BAE 820 Physical Principles of Environmental Systems

Overview of air quality modeling

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From monitoring to modeling

- Air quality monitoring can give important and quantitative information about ambient concentrations and deposition, however, it can only describe air quality at specific locations and times, without giving clear guidance on the identification of the causes of the air quality problem.
- Air quality modeling uses mathematical and numerical techniques to describe the causal relationship between emissions, meteorology, atmospheric concentrations, deposition, and other factors. It aims to provide a more complete deterministic description of air quality problems, including analysis of causes, and guidance on mitigation strategies.

Typical applications of air quality modeling

- Research: modeling can be used to identify key factors to air quality problems.
- Mitigation: modeling can be used to estimate the effectiveness of various mitigation strategies and therefore can assist in the design and decision of effective strategies.
- Permitting: when issuing emission permits for new sources, modeling can be used to predict future pollutant concentrations for comparison with air quality guidelines.

Types of air quality modeling

- Dispersion modeling - used to estimate the concentration of air pollutants at specified ground-level receptors surrounding emissions sources.
- Photochemical modeling - used to simulate the impacts from all sources by estimating pollutant concentrations and deposition of both inert and chemically reactive pollutants over large spatial scales.
- Receptor modeling – are observational techniques which use the chemical and physical characteristics of gases and particles measured at source and receptor to both identify the presence of and to quantify source contributions to receptor concentrations.

Dispersion modeling Introduction

- Dispersion modeling uses mathematical formulations to characterize the atmospheric processes that disperse a pollutant emitted by specific sources.
  - Input: emission source data and meteorological data
  - Output: concentrations of air pollutants at selected downwind receptor locations
- Dispersion models are typically used in the permitting process to determine the compliance with National Ambient Air Quality Standards (NAAQS) and other regulatory requirements such as New Source Review (NSR) and Prevention of Significant Deterioration (PSD) regulations.

Dispersion modeling
Emission source data

- Point sources:
  - are defined in terms of size and may vary between regulatory programs.
- Line sources:
  - most frequently considered are roadways and streets along which there are well-defined movements of motor vehicles.
  - may be lines of roof vents or stacks.
- Area and volume sources:
  - are often collections of a multitude of minor sources with individually small emissions that are impractical to consider as separate point or line sources.
  - large area sources are typically treated as a grid network of square areas, with pollutant emissions distributed uniformly within each grid square.

Dispersion modeling
Meteorological data

- The meteorological data used as input to a dispersion model should be selected on the basis of spatial and temporal representativeness to characterize the transport and dispersion conditions in the study area.
- For long range transport assessments or for assessments where the transport winds are complex and the application involves a non-steady-state dispersion model, use of output from prognostic mesoscale meteorological models is encouraged.

Dispersion modeling
Various levels of sophistication

- Screening models:
  - consists of relatively simple estimation techniques that generally use preset, worst-case meteorological conditions to provide conservative estimates of the air quality impact of a source.
  - the purpose of such techniques is to eliminate the need of more detailed modeling for those sources that likely will not cause air quality problems.
- Refined models
  - provide more detailed treatment of physical and chemical atmospheric processes, require more detailed and precise input data, and provide more specialized concentration estimates.

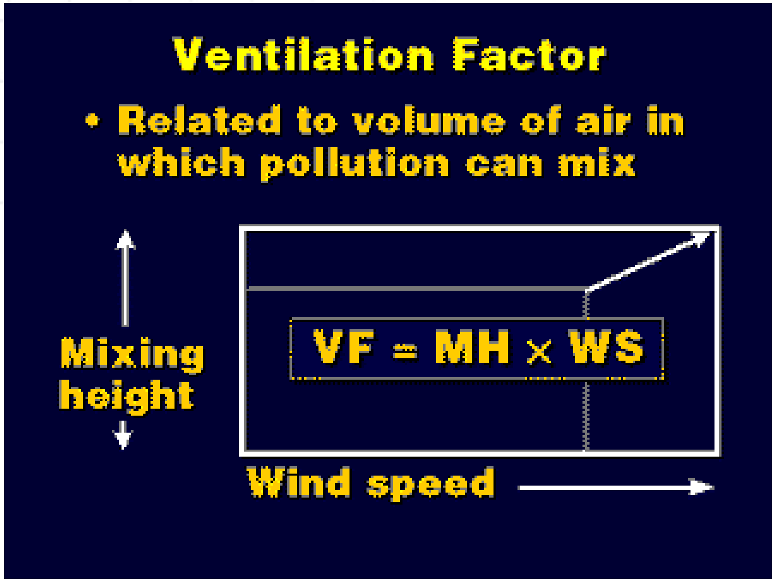
Dispersion modeling
Various modeling approaches

