Simulation of Atmospheric Chemical and Physical Processes

Yun Lin[1], Jiaxi Hu[1], Renyi Zhang[1,2]

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Introduction

Zhang's group research has covered a wide variety of areas in atmospheric chemistry and physics and, in particular, the impacts of global air pollution on human health, ecosystems, and climate:

(i) Photochemical oxidation of hydrocarbons emitted from anthropogenic and biogenic sources has major implications for local and regional air quality. We conduct laboratory work to investigate the hydrocarbon oxidation reactions initiated by hydroxyl radical OH and other radical species, focusing on the formation of intermediate radicals and their subsequent degradation reactions. In addition, calculations using quantum chemical and kinetic rate theories are performed to study the structures, energetics, and isomeric branching to assess the preferred pathways of the organic radicals. Our objective is to quantitatively understand the kinetics and mechanism of atmospheric volatile organic compounds (VOCs) and their roles in tropospheric ozone and secondary aerosol formation.

(ii) Aerosols in the atmosphere profoundly impact human health, radiative transfer, weather, and climate. We combine experimental and theoretical approaches to investigate nucleation, growth, and transformation of aerosols at the fundamental molecular level. These include elucidation of the formation of thermodynamically stable clusters from molecular complexes and clusters, the growth of stable clusters to nano- and submicrometer-sized particles, and transformation and properties of submicrometer-sized particles. The chemical and physical properties of aerosols are measured to assess their effects on weather, human health, visibility, and climate.

(iii) We develop state-of-the-art instrumentation to measure trace gaseous compounds and aerosols in the atmosphere. Our instruments have been deployed to study multi-phase atmospheric chemical processes in Houston and Mexico City. Most recently, our team participated in air quality studies in Beijing during the 2008 summer Olympic Games (CAREBeijing-08) and in Guangzhou during the field campaign, the Program of Regional Integrated Experiments of Air Quality in the Pearl River Delta (PRIDE-PRD).

(iv) Air pollutants emitted from anthropogenic and natural sources are transported in the atmosphere while undergoing chemical transformation, affecting human health, agricultural activity, and climate. An understanding of the chemistry and transport of air pollutants is critical for devising strategies to improve urban, rural, and regional air quality. We employ chemical transport models (CTMs) to investigate formation of ozone and particulate matter and air quality on the urban and regional scales. We also investigate aerosol-cloud-climate interaction using cloud-resolving models, mesoscale models as well as global climate models.

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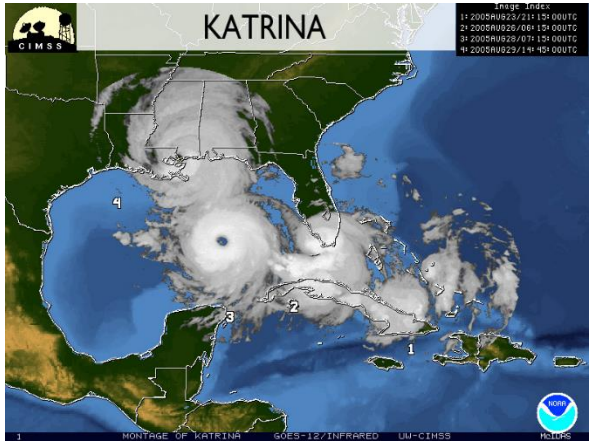
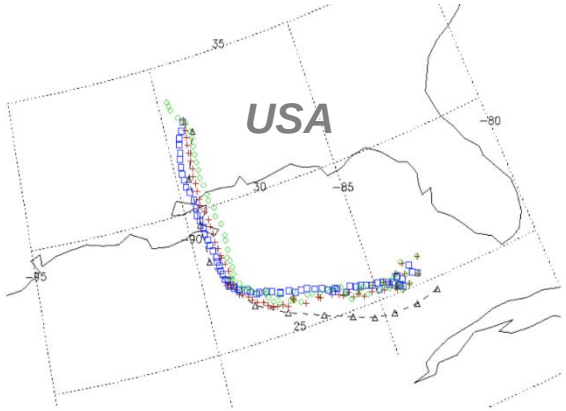
Weather Research & Forecasting Simulations

