An Introduction to Human Exposure Modeling

MODULE III
Atmospheric Dispersion Modeling:
III-1. Elementary Concepts and Examples

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Draft Version

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Module III-1 Structure and Objectives

- Elementary introduction to fundamental concepts and basic equations
- Presentation of examples from simple and comprehensive model applications

Overview of simple atmospheric dispersion models
- Box models
- Empirical (“Gaussian”) plume models

Elementary physics of atmospheric turbulence
- Essential concepts and terminology; types of turbulent dispersion

Formal development of atmospheric dispersion (and air quality) models
- The Eulerian approach
- The Lagrangian approach
- The Gaussian plume model revisited

Example applications
- Simple and advanced models of dispersion from localized (point) sources
- Regional photochemical modeling
- Linking atmospheric dispersion with exposure and risk estimation (demonstration for the WTC plume)

Advanced analytical/numerical modeling methods are covered in Mod III-2
The Simplest Atmospheric Model for Quantifying Airborne Contaminant Levels: “Emissions in a Box”

- The simple homogeneously mixed box model for area emissions $M_A$

$$C_A = \frac{M_A}{uA}$$

- For line source with strength (per unit length) of $Q_L$

$$C_A = \frac{Q_L L}{uW H}$$

- Note, however, that some of the most sophisticated numerical models in essence result from the combination of thousands of box models...
The Empirical Gaussian Plume:
More Realistic than the Uniform Box but Still Very Simple (i)

- Basic assumption about time averaged concentration:
  - It is proportional to source strength
    \[ \bar{C} \propto Q \]
  - It is also inversely proportional to average wind speed
    \[ \bar{C} \propto \frac{1}{u} \]
  - It follows a normal distribution (Gaussian function) in the cross-wind direction
    \[ p(x) = \frac{1}{\sqrt{2\pi} \sigma} \exp \left[ -\frac{(x-a)^2}{2\sigma^2} \right] \]
The Empirical Gaussian Plume: More Realistic than the Uniform Box but Still Very Simple (i)

- Resulting dispersion equation

\[
\bar{C} = \frac{Q}{u} \left\{ \frac{1}{\sqrt{2\pi}\sigma_y} \exp\left[ -\frac{y^2}{2\sigma_y^2} \right] \right\} \left\{ \frac{1}{\sqrt{2\pi}\sigma_z} \exp\left[ -\frac{(z - \bar{z})^2}{2\sigma_z^2} \right] \right\}
\]

Or

\[
\bar{C} = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left\{ -\frac{1}{2} \left[ \left( \frac{y}{\sigma_y} \right)^2 + \left( \frac{z - \bar{z}}{\sigma_z} \right)^2 \right] \right\}
\]
Empirical parameterizations are used to account for magnitude/rate of Gaussian plume “spread”
Atmospheric conditions (wind speed, shear, thermal stratification) determine the overall behavior of a plume.
Sometimes the 3-d structure of the atmosphere requires a more detailed understanding and description of dispersion dynamics.
Physical Picture of Atmospheric Dispersion: The Basics

- Puffs: the results of instantaneous releases
- Plumes: the results of continuous releases
  - Can be approximated by a series of puffs
- Atmospheric turbulence has both thermal and mechanical origins
- Dispersion of a puff (or a plume segment) is a multiscale process determined by its size relative to atmospheric eddies
  - Eddies < puff ⇒ Significant dilution
  - Eddies > puff ⇒ Limited dilution – mostly meandering (bulk transport)
  - Eddies ~ puff ⇒ Dispersed and distorted
- Molecular diffusion has minor role in atmospheric dispersion (eddy diffusion)
- Instantaneous vs time averaged views of puffs/plumes can be very different
  - Instantaneous or relative dispersion vs absolute dispersion
- Description of plume depends on time scale (averaging)
- Time averaged concentrations are typically used for continuous sources (typical industrial emissions) but can be meaningless for fluctuating releases of hazardous contaminants
Fluctuations of Real World Plume/Puff Concentrations Are Due to Meandering (Large Eddies) and Internal “Patchiness” (Small Eddies)
Systematic Air Pollution (or Atmospheric Hazard) Assessment: First Essential Steps - Emissions Characterization and Multiscale Numerical Atmospheric Contaminant Dispersion and Deposition Modeling

3-D numerical grids are used to compute transport/fate in Eulerian or Lagrangian frameworks.

