McNeill Group: Atmospheric Chemistry, Air Pollution, and Climate

http://mcneill-lab.org

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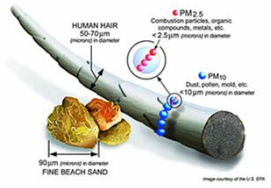
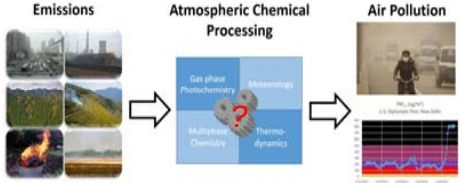
Atmospheric Aerosols

- Condensed-phase particles suspended in a gas
- Diameters range from a few nm to tens of µm
  - EPA regulates particles below 10 µm in diameter[1]
- Human health, air quality, and climate effects due to ability to penetrate deep within lungs, scatter and absorb light, and act as cloud condensation nuclei (CCN)



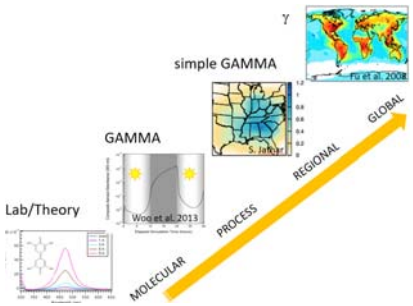
Atmospheric Chemistry and Air Quality

There is a complex, *nonlinear*, incompletely understood connection between pollution sources & air quality. We perform lab and modeling studies to elucidate that connection between human activities, air quality, and climate.



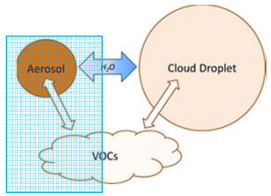
Lab activities provide molecular-level kinetic and mechanistic information about atmospheric processes.

McNeill group modeling activities bridge the scale between the molecular-level information obtained in laboratory studies, and the regional and global scales



Aqueous Aerosol SOA (aaSOA)

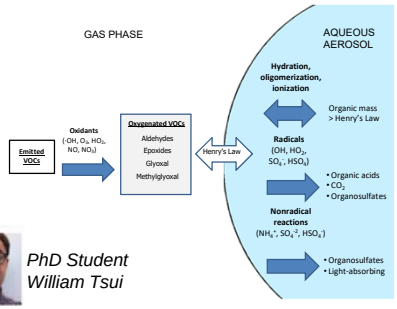
- Water-soluble VOC uptake into aerosol water followed by particle-phase reactions yield low-volatility material
- Evidence from the field:
  - Correlation of water-soluble organic carbon (WSOC) with aerosol liquid water[3]
  - Oligomers, organosulfates
- Likely important in areas with high aerosol sulfate, humidity, and BVOCs (e.g. SE USA)



Gas-Aerosol Model for Mechanism Analysis (GAMMA)

- Photochemical box model with coupled gas and aqueous aerosol chemistry
- Aqueous aerosol-phase SOA formation from gas-phase oxidation of isoprene, acetylene, toluene, xylenes
- Latest mechanisms of aqueous-phase brown carbon and organosulfate formation incorporated

McNeill et al., *ES&T* (2012)
Woo et al., *Faraday Discuss.* (2013)



PhD Student
William Tsui

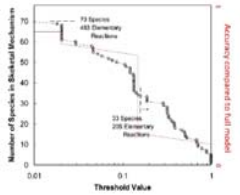
AMORE (Atmospheric Chemistry MOdel REduction)

New EPA-funded project (student needed!)

An efficient and automated approach for updating and condensing atmospheric chemical mechanisms for use in large-scale air quality, atmospheric chemistry, and climate models is needed.

We are developing **AMORE:** An automated tool for flexibly generating accurate reduced chemical mechanisms for use in atmospheric chemistry and air quality models.

Two-step model reduction: graph theory-based strongly-connected component analysis followed by simplified quasi-steady state analysis



Clean Air Toolbox for Cities Initiative

http://aqtoolbox.org @aqtoolbox

Prof McNeill is leading a cross-campus initiative for solutions-oriented on **clean air in India and Africa.**

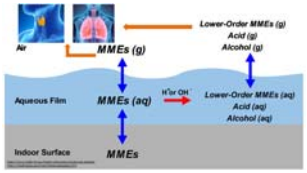
Pilot activities involving low-cost air pollution monitoring field work, data science, and capacity-building are taking place in 10 cities across sub-Saharan Africa and India

Phthalates and Indoor Air Quality

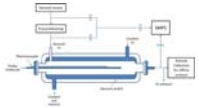
PhD Student
Do Young Maeng

- Man-made esters (MMEs) are abundant in indoor air,[8] as they are commonly used in consumer products and building materials.
- Various MMEs themselves are harmful to human health, but they can also undergo hydrolysis in damp surfaces and form products even more dangerous to our health.

- To better assess and predict indoor air quality, we:
  - Investigate the kinetics of MME hydrolysis reactions via experimental studies
  - Adapt GAMMA for indoor environments



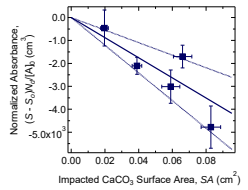
Solar Geoengineering Impact on the Ozone Layer



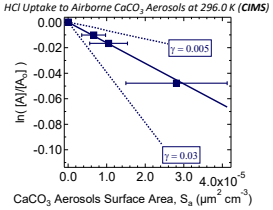
PhD Student
Han Huynh

- Calcite ($CaCO_3$) aerosols were proposed as an alternative to sulfate aerosols to temporarily reduce global temperature with a lower risk of destroying the ozone layer.
- Little experimental data is available for $CaCO_3$ heterogeneous chemistry with stratospheric trace gases (e.g. HNO_3, HCl).
- Using FTIR, we detected absorbed H_2O on $CaCO_3$ surface under dry conditions, leading to $Ca(OH)HCO_3$ structure and to high reactivity with HNO_3 (*0.013 ≤ γ_{HNO3} ≤0.14*) and with HCl (*0.0011 ≤ γ_{HCl} ≤0.012*).
- Using quadrupole CIMS, we determined a high uptake coefficient for HCl (*0.013 ± 0.001*).

*HCl Uptake to Impacted $CaCO_3$ Particles at 296.0 K (**FTIR**)*



*HCl Uptake to Airborne $CaCO_3$ Aerosols at 296.0 K (**CIMS**)*



SOA Formation via Photosensitized Reactions

- Flow tube experiments show particles containing humic acid grow in the presence of VOCs and UV light.
- We will perform chamber experiments in our new, custom-built photochemical reactor for varying, atmospherically relevant temperatures, relative humidities, and photosensitizer and VOC concentrations.