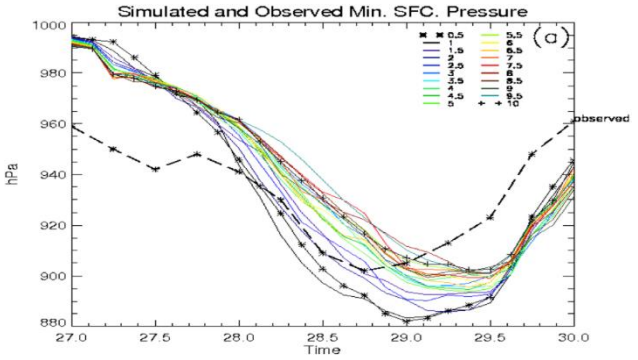
❖ Anthropogenic aerosols effects on tropical cyclones: Hurricane Katrina 2005 as case study

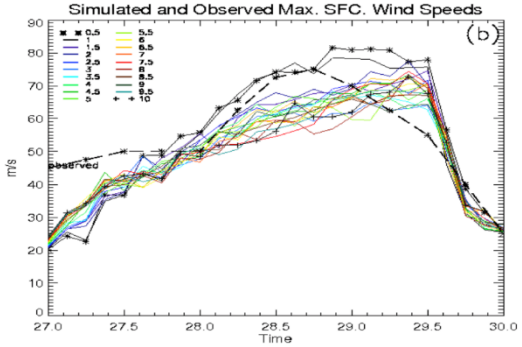
WRF simulations show that the coupled microphysical and radiative effects of anthropogenic aerosols have distinct influences on tropical cyclones, including weakened intensity and early dissipation.





- Time tracks of the observed (black) and simulated hurricane center for C-case (blue), P-case (dark red), and PR-case (green).





- Time evolution of (a) minimum surface pressure and (b) maximum wind speed at the lowest model level for the hurricanes of 20 ensemble simulations. The black line corresponds to the observed values of the hurricane Katrina.