Model Derivation from Fundamental Principles: The Eulerian Approach (i)

- Fixed coordinate system ("grid")
- Continuity (mass balance) equation for concentration $c_i$
  \[
  \frac{\partial c_i}{\partial t} + \frac{\partial}{\partial x_j} u_j c_i = D_i \frac{\partial^2 c_i}{\partial x_j \partial x_j} + R_i(c_1, \cdots, c_N, T) + S_i(x, t)
  \]

- Wind velocities $u_j$ consist of 2 components:
  - Deterministic
  - Stochastic
  \[
  u_j = \bar{u}_j + u_j'
  \]
  - $u_j'$ random $\Rightarrow$ $c_i$ random $\Rightarrow$ No deterministic solution
  - Even determination of mean concentration runs into a closure problem
Many additional assumptions/approximations

- Chemically inert ($R_i=0$) contaminants are simplest to model
- $K$ theory (or mixing-length theory) is the simplest closure approximation

\[ \overline{u_j c} = - \sum_k K_{jk} \frac{\partial \overline{c}}{\partial x_k} \]

- Where $K_{jk}$ is the eddy diffusivity, a function of location and time

- Molecular diffusion is negligible
- The atmosphere is incompressible

\[ \frac{\partial \overline{u_j}}{\partial x_j} = 0 \]

- Resulting semiempirical inert Atmospheric Dispersion Equation (ADE)

\[ \frac{\partial \overline{c}}{\partial t} + u_j \frac{\partial \overline{c}}{\partial x_j} = \frac{\partial}{\partial x_j} \left( K_{jj} \frac{\partial \overline{c}}{\partial x_j} \right) + S(x,t) \]
Model Derivation from Fundamental Principles: The Eulerian Approach (iii)

- **Analytical solutions of the ADE for idealized problems**
  - An instantaneous source (puff)
    
    \[
    \bar{c}(x, y, z, t) = \frac{S}{8(\pi t)^{3/2} (K_{xx} K_{yy} K_{zz})^{1/2}} \exp \left[ - \frac{(x - ut)^2}{4K_{xx}t} - \frac{y^2}{4K_{yy}t} - \frac{z^2}{4K_{zz}t} \right]
    \]
  
  - A continuous steady state source
    
    - Plume is comprised of many puffs each of which has a concentration distribution that is sharply peaked about its centroid at all travel distances
    
    - Slender plume approximation – the spread of each puff is small compared to the downwind distance it has traveled
    
    \[
    \bar{c}(x, y, z) = \frac{q}{4\pi(K_{yy} K_{zz})^{1/2}} \exp \left[ - \frac{u}{4x} \left( \frac{y^2}{K_{yy}} + \frac{z^2}{K_{zz}} \right) \right]
    \]
Model Derivation from Fundamental Principles: The Lagrangian Approach (i)

- Concentration changes are described relative to the moving fluid.
- A single particle
  - A single particle which is at location $\mathbf{x}'$ at time $t'$ in a turbulent fluid
  - Follow the trajectory of the particle, i.e., its position at any later time
  - Probability that particle at time $t$ will be in volume element of $x_1$ to $x_1+dx_1$, $x_2$ to $x_2+dx_2$, $x_3$ to $x_3+dx_3$

$$\psi(x_1, x_2, x_3, t)dx_1 dx_2 dx_3 = \psi(x, t)dx$$

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \psi(x, t)dx = 1$$

- Ensemble of particles
  - Ensemble mean concentration

$$\bar{c}(x, t) = \sum_{i=1}^{m} \psi_i(x, t)$$
Lagrangian Approach

- **Solutions**

  - Instantaneous point source of unit strength at its origin, mean flow only in x direction

  \[
  -c(x, y, z, t) = \frac{1}{(2\pi)^{3/2} \sigma_x(t)\sigma_y(t)\sigma_z(t)} \exp\left[ -\frac{(x - ut)^2}{2\sigma_x^2(t)} - \frac{y^2}{2\sigma_y^2(t)} - \frac{z^2}{2\sigma_z^2(t)} \right]
  \]

