# Atmospheric Aerosol Chemistry and Modeling

MATH 6397-11954 and CHEM 6397-08235 (Spring 2002)


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|---|---|
| **Time:** | 5:30-7:00 p.m. TTH |
| **Room:** | 28 H |
| **Instructor:** | J.W. He & ADJ Haymet |
| **Office:** | 684 PGH & 221 Fleming |
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| **Office hours:** | 1:00-2:00 p.m. Tuesday or by appointment |


## Text Book

**Fundamentals of Atmospheric Modeling**, M. Z. Jacobson. Paperback Cambridge Univ. Pr. 1998. ISBN 0521637171. List price: $49.95

## Course Description

Atmospheric aerosols are comprised of a complex mixture of a variety of organic and inorganic substances that can be of primary or secondary nature and span several orders of magnitude in size. This complexity together with significant gaps in knowledge of the formation and transformation processes provides an ambitious task for the development of atmospheric models for particulate matter. However potential impacts of these particles and the new standards for particulate matter require the development and application of sophisticated Air Quality Models for particles.

The goal of this course is to identify the lessons that can be learned from the current state of particulate matter models and the needs for further development of these models. A key question here is to define the level of model complexity that is required to obtain sufficient information on atmospheric particles while keeping the computational burdens feasible. Therefore the following questions will be addressed:

- Which processes need to be included into a PM air quality model?
- What are the required input data for PM modeling?
- Where are the most important knowledge gaps?
- How important is the contribution of secondary organic particles resulting from anthropogenic and biogenic precursors to the PM load?
- How large is the primary particle contribution to the PM load over Texas?
- Which contributions are most likely to be responsible for violation of PM air quality standards?
- Which numerical implementations are suitable for aerosol modeling?

## Course Policies

Exams: A paper at the end of the semester.

## Reference Books

1. NARSTO Assessment of the Atmospheric Science on Particulate Matter. Draft. August 2001

2. Atmospheric Chemistry and Physics: From Air Pollution to Climate Change. Seinfeld, J.H., and Pandis, S.N. John Wiley and Sons, Inc., New York, 1997.

3. Population Balances: Theory and Applications to Particulate Systems in Engineering. Ramkrishna, D. Academic Press. 2000

4. J. E. Dennis, Jr. and Robert B. Schnabel. Numerical Methods for Unconstrained Optimization and Nonlinear Equations. SIAM, 1996.

5. Hairer, E., and Wanner, G. 1996. Solving Ordinary Differential Equations II. Stiff and Differential-Algebraic Problems. Springer-Verlag, Berlin, 2nd edition.

6. Uri M. Ascher and Linda R. Petzold. Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations. SIAM, 1998.

# Course Outline[1]

**Lecture 1:** Introduction to the atmospheric science of particulate matter

**Lecture 2:** Introduction to atmospheric aerosol processes

**Lecture 3:** Emission inventories and particle measurements: overview

**Lecture 4:** Spatial and temporal characterization of particulate matter concentration and composition

**Lecture 5:** Health effects and visibility effects of particulate matter

**Lecture 6:** mathematical description of particle components and size distribution.

**Lecture 7:** Mathematical description of atmospheric aerosol processes (I): nucleation, coagulation, deposition/sublimation, sedimentation and dry deposition.

**Lecture 8:** Mathematical description of atmospheric aerosol processes (II): condensation/evaporation and general dynamics equation for aerosols

[1]This syllabus is subject to change. Changes will be announced in class.

**Lecture 9:** Introduction to population balance framework: theory and applications to PM modeling

**Lecture 10:** Basic implements of population balances

**Lecture 11:** Mathematical formulation of population balance models

**Lecture 12:** Methods of solution of population balance equations (I)

**Lecture 13: (Dr. Jason Ching, EPA)** Current status of PM chemical transport models

**Lecture 14:** Methods of solution of population balance equations (II)

**Lecture 15 :** Methods of solution of population balance equations (III)

**Lecture 16:** Chemical equilibrium and dissolution processes

**Lecture 17:** Foundation of chemical equilibrium computation

**Lecture 18:** Mathematical structure of the chemical equilibrium problem

**Lecture 19:** Methods based on optimization techniques (I)

**Lecture 20:** Methods based on optimization techniques (II)

**Lecture 21:** Methods based on the solution of non-linear equations (I)

**Lecture 22:** Methods based on the solution of non-linear equations (II)

**Lecture 23:** Aqueous chemistry

**Lecture 24:** Foundation of solving stiff ordinary differential equations (I)

**Lecture 25:** Foundation of solving stiff ordinary differential equations (II)

**Lecture 26:** Introduction to singular perturbation problems

**Lecture 27:** Foundation of solving differential-algebraic problems (I)

**Lecture 28:** Foundation of solving differential-algebraic problems (II)