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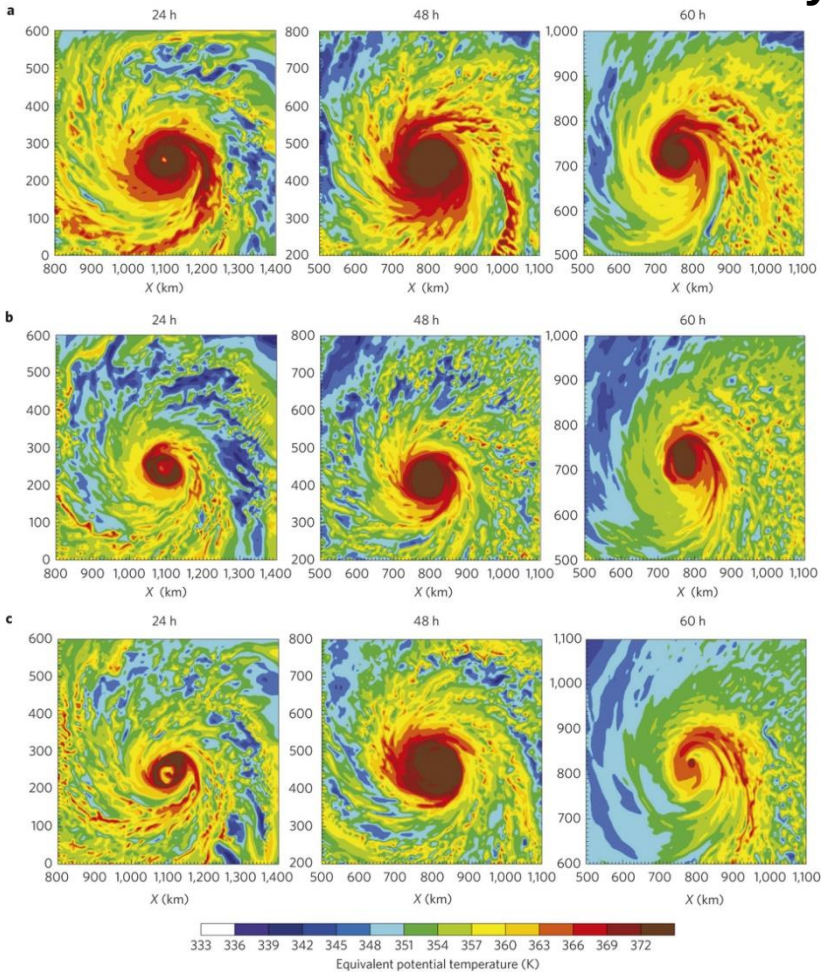
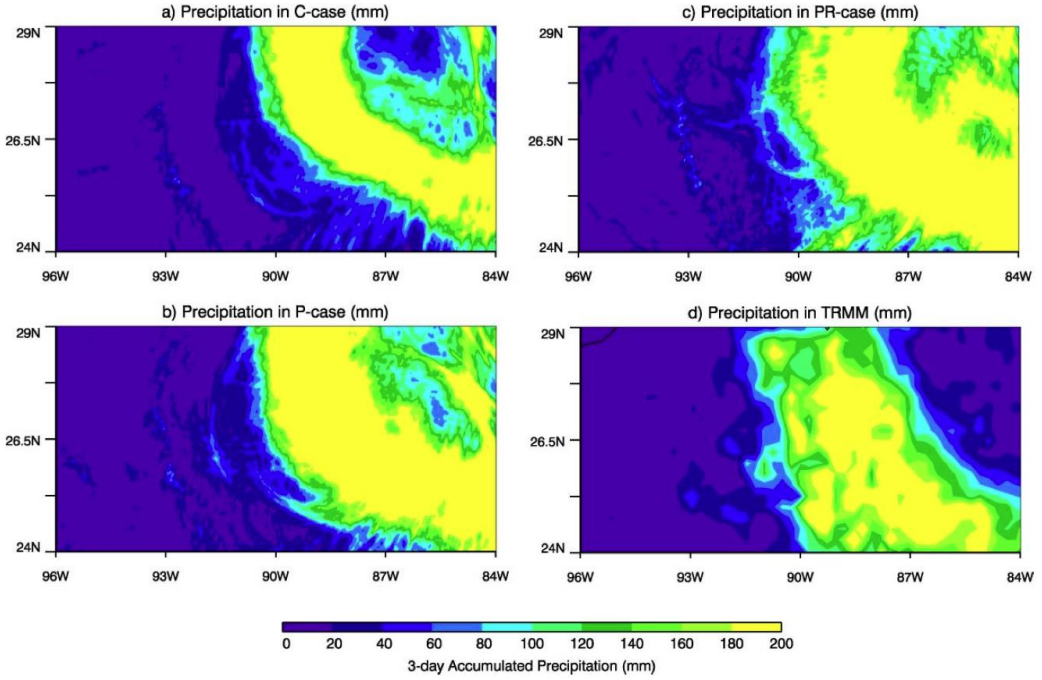
Weather Research & Forecasting Simulations

❖ **Anthropogenic aerosols effects on tropical cyclones: Hurricane Katrina 2005 as case study**





Three-day accumulated precipitation from simulations and TRMM satellite measurement (d).