  - Continuous source

  \[
  -c(x, y, z) = \frac{q}{2\pi u \sigma_y \sigma_z} \exp\left[ -\frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2} \right]
  \]
Eulerian vs Lagrangian Approaches: A Superficial Comparison

- **Eulerian**
  - Fixed coordinates
  - Focus on the statistical properties of fluid velocities
  - Eulerian statistics are readily measurable
  - Directly applicable when there are chemical reactions
  - Closure problem – no generally valid solutions

- **Lagrangian**
  - Moving coordinates
  - Focus on the statistical properties of the displacements of groups of particles
  - No closure problem
  - Difficult to accurately determine the required particle statistics
  - Not directly applicable to problems involving nonlinear chemical reactions
Eulerian vs Lagrangian Approaches

- Reconciliation of idealized solutions from the two approaches
  - Instantaneous sources
    \[ \sigma_x^2 = 2K_{xx}t, \quad \sigma_y^2 = 2K_{yy}t, \quad \sigma_z^2 = 2K_{zz}t \]
  - Continuous sources
    \[ \sigma_y^2 = \frac{2K_{yy}x}{u}, \quad \sigma_z^2 = \frac{2K_{zz}x}{u} \]

- Limitations of both approaches
  - Lack of exact solutions except for idealized (steady state, homogeneous) situations
  - Non-physical limits
  - Real-world atmospheric dispersion is a nonlocal phenomenon: Eulerian and Lagrangian approaches are limiting simplifications of a more general description
Back to the Gaussian Dispersion Model (i)

- Can be “formally” derived as Lagrangian solutions
  - For an instantaneous source (a puff)

\[
\bar{c}(x, y, z, t) = \frac{Q}{(2\pi)^{3/2} \sigma_x(t) \sigma_y(t) \sigma_z(t)} \exp \left[ -\frac{(x-\bar{u}t)^2}{2\sigma_x^2(t)} - \frac{y^2}{2\sigma_y^2(t)} - \frac{z^2}{2\sigma_z^2(t)} \right]
\]

- For a continuous source at a release height of \( H \)

\[
\bar{c}(x, y, z) = \frac{q}{2\pi u \sigma_y \sigma_z} \exp \left[ -\frac{y^2}{2\sigma_y^2} - \frac{(z-H)^2}{2\sigma_z^2} \right]
\]

Or

\[
\bar{c}(x, y, z) = \frac{q}{2\pi u \sigma_y \sigma_z} \exp \left[ -\frac{y^2}{2\sigma_y^2} \right] \exp \left[ -\frac{(z-H)^2}{2\sigma_z^2} \right]
\]
Back to the Gaussian Dispersion Model (ii)

- Ground reflection

\[
- c(x, y, z) = \frac{q}{2\pi u \sigma_y \sigma_z} \exp \left(- \frac{y^2}{2\sigma_y^2} \right) \exp \left(- \frac{(z-H)^2}{2\sigma_z^2} \right) + \exp \left(- \frac{(z+H)^2}{2\sigma_z^2} \right)
\]

- Special cases
  - Ground level receptor \((z=0)\)
  - Center line \((y=0)\)
  - Ground level source \((H=0)\)
Dispersion Coefficients ($\sigma$) in the Gaussian Plume Model: they depend on travel time

- **Factors Affecting dispersion coefficients**
  - Wind velocity fluctuation
  - Friction velocity $u_*$
  - Monin-Obukhov length $L$
  - Coriolis parameter
  - Mixing height
  - Convective velocity scale
  - Surface roughness

- **Pasquill-Gifford Curves** condense all above factors into 2 variables – stability class and downwind distance
  - Charts
  - Numeric formulas
  - Averaging time
    - 3-10 minutes
    - EPA specifies 1 hour
COMPREHENSIVE APPLICATION EXAMPLE I:

Contaminant Dispersion Models Linked With GIS-Based Information on Monitors and Receptors