- Dispersion of air pollutants in the troposphere is mainly governed by advection (wind) field. Other processes like turbulent diffusion, chemical reaction and deposition of air pollutants also play important role in the spatiotemporal evolution of dispersion pattern.

- For simulating the dispersion of air pollutants, various modelling approaches have been developed with specific requirements for the different spatial scales from local to regional models, and deficiencies with respect to particle dispersion and aerosol dynamics within different scales.
  - Box model
  - Gaussian plume
  - Lagrangian
  - Eulerian
  - Computational Fluid Dynamics (CFD)

Dispersion modeling
Box models

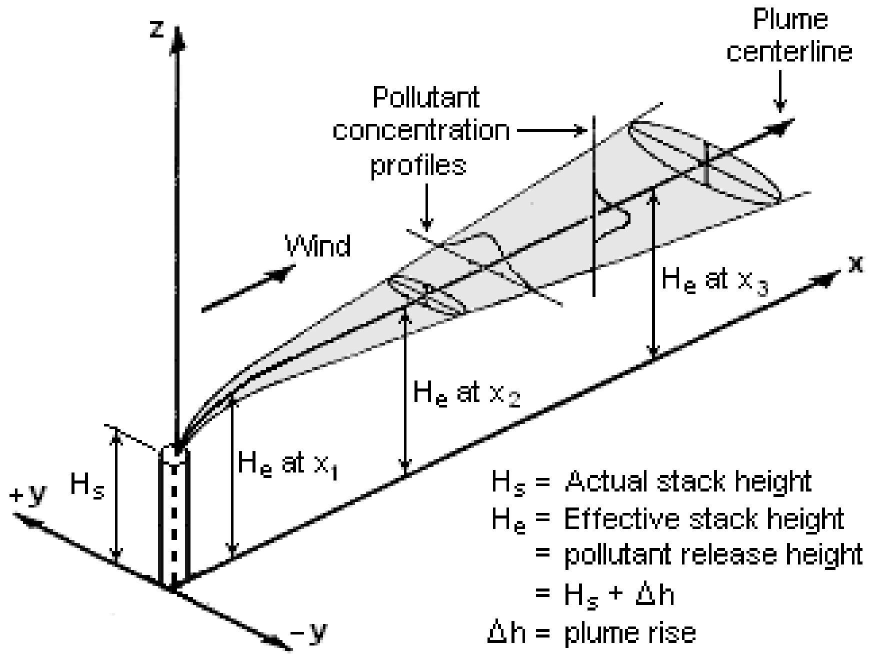
- Box models are derived from the concept of CSTR.
- The ventilation factor gives us a way of relating the pollution concentration to the parameters that control dispersion of the pollution in the local environment.
- Basically, increasing either the mixing height or the wind speed increases the effective volume in which pollutants are allowed to mix.



- Global mixing model
  - Stratosphere
  - Troposphere
- Indoor box model

Dispersion modeling
Gaussian plume

- Assuming a homogenous, steady-state flow and a steady-state point source, the turbulent dispersion equation can be analytically integrated and results the well-known Gaussian plume distribution.

