Beltsville PBL Air Quality Modeling Atmospheric Chemistry

Objective: To provide students with hands-on experience with relevant meteorology, tropospheric atmospheric chemistry, the interactions between the PBL and atmospheric chemistry, the components of numerical models and the evaluation of simulations with observations. Students are responsible for picking their modeling and graphical platforms to be used in the workshop.

Overview

Air quality is an Important factor in human health and reducing the concentrations of air pollutants is a worthy goal. The development of air quality improvement strategies is a very broad field that links science, engineering, law and governmental agencies. In this workshop we discuss some aspects of the science and modeling behind the development of public policy and air quality forecasting with an emphasis on processes that occur in the planetary boundary layer.

The solar extraterrestrial flux and the balance between incoming and outgoing energy affects the Earth's temperature. The solar extraterrestrial flux is the cause of photolysis reactions which are one important class of reactions that affect air quality. The photolysis of nitrogen dioxide (NO_2), ozone (O_3), formaldehyde (HCHO) and other trace gases is a major factor that determines atmospheric composition. Solar radiation provides the actinic flux that produces photolysis. The sun's temperature and composition affect the extraterrestrial solar radiation flux. Atmospheric factors, such as stratospheric ozone and aerosol scattering affect the actinic flux that reaches the planetary boundary layer (PBL). Students will learn about these and other factors that determine photolysis frequencies, rates and reaction products.

The production of air pollutants is affected strongly by meteorology and temperature. High mixing ratios of ozone occur on days with stagnant high-pressure systems where the atmosphere is very stable, skies are clear, there is high humidity and temperatures are high. Air quality models simulate these processes that affect air quality. The processes include emissions, transport, gas-phase chemistry, deposition to surfaces, and the physics and chemistry of clouds and aerosols.

For example, the known chemical reactions that occur in the PBL are translated into differential equations. These differential equations are incorporated in a chemical module where the equations are solved numerically to simulate the chemical transformations that produce ozone, particulate matter (also called aerosols), acids and other air pollutants. The numerical routines are a research focus because the differential equations describing gas-phase chemistry are very stiff making solutions unstable or very computational resource intensive.

The mixing layer height is an important aspect of the PBL. The mixing layer height is a major factor that determines the chemical concentrations of emissions near the Earth's surface. This affects the rates of formation of pollutants produced by chemical reactions because many of the formation reactions are concentration dependent. It is critical to link the chemical module with other modules such as a mixing-layer module to simulate the effects of a rising boundary height on air pollutant formation.

Comprehensive, meteorological 3-D air quality models are available to simulate air quality over scales that range from local to the global. In the United States there are three models that are very commonly used: The Community Multiscale Air Quality model (CMAQ), the Weather Research and Forecasting model with Chemistry (WRF-Chem) and the Comprehensive Air Quality Model with eXtensions (CAMX). The HYSPLIT model is another widely used and affective tool that is used to produce backwards and forward wind trajectories to trace the long-range flow of emissions to a receptor site. 3-D meteorological and air quality models require the initial state of the atmosphere to begin their simulations. Assimilation of observations may be used to determine the required initial state. Sensitivity analysis is closely related to data assimilation and used to investigate model uncertainties and responses to changes in emissions. Statistics need to be used to evaluate model simulations against observations and this important aspect will be discussed.

The units to be covered are given below. Students are encouraged to download all of the units and associated dataset (if any) in advance of the workshop. Please download some of key references listed below the table too.

#	Topic	# pages
1.	Solar Actinic Flux Measurements, Photolysis, Simulation and Impact on Air Quality	15
2.	Meteorological Boundary Layer Box Models	TBD
3.	Atmospheric Chemistry / Air Quality Box models	12
4.	Meteorological Boundary Layer 1-D Models	TBD
5.	Atmospheric Chemistry / Air Quality 1-D models	5
6.	Application Box Models: Impact Climate Change and Air Quality	4
7.	Air Pollution Meteorology	15
8.	3-D Air Quality Models – processes: emissions, transport, deposition, cloud / aerosol physics – chemistry	28
9.	3-D Air Quality Models WRF-Chem, CMAQ, CAM-X	6
10.	Evaluation of Meteorological and Air Quality Simulations with Observations	7
11.	3-D Air Quality Modeling and Data Assimilation	7
12.	Applications of 3-D Air Quality Models to Estimate Health Impacts – Linking to Health Effects Codes	3
13.	Beltsville PBL Air Quality Modeling – Atmospheric Chemistry Applications of 3-D Models to Air Quality Analysis and Public Policy	13

Please Download these free publicly available references prior to the workshop.

A free meteorology textbook:

Stull, R. (2017) Practical Meteorology: An Algebra-based Survey of Atmospheric Science -version 1.02b. Univ. of British Columbia. 940 pages. isbn 978-0-88865-283-6 . https://www.eoas.ubc.ca/books/Practical_Meteorology/

"Guidelines for Developing an Air Quality (Ozone and PM2.5) Forecasting Program, EPA-456/R-03-002," https://www3.epa.gov/airnow/aq_forecasting_guidance-1016.pdf

One of the first extensive presentations on air quality modeling:

McRae, G.J. and Goodin, W.R. and Seinfeld, J.H. (1982) Mathematical modeling of photochemical air pollution, Environmental Quality Laboratory Report, 18. California Institute of Technology , Pasadena, CA. https://resolver.caltech.edu/CaltechEQL:EQL-R-18 see also https://authors.library.caltech.edu/25729/

Parrish, D.D. and W.R. Stockwell (2015) Urbanization and Air Pollution - Then and Now, *Eos Trans. AGU*, *96*, 2015. doi:10.1029/2015EO021803 available at: https://eos.org/features/urbanization-air-pollution-now

Stewart, D.R., E. Saunders, R.A. Perea, R. Fitzgerald, D.E. Campbell and W.R. Stockwell (2017) Linking Air Quality and Human Health Effects Models: An Application to the Los Angeles Air Basin, *Environmental Health Insights, 11,* 1–13*,* open access at doi: 10.1177/1178630217737551

Stockwell, W.R., C.V. Lawson, E. Saunders and W.S. Goliff, A Review of Tropospheric Atmospheric Chemistry and Gas-Phase Chemical Mechanisms for Air Quality Modeling, *Atmosphere*, *3*, 1–32, 2012. doi:10.3390/atmos30100012011 open access: available at https://www.mdpi.com/2073-4433/3/1/1