MET & GIS (TOPO, RECEPTOR) DATA

- Real Time/On Line
- Other Lab & Field Data

Research Lab Modeling Prognostic/Diagnostic

- Evaluation of Assumptions
- Systematic Simplification

Response Center Modeling

- Query Real Time
- Real Time Assimilation
- Correction & Decision Support (Real Time)

"Field Model" (on Wireless Laptop or PDA)

- Real Time
- Real Time/On Line
- Off-Line Scenario Based

Trained EM Personnel
Center Scientists
Research Scientists

Contaminant Dispersion Models Linked With GIS-Based Information on Monitors and Receptors

Real Time
Trained EM Personnel
Real Time/On Line
Center Scientists

Off-Line Scenario Based
Research Scientists

Model Application & Operators

SOURCE & CONTAMINANT DATA

Controlled Experiments & Research Monitoring Network

Real-Time Sensor & Monitor Data
Contaminant Dispersion Models Linked With GIS-Based Information on Monitors and Receptors

**Real Time**
- MET & GIS (TOPO, RECEPTOR) DATA
  - Real Time/On Line
  - Other Lab & Field Data

**Simple/Fast**
- Comprehensive Diagnostic
  - All Available
- Fast
  - On-Line Real Time
- Minimal
  - Real Time
- Trained EM Personnel
- Real-Time Sensor & Monitor Data

**Model Complexities & Data Requirements**
- Query Real Time
- Evaluation of Assumptions
- Systematic Simplification
- Real Time Assimilation
- Correction & Decision Support (Real Time)
- Guidance & Decision Support

**SOURCE & CONTAMINANT DATA**
- Controlled Experiments & Research Monitoring Network
- Real-Time Sensor & Monitor Data

**Model Application & Operators**
- Real Time
- Real Time/On Line
- Off-Line Scenario Based
- Center Scientists
- Research Scientists

**Other Lab & Field Data**
- e.g. CAMEO/ALOHA (EPA)
- e.g. LLNL-NARAC Model (DOE)
- e.g. VLSTRACK (NSWC), HPAC/SciPUFF (DSWA)
- e.g. MENTOR/RAMS (CCL-EOHSI)
- e.g. VLSTRACK (NSWC), HPAC/SciPUFF (DSWA)
- e.g. MENTOR/RAMS (CCL-EOHSI)
- e.g. LLNL-NARAC Model (DOE)
- e.g. CAMEO/ALOHA (EPA)
A Framework for Model/Data Fusion with Application to Both Forward and Inverse Problems

1ST Level Transport Problem

MONITORS

SOURCE

SENSITIVE RECEPTORS

2ND Level Transport Problem

Bayesian Model/Data Fusion

EXPOSURE & RISK ANALYSIS
Real Time Meteorological Monitors in New Jersey and Delaware

Meteorological Stations within 10 km of NJ
- No Real Time Data
- Online Hourly Data

Projection: UTM NAD 1983 Zone 18N
NE: 41.47N 73.34W
SW: 38.83N 75.97W

Meteorological Stations of Delaware
- No Real Time Data
- Online Hourly Data

Projection: UTM NAD 1983 Zone 18N
NE: 40.02N 74.26W
SW: 38.22N 76.03W
Example Ia: Calculations with ALOHA Model for Hypothetical Release in New Jersey

Legend
- NJ_Schools

Chemical Release Model
- Uncertainty Region
- Above LOC Region
- NJ_Hospitals

July 12, 1995, 2:00 pm

July 12, 1995, 7:00 pm
Simulation of the Same Case Study With a Comprehensive System that Accounts for Sea Breezes (RAMS-HYPACT)
Simulation of the Same Case Study With a Comprehensive System that Accounts for Sea Breezes (RAMS-HYPACT)

v = 87.30 km
l = 1220 GMT
NJ-xz.avi
Vertical Wind Structure of Sea Breeze (from RAMS-HYPACT)
Example Ib: Hypothetical Anthrax Release Simulation Results, Modeled Using ISC and CALPUFF

Continuous release modeled with ISC at 250m resolution (08:00 & 16:00 – zero concentration at 12:00)

