Kinetics and photochemistry of the atmosphere

Spring 2023: March 20 through May 12, 2023. Class meets on Mondays and Wednesdays between 1:00 and 3:15 PM. For Graduate Students Interested in Atmospheric Chemistry. Post-doctoral fellows are welcome.

Instructor: A. R. (Ravi) Ravishankara

Do you wonder why nitrogen oxides can deplete ozone in the stratosphere but make ozone in the troposphere? Do you know how rapidly chemicals are formed and destroyed in the Earth's atmosphere? <u>Are you curious but feel hesitant to ask?</u> If yes, this is the course for you!

Course Objective:

Students will understand the fundamentals of gas phase and heterogeneous/multiphase chemical kinetics and photochemistry essential for dealing with chemical transformations in the atmosphere. We will learn about the "what, how, and why" of these processes. The overarching goal is to provide the students with a *working knowledge* of kinetics and photochemistry needed to understand atmospheric chemical processes, literature, and chemical modeling. It will also cover how information is obtained through laboratory and field observations. It will also provide a rudimentary knowledge of the theory behind chemical reactions and photochemistry. The focus will be on reactions of free radicals and molecules of interest to the atmosphere and those reactions that determine the chemical composition of the troposphere and stratosphere.

Let us make this an enjoyable learning experience!

Tentative Learning Objectives:

Overall objective is that the student understands gas phase and multiphase chemistry that is used in today's atmospheric chemistry and develops a working knowledge of the kinetics and photochemistry of the Earth's troposphere and stratosphere.

(Dates for specific topics will be decided based on what you already know. I may have to finetune the material depending on your preparation level for this class.)

- Week 1: Structure and composition of the atmosphere as it relates to chemical processes. Fundamental gas phase kinetics. Order, molecularity, rate equations, bimolecular reactions, and theories of bimolecular reactions (needed to understand kinetics). Positive and negative activation energies. Network of reactions.
- Week 2: Connections between thermodynamics and kinetics. Ways to "guestimate" rate coefficients of chemical reactions. Association and dissociation reactions. Pressure dependence of reactions. Fall off curves. How to fit the fall-off curves and use them. How the rate coefficients are measured.
- Weeks 3: Basics of atmospheric photolysis rate coefficient and their calculations. Obtaining the solar flux at various altitudes in the atmosphere. TUV and Fast Jx calculations. Absorption cross sections, quantum yields, and how one gets these parameters. We will integrate all this information to calculate the rates of photolytic processes.

- Week 4: Chemical reaction mechanisms. Their uses and abuses. Steady-state approximation. Lifetimes, turnover times, etc. Use of various kinetics and photochemistry evaluations. Uncertainty analyses and how to interpret uncertainties in data evaluations.
- Week 5: Heterogeneous and multiphase reactions. Chemical composition and properties of aerosols, cloud droplets, and surfaces. Uptake coefficient. Representations in terms of fundamental parameters. Use of the derived uptake coefficients in models and mechanisms.
- Weeks 6 and 7: Integration of previous concepts and their application to tropospheric and stratospheric chemistries.
- Week 8 (Exam week): Take home exams to be returned before 9 May 2023 (Tuesday)