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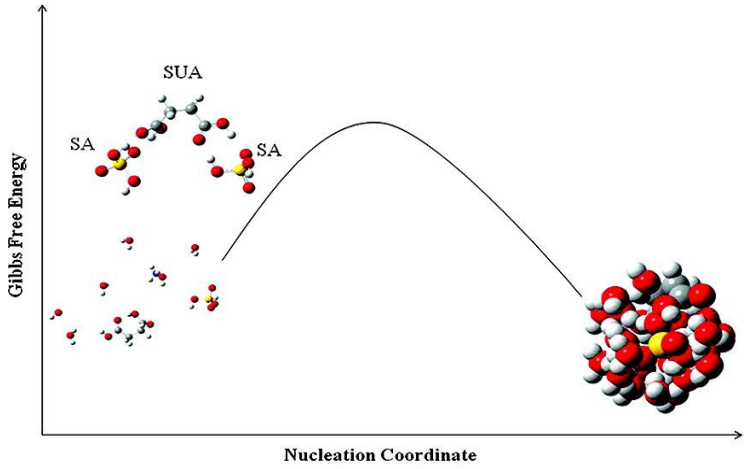
Quantum Chemical Calculations

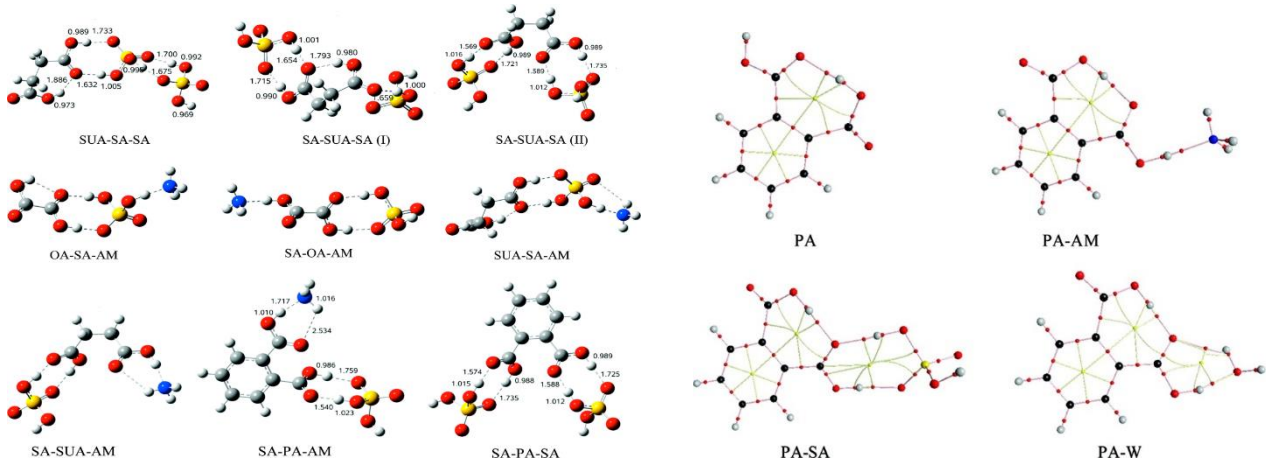
- **Many chemical species such as organic acids and amines are believed to play an important role in the formation and growth of atmospheric secondary organic aerosols.**



Atmospheric Aerosol Nucleation

In the following studies we use Gaussian 09, QTAIM with AIM2000 software to conduct natural bond orbital (NBO), topological, geometrical, and thermochemical analysis on hydrated clusters formed by organic acids and amines.

- **Interaction of Dicarboxylic Acids with Common Aerosol Nucleation Precursors**



- Molecular graphs of PA, PA-AM, PA-SA, and PA-W complexes showing the BCPs, ring critical points, bond path, and ring path.