Continuous release modeled with CALPUFF at 250m resolution (08:00, 12:00 & 16:00)
Hypothetical Anthrax Release Simulation Results, Modeled Using CALPUFF

Continuous release modeled with CALPUFF at 1km resolution (08:00, 12:00 & 16:00)

Continuous release modeled with CALPUFF at 250m resolution (08:00, 12:00 & 16:00)
Example Ic: Potential Environmental Impact of Forest Fires in the Vicinity of the Savannah River Site
3-D Views of the Smoke Plume
(Superimposed to the ABL Wind Field)

the smoke plume at 2200 GMT (5:00 PM local time)

the smoke plume at 0800 GMT (3:00 AM local time, next day)
3-D Views of the Smoke Plume (Superimposed to the ABL Wind Field)

Click to animate
COMPREHENSIVE APPLICATION EXAMPLE II:
Regional/Multiscale Modeling of Photochemical Air Pollution for Regulatory Control Strategy Development
Physical/chemical transformations (e.g. involving \( \cdot \text{OH} \)) over multiple spatial/temporal scales “link” gaseous/particulate pollutant dynamics in an “one-atmosphere” system.
The Ozone Problem is Persistent Across the US – Particularly Critical for New Jersey (Statewide Nonattainment of the Standard)

Counties Designated Nonattainment for Ozone (Source, USEPA, 2002)

Photochemistry 000: Dissociation of nitrogen dioxide by sunlight forms equal numbers of nitric oxide molecules and oxygen atoms which convert oxygen to ozone. Ozone and nitric oxide react to reform nitrogen dioxide.
In air contaminated with reactive hydrocarbons and hydroxyl radicals, peroxy radicals are formed. These oxidize nitric oxide to nitrogen dioxide. This process leaves very little of the nitric oxide to react with ozone and in this way ozone builds up to large concentrations.
Nested OTAG (Ozone Transport Assessment Group) Modeling Domains: Efforts in the Mid-Late ’90s Applied Mostly UAM-V to Ozone Episodes from 1988 to 1995; Currently we are Focusing on the Summer of 1999 Using CMAQ
Census Tracts within the “Intermediate” Grid of CMAQ/MENTOR: The “NE Corridor” (Boston-Washington) Area “Behaves” as One Sprawling Metropolis
UAM-V Simulation of Summer 1995
Layer 1

Base1c: 2007 Hrly Ozone, Layer 1

Base1c (bas1cD2): July 95 Episode
OTAG: Northeast Modeling and Analysis Center (NEMAC)

Click to animate
UAM-V Simulation of Summer 1995
Layer 5

Lyr 5 Hrly Ozone: Base07

Base07: 07BasicD2; July 95
OTAG: Northeast Modeling and Analysis Center (NEMAC)

July 10, 1995 0:00:00
Min=−999 at (1,1), Max= 125 at (50,17)
Example: Daily Maxima of 8-hr Average Ozone Concentrations (7/16/1999) for the Inner OTAG Domain (Calculated Using Models-3/CMAQ)
CMAQ Simulation of Ground-Level Ozone, July 11-24, 1999
Base Case

Surface Layer Ozone
CB4 Chemistry 38km Grid Resolution
Emissions: Base Case

Jul 11, 1999 0:00:00
Min = 35 at (1,1), Max = 85 at (1,1)

38km-base.zvi
CMAQ Simulation of Ground-Level Ozone, July 11-24, 1999
NOX Emissions Reduced by 50%

Surface Layer Ozone
CB4 Chemistry 36km Grid Resolution
Emissions: 50% Cut for NOx, 0% for VOC

July 11, 1999 0:00:00
Min= 35 at (1,1), Max= 35 at (1,1)

36km-50nox.avi
CMAQ Simulation of Ground-Level Ozone, July 11-24, 1999
VOC Emissions Reduced by 50%

Surface Layer Ozone
CB4 Chemistry 36km Grid Resolution
Emissions: 0% Cut for NOx, 50% for VOC

July 11,1999 0:00:00
Min= 35 at (1,1), Max= 35 at (1,1)

