MEA 593J: Air Quality Modeling and Forecasting
MEA 793J: Advance Air Quality Modeling and Forecasting
Department of Marine, Earth and Atmospheric Sciences
Fall 2004

Class Time:	Tuesday/Thursday, 1:05-2:20 pm	**Instructor**:	Dr. Yang Zhang
Class Location:	Room 1109 Jordan Hall	Office:	Room 5151 Jordan Hall
Office Hours:	1:30-3:00 pm Fridays	Phone:	919-515-9688
	(or by appointment)	Fax:	919-515-7802
		Email:	yang_zhang@ncsu.edu

Objectives

This graduate level course in air quality modeling and forecasting describes the chemistry and physics of the atmosphere, numerical methods and computational techniques required for a scientist to study air pollution and meteorology. It offers a comprehensive examination of contemporary numerical/computational techniques for simulating/forecasting important gas and aerosol processes. It is targeted for students from atmospheric science, engineering, mathematics, statistics, and computer sciences who would like to learn about air quality modeling and who are prospective air quality modelers and forecasters. Upon completion of this course, the students should have a knowledge of important atmospheric chemical processes and numerical methods to simulate them in air quality models and should be able to conduct model simulations (box and 3-D) and develop their own computer codes to simulate one or more atmospheric processes. Students who are interested in pursuing an environmental/air quality position upon graduation are highly recommended to take this course to acquire air quality background required for such positions.

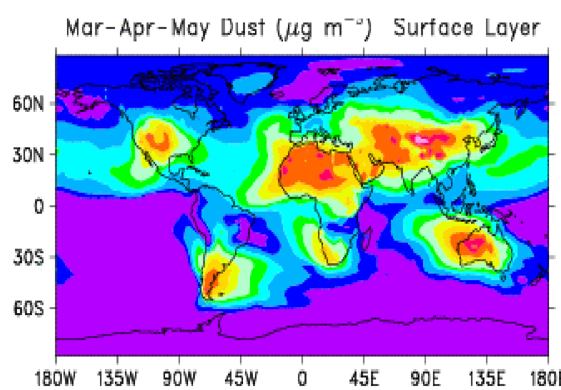
Textbook

Fundamentals of Atmospheric Modeling, M.Z. Jacobson, Cambridge University Press, New York, 1999, 656 pp, reprinted 2000 edition.

Course Description

The course provides the fundamentals of numerical modeling of urban, regional, and global air quality. It covers the chemistry, physics, and transport required for the understanding, development, application and evaluation of air quality models. It will review history and current status of air quality modeling and forecasting and provide students with hands-on computer practicing. Different computer modeling techniques for solving major atmospheric processes used in current air quality models will be reviewed and discussed. Course topics will include:

- **Atmospheric thermodynamics/structure**
- **Numerical solutions to ODEs and PDEs**
- **Atmospheric chemical kinetics**
- **Urban, tropospheric/stratospheric chemistry**
- **Modeling gas-phase chemistry**
- **Modeling radiation transfer**
- **Modeling chemistry of clouds**
- **Modeling dynamics and chemistry of aerosols**
- **Model design, applications and evaluation**
- **Air quality forecasting**



Prerequisites: CE/MEA 479/579, FORTRAN77/90 or consent of instructor.

Grading

Letter grades, on the +/- scale, determined by:

Mid exam:	30%
Homework:	30%
Term Project:	40%

Grade will be upgraded based on bonus points gained (see below for details)

Homework

(1) It must be neat and easily understood in terms of writing and presentation. It will be graded as a final report to the client and returned without grading if it does not follow this requirement.

(2) Homework will be handed out and collected on specific dates at the beginning of the class. Missed assignments and exams cannot be made up without an official university excuse. From 3PM on the due date until noon one day after the due date there will be an automatic deduction of 25 points from the grade. For the next 24-hour period (noon-to-noon) another 25 points will be deducted. This process will continue. Once a graded homework set has been returned, late homework will not be accepted. If you are sick or some special condition arises, please contact me.

(3) Reading assignments should be completed within the assigned schedule. Some test problems will be based on reading assignments.