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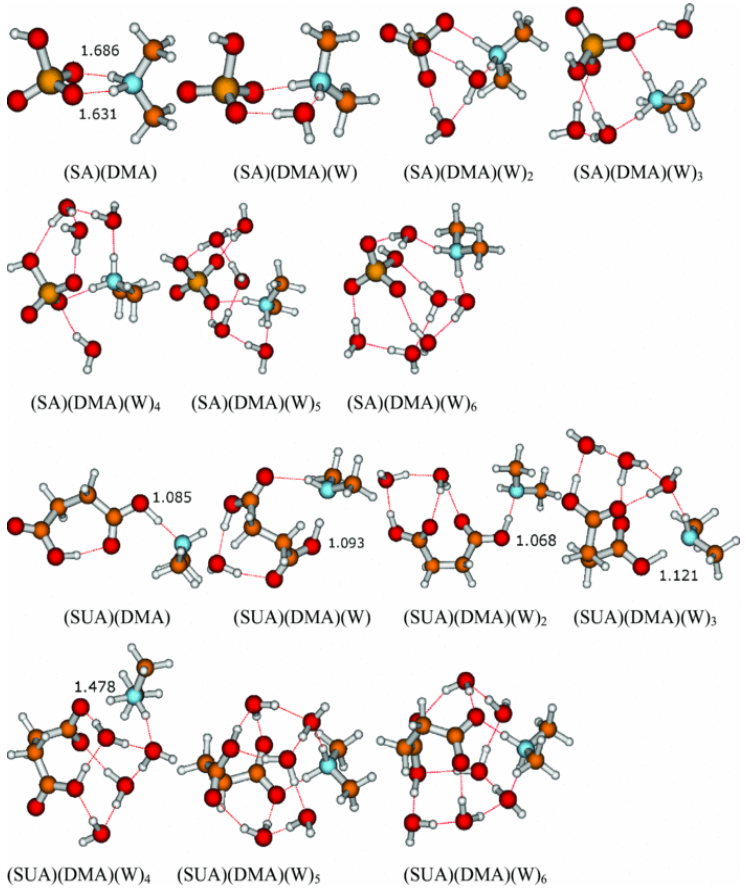
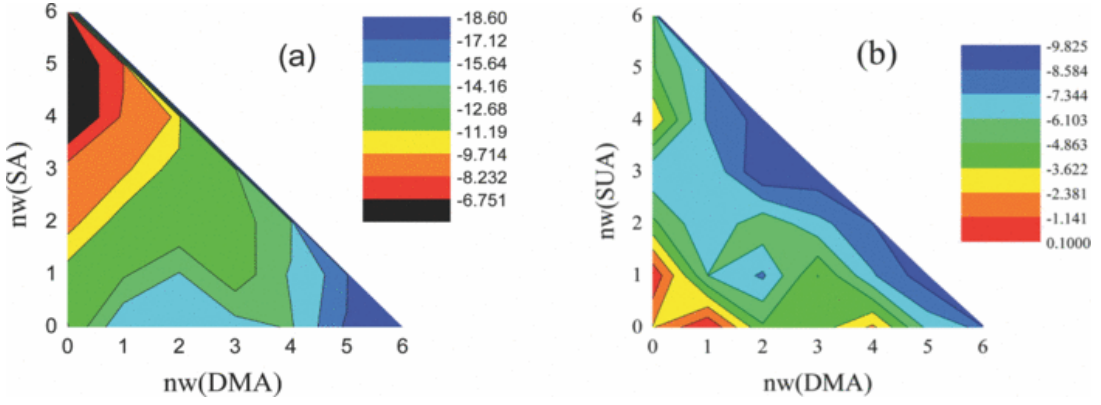
Quantum Chemical Calculations

❖ **Hydrated molecular clusters of amines and dicarboxylic acids**



- Optimized geometries of sulfuric/succinic acids and dimethylamine clusters in hydrate and anhydrate forms.



- Contour plots of the free energies of reactions of sulfuric/succinic acid with dimethylamine hydrated clusters versus the number of water molecules in sulfuric/succinic acid and dimethylamine cluster.