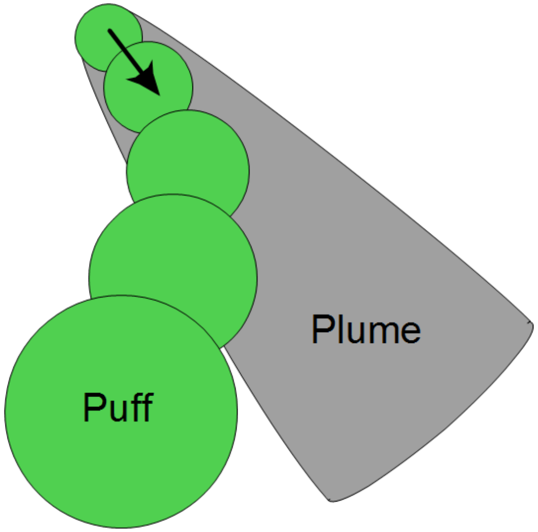


$$u\frac{\partial C}{\partial x} = D_y\frac{\partial^2 C}{\partial x^2}+D_z\frac{\partial^2 C}{\partial x^2}$$

$$C\ (x,y,z) = \frac{Q}{2\pi u \sigma_y \sigma_z}\exp(\frac{y^2}{2{\sigma_y}^2})\ [\exp(-\frac{(z-h)2}{2{\sigma_z}^2})+\exp(-\frac{(z+h)2}{2{\sigma_z}^2})]$$

Dispersion modeling
Lagrangian models

- Lagrangian models are based on the idea that pollutant particles in the atmosphere move along trajectories determined by the wind field, the buoyancy and the turbulence effects.
- The models either estimate the particle as a single drifting point, and the final distribution of numerous particles is used to estimate concentration fields (trajectory models), or assume a Gaussian dispersion inside each particle and the final concentration field is given as a superposition of these Gaussian distributions (puff models).
- Deposition and radioactivity can be taken into account as a time-dependent decay term within each particle.



Dealing with changing wind and emission data.

Dispersion modeling
Eulerian models

- The main idea of any Eulerian models is to solve numerically the atmospheric transport equation. The atmospheric transport equation is mathematically a second order partial differential equations (PDE), and its solution with the appropriate initial and boundary conditions provides the spatiotemporal evolution of the concentration, i.e., $c = c(t,x)$
- There are several numerical methods to solve PDE, one of the most powerful and common method is the so-called "method of lines". The method consists of two steps: (i) spatial discretization and (ii) the temporal integration of the derived ordinary differential equations (ODEs). Spatial discretization of PDE is performed on a mesh (grid). This reduces the PDE to a system of ODEs in one independent variable, time. The system of ODEs can then be solved as an initial value problem, and a variety of powerful methods and software tools exist for this purpose.

Dispersion modeling
Computational Fluid Dynamics models

- Eulerian and Lagrangian models models are tightly connected to numerical weather prognostic (NWP) models that provide wind field and other meteorological data in order to perform dispersion calculations. Grid resolution of NWP models is in a range of 1 to 10 km, however, many dispersion problems are concentrated on a smaller scale. Wind field datasets from NWP models have far too coarse resolution to represent the wind field within an urban area.
- The more efficient computers led to rapid development of the Computational Fluid Dynamics (CFD) technology, a general purpose engineering tool for numerical flow simulation. They provide a tool to solve various PDEs.
- Key parameters of a CFD model are the mesh, the solver, the turbulence model, and a visualization tool to create 3D plots and slices of the computed fields.

Recommended approaches for different scales and applications of atmospheric dispersion modelling

Application	< 1 km	1 – 10 km	10 – 100 km	100 – 1000 km
Online risk management (fast runtime is important)	-	Gaussian	Puff	Eulerian
Complex terrain	CFD	Lagrangian	Lagrangian	Eulerian
Reactive materials	CFD	Eulerian	Eulerian	Eulerian
Source-receptor sensitivity	CFD	Lagrangian	Lagrangian	Lagrangian
Long-term average loads	-	Gaussian	Gaussian	Eulerian
Free atmosphere dispersion (volcanoes)	-	Lagrangian	Lagrangian	Lagrangian
Convective boundary layer	(CFD)	Lagrangian	Eulerian	Eulerian
Stable boundary layer	CFD	Lagrangian	Eulerian	Eulerian
Urban areas, street canyon	CFD	CFD	Eulerian	Eulerian

(Reference: Lafzi et al., 2013)