(4) "Bonus" problems may be given for some topics, they are optional homework for students who are willing to spend more time on this course. For students signed up for 593J, your grade will be upgraded if you work on those additional problems. For students signed up for 793J, some of the bonus problems may be obligatory, your grade will be upgraded if you work on remaining bonus problems. The following table illustrates how you can earn bonus scores and how it will upgrade your base grade.

Base grade*	**Homework Bonus pts, (total 200 pts; counted as 15 pts in final grade)**	**Homework Bonus pts in final bonus pts**	**Mid-term Bonus pts, (total 30 pts counted as 5 pts in final grade)**	**Mid-term Bonus pts in final bonus pts**	**Total bonus pts (full bonus pts = 15+5= 20)**	**Final grade (bonus pts are added)**
75 (B)	80	6	20	3.33	9.33	84.33 (B+)
83 (B+)	80	6	20	3.33	9.33	89.33 (A-)
89 (A-)	80	6	20	3.33	9.33	98.33 (A)
95 (A)	80	6	20	3.33	9.33	104.33 (A+)

* The scores shown in the above table do not necessarily correspond to the actual grades to be used for this class.

Tests

One midterm (Tuesday, October 12) is planned.

Project

The term project accounts for 40% of your grade. Each team member/individual should spend at least 30-40 hours on the project. The term project will be assigned by mid-October and the report and computer codes should be handed in by Tuesday, December 7. You can pick up a suggested topic or choose your own upon my approval. The final report should be prepared as a report to a client. It should be typed with a font size clear and readily legible (12-point, 1 ½ line spacing). Excluding the computer code itself, the written report should be 8-10 pages in length including Figures, Tables and references. In addition, each student is required to give a 10-minute oral presentation (including questions) on the course project (Nov. 30 and Dec. 2). Your presentations will be evaluated by students and invited MEAS faculty members in terms of technical quality, clarity and organization.

Project Grading
The project, itself, will be graded according to the following criteria:

Projects without or with minor code modification/development (for 593 J students)

Written Report of work (80%):	
Organization	10%
Clarity	10%
Comprehensiveness	10%
Technical quality	20%
Up-to-date of the survey	10%
Following specific instruction	10%
Inclusion of references cited	10%
Oral presentation of work	10%
Effort in overall project	10%
Total	100%

Projects with code modification/development (for 793 J students)

Computer coding (35%)	
Rigor/capability of code	10%
Coding style*	10%
Coding efficiency	5%
User friendliness of code	5%
Demonstrated application of code	5%
Written report of work (45%)	
Organization	10%
Clarity	10%
Technical quality	20%
Following specific instruction	3%
Inclusion of references cited	2%
Oral presentation of work	10%
Effort in overall project	10%
Total	100%

* The grade for coding style depends primarily on the abundance and clarity of comments, on the existence and clarity of definitions given for all variables, and on indentation and spacing used in the code

Class Absences

If you miss (or plan to miss) a class, contact me as soon as possible to identify the materials to be covered during your absence. You are expected to make up the materials by reading the appropriate sections(s) in the textbook, doing the home assignments and meeting with me as necessary to discuss the materials. See the university attendance regulation at http://www.ncsu.edu/policies/academic_affairs/pols_regs/REG205.00.4.php)

Academic Integrity:

The university provides a detailed policy on academic integrity (see http://www.ncsu.edu/policies/student_services/student_discipline/POL11.35.1.php It is understood that when you sign and submit your homework, term project and exams, you are implicitly agreeing to the university honor pledge: "I have neither given nor received unauthorized aid on this test or assignment."

Students with Disabilities:

Reasonable accommodations will be made for students with verifiable disabilities. In order to take advantage of available accommodations, students must register with Disability Services for Students at 1900 Student Health Center, Campus Box 7509, 515-7653. See http://www.ncsu.edu/provost/offices/affirm_action/dss/.

Additional Reading Materials (reserved in Natural Resources Library):

1. Finlayson-Pitts, B.J. and J.N. Pitts, Jr., "Atmospheric Chemistry," Wiley-Interscience, 2000.
2. P. Warneck, "Chemistry of the Natural Atmosphere (Second Edition)," Academic Press, 1999.
3. Jacobson, M.Z., "Atmospheric Pollution," Cambridge University Press, ISBN 0521010446, 2002.
4. Seinfeld, J.H. and S.N. Pandis, "Atmospheric Chemistry and Physics: from air pollution to climate change", John Wiley & Sons, Inc., ISBN 0471-178152.
5. McElroy, M.B., "The Atmospheric Environment: Effects of Human Activity", Princeton University Press, ISBN 0-691-00691-1, 2002.