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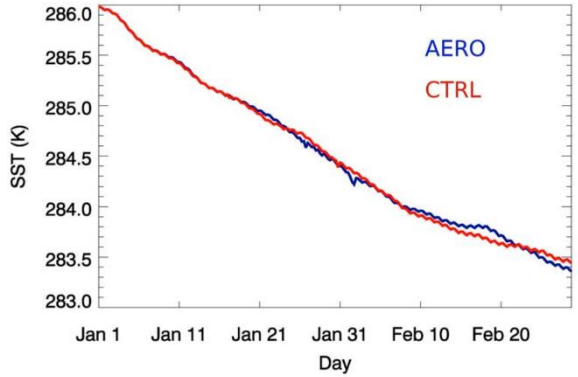
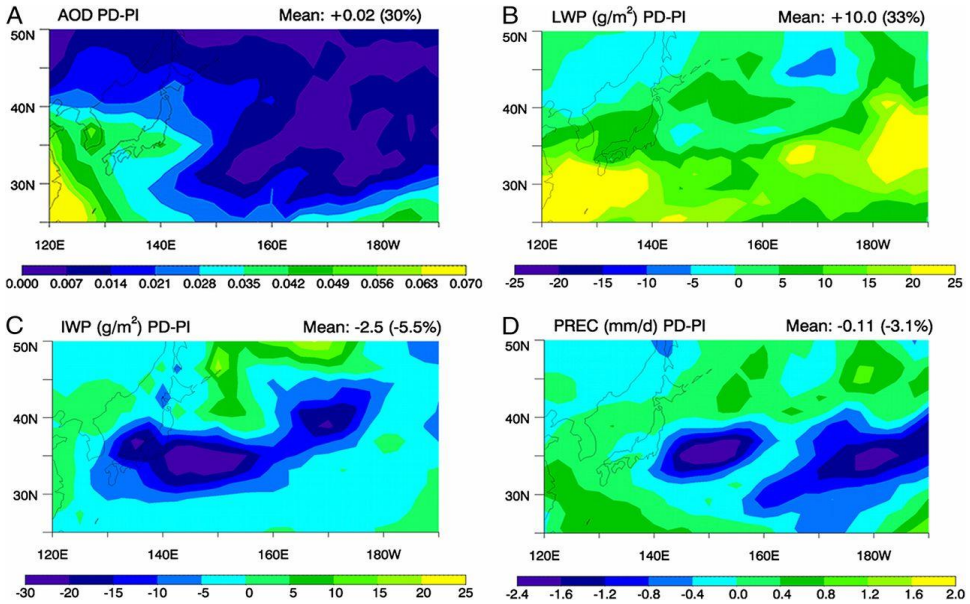
GCM Simulations

❖ **The effects of anthropogenic aerosols on Pacific storm track using a multiscale global climate model**



- Simulated SST from CAM-slab ocean model. SST are averaged over the northwest Pacific. In the control simulation (CTRL) and the simulation with additional aerosol forcings (AERO).



- The differences in (A) AOD, (B) LWP, (C) IWP, and (D) precipitation between PD and PI over the northwest Pacific from CAM5 simulations.

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References

- Xu, W.; Zhang, R. Y. Theoretical Investigation of Interaction of Dicarboxylic Acids with Common Aerosol Nucleation Precursors J. Phys. Chem. A 2012, 116, 4539– 4550.
- Xu, W.; Zhang, R. Y. A Theoretical Study of Hydrated Molecular Clusters of Amines and Dicarboxylic Acids. J. Chem. Phys. 2013.
- Wang, Y.; Lee, K. H.; Lin, Y.; Levy, M.; Zhang, R. Y. Distinct Effects of Anthropogenic Aerosols on Tropical Cyclones Nat. Clim. Change 2014, 4, 368– 373.
- Wang, Y.; Zhang, R. Y.; Saravanan, R. Asian Pollution Climatically Modulates Mid-Latitude Cyclones Following Hierarchical Modelling and Observational Analysis Nat. Commun. 2014, 5, 3098.
- Wang, Y., M. Wang, R. Zhang, S.J. Ghan, Y. Lin, J. Hu, B. Pan, M. Levy, J. Jiang, M.J. Molina, Assessing the Effects of Anthropogenic Aerosols on Pacific Storm Track Using A Multi-Scale Global Climate Model, Proc. Natl Acad. Sci. USA, 111(19), 6894-6899 (2014).

Acknowledgements

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