Examples of dispersion models

- AERMOD (developed by EPA) is a steady-state plume model that incorporates air dispersion based on planetary boundary layer turbulence structure and scaling concepts, including treatment of both surface and elevated sources, and both simple and complex terrain.
- CALPUFF (developed by EPA) is a non-steady-state puff dispersion model that simulates the effects of time- and space-varying meteorological conditions on pollution transport, transformation, and removal. CALPUFF can be applied for long-range transport and for complex terrain.
- HYSPLIT (developed by the NOAA Air Resources Laboratory) provides an easy-to-use online interface for single trajectory simulations in order to give a fast estimation of atmospheric dispersion pathways or source regions. It also offers a mixture of a vertical trajectory and a horizontal puff model to determine concentration levels.

Photochemical modeling Introduction

- Photochemical air quality models simulate the changes of pollutant concentrations in the atmosphere using a set of mathematical equations characterizing the chemical and physical processes including chemistry, diffusion, advection, sedimentation (for particles), and deposition (both wet and dry) in the atmosphere.
- Most of current models adopt the three-dimensional Eulerian grid modeling. They solve a finite approximation by dividing the modeling region into a large number of cells, horizontally and vertically, which interact with each other to simulate the various processes that affect the evolution of pollutant concentrations.
- Input of emission and meteorological data are typically specified at hourly intervals for each computational cell in the modeling domain.

Photochemical modeling
Emission processors

- Emission inventories typically have an annual-total emissions value for each emissions source, or perhaps an average-day emissions value. Photochemical models, however, typically require emissions data on an hourly basis, for each model grid cell (and perhaps model layer). Consequently, to achieve the input requirements of the models, emission inventories need to be processed via emission processors by temporal allocation, chemical speciation, spatial allocation, and perhaps layer assignment.
- The Sparse Matrix Operator Kernel Emissions (SMOKE) Modeling System has been recently created allowing emission data processing methods to integrate high-performance computing sparse-matrix algorithms. The purpose of SMOKE is to convert the resolution of the data in an emission inventory to the resolution needed by a photochemical air quality model.

Photochemical modeling
Meteorological models

- Photochemical models generally require hourly, vertically and horizontally resolved wind fields, as well as hourly temperature, humidity, mixing depth and solar insolation fields.
- Recent model applications have found it desirable (because of the sparseness of the data) to use dynamic, or prognostic, meteorological models.

Photochemical modeling
Process descriptions

- Turbulent transport and diffusion
- Removal processes
  - Dry deposition
  - Wet deposition and rain, fog, and cloud processing
- Chemical kinetics
  - Chemical mechanisms are used to provide a computationally viable means of representing the chemical dynamics. The current trend is to add a mechanism compiler to allow the photochemical model to easily switch between or update mechanisms.
- Particulate matter modeling
  - Modeling the formation of secondary species and growth of aerosols

Photochemical modeling
Model applications

- Photochemical air quality models are typically used for regulatory analysis and attainment demonstrations by assessing the effectiveness of air pollution control strategies.
- One of the major applications of photochemical models is to assess the relative importance of VOC and NO_x controls in reducing ozone levels.
- Reactivity assessment: Different VOC species can have a very different impact on the rate and amount of ozone formation. Photochemical modeling has been used to quantify the reactivities of a variety of VOCs.

Example of photochemical modeling

- Community Multi-scale Air Quality (CMAQ) - EPA's CMAQ modeling system is supported by the Community Modeling and Analysis System (CMAS) Center. The CMAQ model includes state-of-the-science capabilities for conducting urban to regional scale simulations of multiple air quality issues, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation.

Receptor modeling

- Receptor models are mathematical or statistical procedures for identifying and quantifying the sources of air pollutants at a receptor location. Receptor models use the chemical and physical characteristics of gases and particles measured at source and receptor to both identify the presence of and to quantify source contributions to receptor concentrations.
  - Chemical Mass Balance (CMB): The CMB uses source profiles and speciated ambient data to quantify source contributions.
  - UNMIX: Chemical profiles of the sources are not required, but instead are generated using a mathematical formulation based on factor analysis.
  - Positive Matrix Factorization (PMF): Using factor analysis the underlying co-variability of many variables (e.g., sample to sample variation in PM species) is described by a smaller set of factors (e.g., PM sources).
- CMB fully apportions receptor concentrations to chemically distinct source-types depending upon the source profile database, while UNMIX and PMF internally generate source profiles from the ambient data.