Computer References

Getting start with NCSU's Linux Cluster:
http://www.ncsu.edu/itd/hpc/Documents/GettingStartedbc.php

Unix Basics:
http://www.ncsu.edu/itd/hpc/Documents/unix_basics/
http://www.ncsu.edu/it/essentials/connections_labs/workstations/unix/

1. Arnold Robbins, Unix in a Nutshell, O'Reilly, ISBN 1565924274, O'Reilly; 3rd edition (November 15, 1999) (available online through netLibrary at NCSU, students must set up free netLibrary accounts to access it) . **(request to order a print copy for NRL)**

2. Matt Welsh, Lar Kaufman, Matthias Kalle Dalheimer, Terry Dawson, Running Linux, ISBN 0596002726, 4th Edition, O'Reilly, (December 15, 2002) **(will soon be reserved at NRL)**

3. Ellen Siever, Aaron Weber, Stephen Figgins, Linux in a Nutshell, O'Reilly; 4th edition, (June 2003)

FORTRAN 90 tutorial and references
http://www.cs.mtu.edu/~shene/COURSES/cs201/NOTES/fortran.html
http://www.qmw.ac.uk/~cgaa260/BUILDING/INTR_F90/OUTLINE.HTM
http://www.scd.ucar.edu/tcg/consweb/Fortran90/F90Tutorial/tutorial.html

1. Stephen J. Chapman, Introduction to Fortran 90/95, ISBN 0070119694, McGraw-Hill Science/Engineering/Math; 1st ed edition (September 1, 1997) (beginners) **(request to order a copy for NRL)**

2. T.M.R. Ellis, Ivor R. Phillips, Thomas M. Lahey, Fortran 90 Programming (International Computer Science Series), ISBN: 0201544466, Addison-Wesley Pub Co; 1st edition (May 31, 1994) (beginners)

3. Stephen J. Chapman, Fortran 90/95 for Scientists and Engineers, ISBN 0-07-282575-8, Elizabeth A. Jones, 2004 (beginners/experienced users, intermediate level) **(will soon be reserved at NRL)**

Debugger on HPC Machines
http://www.ncsu.edu/itd/hpc/Documents/debug.php

NCSU helpdesk (Monday - Friday, 8:00 AM - 6:00 PM)
Email: help@ncsu.edu
Telephone: 919-515-HELP (4357)
Fax: 919-513-1893

Locations of NCSU Unity computer labs
http://www.ncsu.edu/it/essentials/connections_labs/unity_computer_labs/

Numerical packages/softwares:

Netlib –a repository of mathematical software, data (free software for downloading)
http://www.netlib.no/netlib/master/index.html (file index)
http://www.netlib.no/netlib/ode/ (ODE solvers)
http://www.netlib.no/netlib/odepack/ (LSODE solvers)
http://netlib.bell-labs.com/netlib/ode/ (ODE solvers)

Numerical Recipes in Fortran 90 (Text only, no software provided)
http://www.library.cornell.edu/nr/bookf90pdf.html

Web links for Matlab at NCSU:
http://www.eos.ncsu.edu/software/matlab/toolboxes.html
http://www2.ncsu.edu/unity/lockers/users/p/pfackler/ECG561/MPRIMER.htm
http://www.mathworks.com/access/helpdesk/help/techdoc/matlab.shtml

Lecture Topics and Schedule (As of August 24):