Exposure Modeling Course: Air Transport/Dispersion
Computational Chemodynamics Laboratory
Relative Effectiveness of VOC vs NOx Intensive Controls in Reducing Daily Maxima of 8-hr Average Ozone Concentrations: NOx Controls More Effective

Difference of base case results minus NOx-intensive strategy

Daily maxima of 8-hr average ozone concentrations (ppb)

(CMAQ calculations for 7/16/1999)

Difference of base case results minus VOC-intensive strategy

Daily maxima of 8-hr average ozone concentrations (ppb)

(CMAQ calculations for 7/16/1999)
Some of the General Findings for New Jersey (and the Northeast)

- The Eastern United States are one airshed
  - Only regional strategies can work
- The NE Corridor (Boston-Washington) is one sprawling metropolis
  - Managing sprawl and emissions must consider multiple MSAs simultaneously
- New Jersey is always downwind
  - Even if all anthropogenic emissions were eliminated NJ would still be in non-attainment
- NOx controls are more effective regionally than VOC controls
  - But must be implemented carefully regionally/locally
- Different subregions respond differently to the same controls
  - E.g., a strategy that benefits NJ may worsen air quality in NYC
Spatiotemporal patterns of surface benzene concentrations predicted by CMAQ (at 12 km resolution) for January and July of 2001

**January 1, 2001 0:00:00**
Min = 0.01 at (3,35), Max = 1.31 at (31,31)

**July 1, 2001 0:00:00**
Min = 0.03 at (40,1), Max = 1.13 at (14,10)
Spatiotemporal patterns of surface formaldehyde concentrations predicted by CMAQ (at 12 km resolution) for January and July of 2001.
Benzene spatial distributions (annual and seasonal) and sample hourly time series predicted by CMAQ (at 4 km resolution) for 2001

EPA’s CMAQ-4km predicted 2001 hourly benzene in Central Philadelphia

[Images of spatial distributions and time series plots showing benzene concentrations]
Formaldehyde spatial distributions (annual and seasonal) and sample hourly time series predicted by CMAQ (at 4 km resolution) for 2001

Annual Average

Seasonal Average winter

Seasonal Average spring

Seasonal Average summer

Seasonal Average fall

EPA's CMAQ-4km predicted 2001 hourly formaldehyde in Central Philadelphia
COMPREHENSIVE APPLICATION EXAMPLE II:

Environmental Impact of the Contaminants Released from the World Trade Center Collapse and Fires
HAZECAM Photographs: Courtesy NESCAUM

9/11/2001 12:01 PM

9/11/2001 2:01 PM

9/12/2001 3:01 PM

9/13/2001 6:01 AM
SPOT and LANDSAT Images of the WTC Plume at Noon on 9/11 and 9/12
MODIS (MODe rate-resolution Imaging Spectroradiometer) Images from NASA’s Terra Satellite

9-11-01 11:20 AM EDT  9-12-01 12:00 PM EDT
NASA Space Station Images

9/11/2001 12:10 PM

9/11/2001 12:30 PM
NASA GOES-8 Satellite Image of WTC Plume on 9/11/2001

NASA'S GOES-8 satellite 1km visible image taken starting at 12:45 pm EDT, shows debris field of the collapse of the WTC towers and the smoke plume advected south along the coast of NJ that is over 90 miles long.
The Triple-Nested RAMS 4.3 Modeling Domain
with 4 km (D1), 1 km (D2), and 250 m (D3) Horizontal Grid Structure

RAMS4.3 simulations utilized the following data for the initial fields:
- Eta data available every 3 hours over a horizontal grid resolution of 40 km
- ASOS data from 4 nearby airports (Newark, Teterboro, J.F.K., LaGuardia) and Central Park available every hour
- Surface data from NCAR available every 6 hours

Initial RAMS4.3 simulations utilized the following for the surface fields:
- DEM 30 seconds topography data from RAMS database
- 30 seconds vegetation data from RAMS database