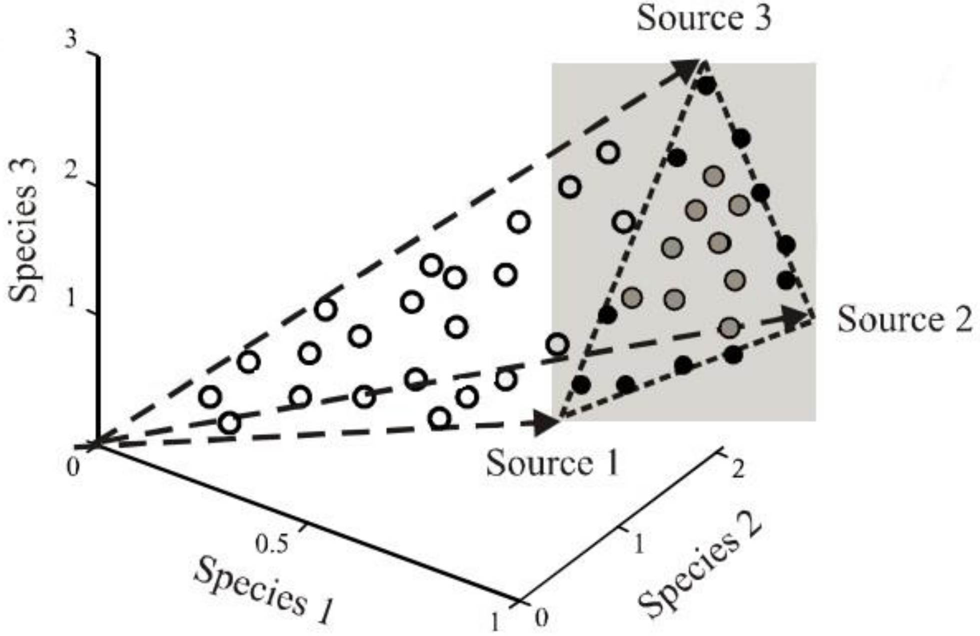
The CMB receptor model

- The CMB receptor model consists of a solution to linear equations that express each receptor chemical concentration as a linear sum of products of source profile abundances and source contributions.
  - Input: source profile abundances (i.e., the mass fraction of a chemical or other property in the emissions from each source type) and the receptor concentrations, with appropriate uncertainty estimates.
  - Output: the amount contributed by each source type represented by a profile to the total mass, as well as to each chemical species.

- CMB is applicable to multi-species data sets, the most common of which are chemically-characterized PM_{10}, $PM_{2.5}$, and Volatile Organic Compounds (VOC).

The Unmix receptor model

Unmix seeks to solve the general mixture problem where the data are assumed to be a linear combination of an unknown number of sources of unknown composition, which contribute an unknown amount to each sample. It is assumed that for each source there are some data points where the contribution of the source is not present or small compared to the other sources. These are called edge points and Unmix works by finding these points.



Plot of three sources and three species case: the grey dots are the raw data projected to a plane, and the solid black dots are the projected points that have one source missing (edge points)

(Reference: Mijic et al., 2010)

The PMF receptor model

- Positive Matrix Factorization (PMF): It is a multivariate factor analysis tool that decomposes a matrix of speciated sample data into two matrices: factor contributions (G) and factor profiles (F).
- These factor profiles need to be interpreted by the user to identify the source types that may be contributing to the sample using measured source profile information, and emissions inventories.
- PMF has been shown to be a powerful receptor modelling tool and has been commonly applied to particulate matter data and recently to VOC data.

The EPA air quality models

- PMF Many air quality models (Executable and implementation guide) are freely available at the EPA website.
- http://www.epa.gov/ttn/scram/aqmindex.htm