Class, Date	Topic	Lecture content	Reading*
1, 08-19	Intro.	Introduction and overview: current AQ status and importance of AQM	MZJ 1.1, LN
2, 08-24	Comp	Fortran/Unix basics, EPA coding standards **(Lab**[**]**) (HMK#1 assigned)**	
3, 08-26	Thermo	Atmospheric structure, composition, thermodynamics - I	MZJ 2.1-2.4, LN
4, 08-31	Thermo	Atmospheric structure, composition, thermodynamics -II	MZJ 2.5-2.7, LN
5, 09-02	Chem	Gas-phase species and chemical kinetics **(HMK#1 due, HMK#2 assigned, Lab)**	MZJ 11, LN
6, 09-07	Chem	Free-tropospheric chemistry	MZJ 12.1, LN
7, 09-09	Chem	Urban photochemistry	MZJ 12.2, LN
8, 09-14	Chem	Stratospheric photochemistry **(HMK #2 due, HMK#3 assigned, Lab)**	MZJ 12.3, LN
9, 09-16	Math	Numerical solutions to PDEs	MZJ 6, LN
10, 09-21	Math	Modeling gas-phase chemistry – I	MZJ 13.1-13.5, LN
11, 09-23	Math	Modeling gas-phase chemistry – II **(HMK #3 due, HMK#4 assigned)**	MZJ 13.6-13.9, LN
12, 09-28	Modeling	Air quality modeling: types, scales, history, current status and steps **(Lab)**	MZJ 21.1, LN
13, 09-30	Modeling	3-D AQM coordinates, framework, structure and science components **(HMK#4 due on Oct. 1)**	MZJ 5, LN
10-05***	Mid-term	Test of all of the above topics	
14, 10-12	Modeling	Model application –I **(Mid-term survey, Term project assigned))**	MZJ 21.2, LN
15, 10-14	Modeling	Model evaluation	LN
16, 10-19	Modeling	Modeling aqueous-phase chemistry **(Lab)**	MZJ 19, LN
17, 10-21***	Aqueous	Model application – II: Air quality forecasting (guest lecturer) **(Lab)**	LN
18, 10-26	Aerosol	Components, Size, Properties **(HMK#5 assigned, Lab)**	MZJ 14, LN
19, 10-28	Aerosol	Thermodynamics – I	MZJ 18.1-18.9, 18.11, LN
20, 11-2	Aerosol	Thermodynamics – II	MZJ 18.10, 18.12-15, LN
21, 11-4	Aerosol	Aerosol dynamics – I: Emissions, nucleation and coagulation	MZJ 15, 16, LN
22, 11-9	Aerosol	Aerosol dynamics – II: Condensation	MZJ 17, LN
23, 11-11	Radiation	Modeling radiation transfer – I **(HMK #5 due)**	MZJ 10.1-10.4, LN
24, 11-16	Radiation	Modeling radiation transfer - II	MZJ 10.5-10.8, LN
25, 11-18	Modeling	Advance air quality modeling - I **(Lab)**	LN
26, 11-23	Modeling	Advance air quality modeling – II	LN
11-30	Course project	Class Presentations – I (group 1)	
12-02	Course project	Class Presentations – II (group 2)	
12-06		**Group 1 term project report due at 10:00 am**	
12-07		**Group 2 term project report due at 5:00 pm**	

* MZJ- Readings are from Jacobson, 1999; LN-lecture notes prepared by the instructor.
** Lab session will be held in #6136, Jordan Hall, unless notified, the lecture will normally start in #1109, then move to #6136.
*** Zhang will be out of town for conference/workshop. Substitute instructor will be in the class.

Course outline

1. Introduction and Overview: AQM importance, types, scales, history and current status
    a. Importance of air quality models
    b. Major air quality model (AQM) types and scales
    c. History of AQM development
    d. Current status of AQMs
2. Fortran/Unix basics and EPA coding standards
    a. Basic Fortran commands
    b. Basic Unix commands
    c. EPA's coding standards
    d. Sample Fortran codes
3. Atmospheric structure, composition, thermodynamics - I
    a. Pressure, density and composition
    b. Temperature structure
    c. Equation of state
    d. Change in Pressure with Altitude
4. Atmospheric structure, composition, thermodynamics - II
    a. Water in the atmosphere
    b. First law of thermodynamics
5. Gas-phase species and chemical kinetics
    a. Atmospheric gases and their molecular structures
    b. Chemical reactions and photoprocesses
    c. Atmospheric chemical kinetics
    d. Stiff system
6. Free-tropospheric chemistry
    a. Photostationary-state relationship
    b. Reactions of hydroxyl and hydroperoxy radicals
    c. Oxidation of organic species
    d. Sulfur photochemistry and nighttime nitrogen chemistry
7. Urban photochemistry
    a. Chemistry of oxidants and radicals
    b. Chemistry of anthropogenic hydrocarbons
    c. Chemistry of biogenic hydrocarbons
    d. Role of VOCs/NO_x in O_3 formation
    e. Major gas-phase mechanisms used in urban/regional models
8. Stratospheric chemistry
    a. Background stratospheric photochemistry
    b. Chlorine and bromine photochemistry
    c. O_3 regeneration rates and Antarctic O_3 depletion
    d. Heterogeneous stratospheric chemistry
9. Numerical solutions to PDEs
    a. ODEs and PDEs
    b. Operator-splitting
    c. Advection-diffusion equations
    d. Finite-difference approximations
10. Modeling gas-phase chemistry – I
    a. Characteristics of chemical ODEs
    b. Analytical solutions to ODEs