Legend
- Meteorological Stations used in RAMS Simulations
  (A) NJ Newark Int. Airport
  (B) NJ Teterboro Airport
  (C) NY Central Park
  (D) NY Laguardia Int. Airport
  (E) NY JFK Int. Airport
Instantaneous Views of the WTC Plume, Simulated Using the RAMS/HYPACT Prognostic Meteorological and Particle Dispersion Models  
Top: 3-d Plume View; Bottom: Surface Layer Wind Fields and Concentration Gradients
(Concentration Fields are Normalized with Respect to Maximum of Each Instance)
WTC Plume Dispersion Modeling Employing the Mesoscale Prognostic RAMS/HYPACT Platform

13:00:00 GMT
11 Sep 01
WTC plume simulated by RAMS-HYPACT
1 of 167
Lowest 20 layers

Click to animate
WTC Plume Dispersion Modeling Employing the Mesoscale Prognostic RAMS/ HYPACT Platform
Surface Layer Wind Fields and Concentration Gradients (Concentration Fields are Normalized with Respect to Maximum of Each Instance)
WTC Plume Dispersion Modeling Employing the Mesoscale Prognostic RAMS/HYPACT Platform

RAMS/HYPACT Simulation Results
Grid 3, September 11, 2001, 1200 EDT

Spot Satellite Image
September 11, 2001, 11:55 EDT
September 11, 2003

Normalized 8-hour averaged (a, b) and 24-hour averaged (c) surface layer concentration fields in Grid 3 calculated with RAMS/HYPACT (concentrations are normalized with respect to the instance max)
September 12, 2003

Normalized 8-hour averaged (a, b, & c) and 24-hour averaged (d) surface layer concentration fields in Grid 3 calculated with RAMS/HYPACT (concentrations are normalized with respect to the maximum of each instance)
Example Test: Time Series of PM2.5 Concentrations Observed at PS 64 in Manhattan Compared with 24-Hour Averaged Surface Layer Concentrations in Grid 3 Calculated with RAMS/HYDAPC
A final reminder: To assess (health) effects of airborne contamination it is not enough to characterize concentrations with respect to time and geographic location. In addition, factors such as: dynamic microenvironmental attributes, demographic and physiological characteristics, activity patterns, etc. differentiate significantly the exposures and doses of individuals (and of selected subpopulations) that result from environmental pollution or a hazardous atmospheric release.

Example: Dependence of inhaled fine PM dose on gender, age, and activity (MET = Metabolic Equivalent of Tasks)
Caveat: Neighborhood Scale Effects Can Modify Significantly Estimates from Atmospheric Transport Models or from Monitor Interpolations (Barriers, Channeling, Local Flows, Trapping): Need for Both CFD & Simplified Models
From Microenvironmental to Personal:
Air Contaminant Dispersion Takes Place Around Us
(and with Ourselves as the Source...)
The Convective Personal Flow Field Affects
Inhalation Intake and Releases from the Body
(Video from G. Settles)
ADDENDUM

Basic Concepts of Atmospheric Thermodynamics:
A Brief Reminder
Adiabatic Processes and the Concept of an Air Parcel

- An air parcel of infinitesimal dimensions that is assumed to be
  - Thermally insulated – adiabatic
  - Same pressure as the environmental air at the same level – in hydrostatic equilibrium
  - Moving slowly – kinetic energy is a negligible fraction of its total energy

- Reversible adiabatic process of air

\[ dq = c_v \, dT + P \, d\alpha \]

Add and subtract \( \alpha \, dP \):
\[ dq = c_v \, dT + d(P \alpha) - \alpha \, dP \]

Use ideal gas law:
\[ dq = (c_v + R) \, dT - \alpha \, dP \]
\[ dq = c_p \, dT - \alpha \, dP \]

Adiabatic process:
\[ dq = 0 \]
\[ c_p \, dT - \alpha \, dP = 0 \]

Combine with ideal gas law:
\[ \frac{dP}{P} = \frac{C_p}{R} \, \frac{dT}{T} \]
Lapse Rate

- Combine hydrostatic equation and ideal gas law

\[
\frac{dP}{dz} = -g \rho = -g \frac{PM}{RT}
\]

\[
\frac{dP}{P} = -\frac{gM}{RT} \, dz
\]

- For adiabatic process

\[
\frac{dP}{P} = \frac{C_p}{R} \frac{dT}{T}
\]

