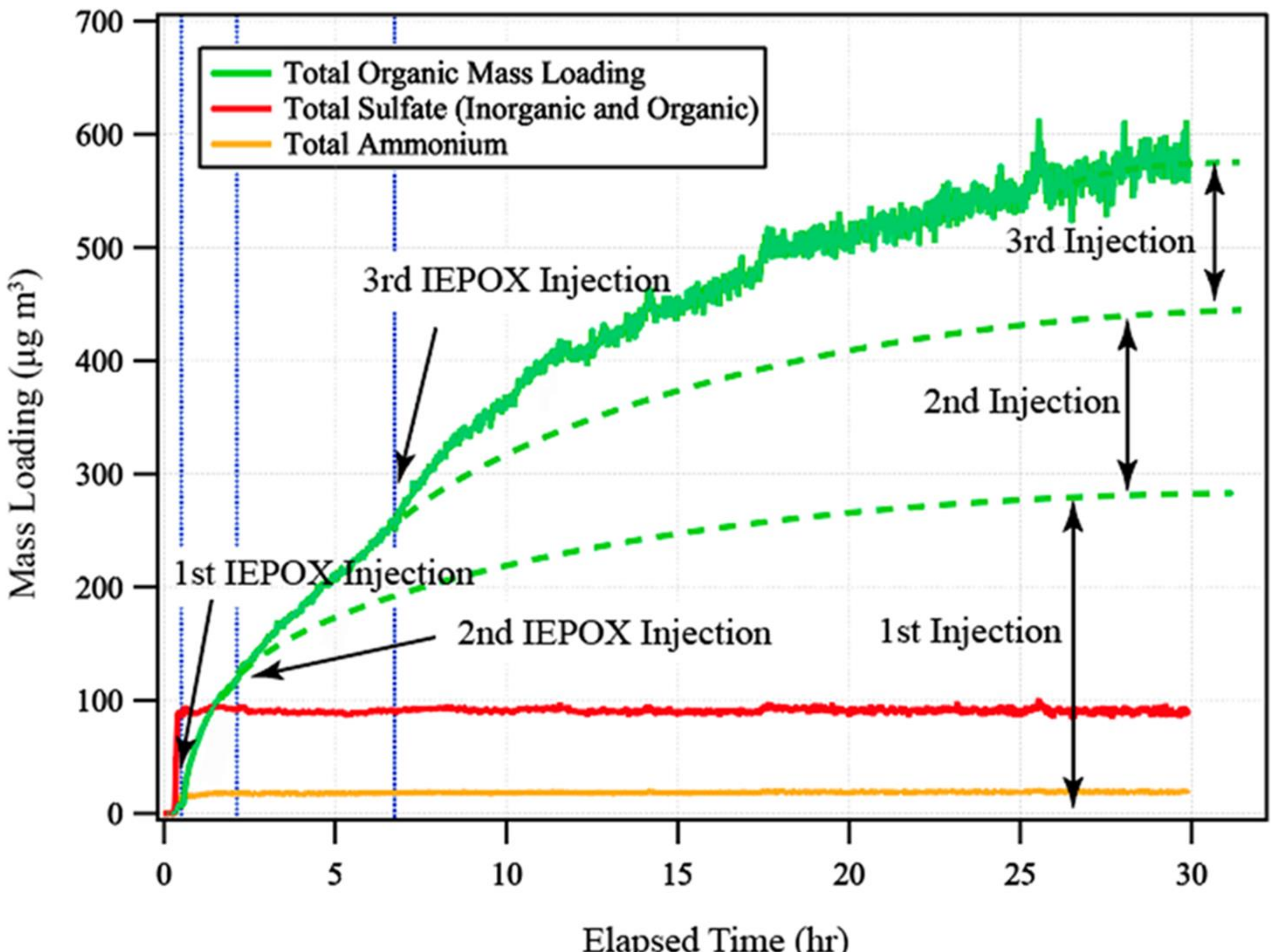
Aerosol Phase

To constrain

Key Assumptions:

- Homogenous aerosol-phase
- Constant aerosol-phase acidity
- Constant uptake coefficient γ_{IEPOX} from previous flow tube measurements

Dissertation: Characterizing the Effects of Aerosol Sulfate, Phase State and Aging on Atmospheric Secondary Organic Aerosol Formation from Isoprene Epoxydiols , Chen, Yuzhi, 2021, ISBN 9798516059315



Zhang, Y.; Chen, Y.; Lei, Z.; Olson, N. E.; Riva, M.; Koss, A. R.; Zhang, Z.; Gold, A.; Jayne, J. T.; Worsnop, D. R., Joint Impacts of Acidity and Viscosity on the Formation of Secondary Organic Aerosol from Isoprene Epoxydiols (IEPOX) in Phase Separated Particles. *ACS Earth and Space Chemistry* ***2019, 3 (12), 2646-2658.***

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Future Work

- 0D box model runs to compare aerosol speciation using CMAQ 5.3.2 parameterization vs updated IEPOX chemical mechanisms.
- Addition of AIOMFAC (Aerosol Inorganic-Organic Mixtures Functional groups Activity Coefficients)