c. Taylor series solutions to ODEs
d. Forward and backward Euler solutions to ODEs

11. Modeling gas-phase chemistry – II
    a. Simple exponential and QSSA solutions to ODEs
    b. MIE solution to ODEs
    c. Gear's solution to ODEs
    d. Family solution to ODEs
12. Air quality modeling: types, scales, history, current status and steps
    a. Major AQM types and scales
    b. Model history and current status
    c. Steps in model formulation
13. 3-D AQM coordinates, framework, structure and science components
    a. Model coordinates
    b. Framework of a 3rd generation AQM
    c. Meteorology modeling
    d. Emission modeling
    e. Science components
14. Model applications - I
    a. AQM type of applications
    b. Urban/regional retrospective applications
    c. Urban/regional air quality forecasting
    d. Global air quality modeling
15. Model evaluation
    a. Type of model evaluations
    b. Meteorological and chemical conditions for model evaluation
    c. Measurement data needed for model evaluation
    d. Examples of model evaluation
16. Model application -II: Air quality forecasting (guest lecturer: John McHenry, BAMS)
    a. Fundamental of air quality forecasting
    b. Real-time Air quality forecasting status
    c. Real-time Air quality forecasting examples
    d. Evaluation of forecasting skills
17. Modeling aqueous-phase chemistry
    a. Aqueous-phase chemical equilibria and Henry's Law
    b. Aqueous-phase kinetic reactions of sulfur compounds
    c. Aqueous-phase kinetics of other compounds
    d. Coupled gas and aqueous-phase modeling system
18. Aerosol component, size and properties
    a. Effects, classification and sources
    b. Size distributions: observations and modeling approaches
    c. Chemical compositions
    d. Single particle dynamics
19. Aerosol thermodynamics - I
    a. Thermodynamic principles
    b. Calculation of the equilibrium constant
    c. Calculation of activity coefficient
    d. Aerosol liquid water content: water equation
    e. Solid formation and deliquescence relative humidity
20. Aerosol thermodynamics - II

a. Method of solving equilibrium equations
b. Major thermodynamic equilibrium modules
c. Non-equilibrium between gas and particle phases
d. Solution to growth equations for a soluble species

21. Aerosol dynamics –I: emissions, nucleation and coagulation
    a. Emissions
    b. Nucleation
    c. Coagulation
22. Aerosol dynamics –II: condensation
    a. Fluxes to and from a single drop
    b. Corrections to growth parameters
    c. Fluxes to a particle with multiple component
    d. Fluxes to a population of particles
    e. Solutions to growth equations
23. Modeling radiation transfer - I
    a. Energy transfer equation
    b. Electromagnetic spectrum
    c. Light processes
    d. Absorption and scattering by gases and particles
24. Modeling radiation transfer - II
    a. Visibility
    b. Optical depth
    c. Solar zenith angle
    d. The radiative transfer equation
25. Advance air quality modeling- I: CMAQ and CAMx
    a. Overview of CMAQ and CAMx
    b. Structure and Application of CMAQ
    c. Structure and application of CAMx
26. Advance air quality modeling- II
    a. Types of probing tools for air quality models
    b. Applications of probing tools
    c. Fine scale AQ-exposure modeling
    d. Global air quality-climate modeling