- Therefore

\[
\frac{dT}{dz} = -\frac{gM}{C_p} \, dz
\]

\[
\frac{dT}{dz} \text{ is Dry Adiabatic Lapse Rate (DALR)}
\]
Dry and Wet Adiabatic Lapse Rate

- **Dry adiabatic lapse rate (DALR)**
  \[
  \frac{dT}{dz} = -\frac{gM}{C_p} = -\frac{9.81 \text{ m/s}^2 \times 29 \text{ g/mol}}{3.5 \times 8.314 \text{ m}^3 \cdot \text{Pa/mol} \cdot \text{K}} \times \frac{\text{kg}}{1000 \text{ g}} \times \frac{\text{Pa} \cdot \text{m} \cdot \text{s}^2}{\text{kg}}
  \]
  \[
  = -0.00978 \frac{\text{K}}{\text{m}} = -9.78 \frac{\text{C}}{\text{km}} = -5.37 \frac{\text{F}}{1000 \text{ ft}} \approx -10 \frac{\text{C}}{\text{km}}
  \]

- Or on a unit mass basis
  \[
  \frac{dT}{dz} = -\frac{g}{c_p} = \frac{9.81 \text{ m/s}^2}{1004 \text{ J/kg} \cdot \text{K}} = -9.8 \frac{\text{K}}{\text{km}}
  \]

- **Effect of moisture**

  Because
  \[
  C'_{p} = (1 - w)C_{p,Air} + wC_{p,Water Vapor}
  \]
  \[
  C_{p,Water Vapor} > C_{p,Air}
  \]
  \[
  C'_p > C_p
  \]
  Wet adiabatic lapse rate < DALR (temperature decreases slower as air parcel rises)
Potential Temperature

- Current state: $T$, $P$
- Adiabatically change to: $T_o$, $P_o$

\[ T_o = T \left( \frac{P_o}{P} \right)^{\left( \frac{\gamma-1}{\gamma} \right)} \]

- Set $P_o = 1000$ mb, $T_o$ is potential temperature $\Theta$
- If an air parcel is subject to only adiabatic transformation, $\Theta$ remains constant
- Potential temperature gradient

\[ \frac{\Delta \Theta}{\Delta z} = \left( \frac{dT}{dz} \right)_{\text{actual}} + DALR \]
Contaminants released in the Atmosphere are Transported/Dispersed by Winds and Turbulence

- Turbulent flows – irregular, random, and cannot be accurately predicted
- Eddies (or swirls) – Macroscopic random fluctuations from the “average” flow
  - Thermal eddies
  - Convection
  - Mechanical eddies
  - Shear forces produced when air moves across a rough surface
Lapse Rate and Stability

- Neutral
- Stable
- Unstable
Richardson Number and Stability

- **Stability parameter**

- **Richardson number**
  - Stable
  - Neutral
  - Unstable

\[ s = \frac{g}{T} \left( \frac{\Delta \Theta}{\Delta z} \right) \]

\[ Ri = \frac{g \left( \frac{\Delta \Theta}{\Delta z} \right)}{T \left( \frac{d u}{dz} \right)^2} \]
Stability Classification Schemes

- Pasquill-Gifford Stability Classification
  - Determined based on
    - Surface wind
    - Insolation
  - Six classes: A through F

- Turner’s Stability Classification
  - Determined based on
    - Wind speed
    - Net radiation index
  - Seven classes
  - Feasible to computerize
Inversions

- Definition
- Types
  - Radiation inversion
  - Evaporation inversion
  - Advection inversion
  - Frontal inversion
  - Subsidence inversion
- Fumigation
Planetary Boundary Layer

- Turbulent layer created by a drag on atmosphere by the earth’s surface
- Also referred to as mixing height
- Inversion may determine mixing height
Planetary Boundary Layer

- Neutral conditions
  - Mixing height

- Increased wind speed and surface roughness cause higher $h$.

$$h \approx \alpha \frac{u_*}{f}$$
Planetary Boundary Layer

- Unstable conditions
  - Mixing height

\[ h = \left[ \frac{2\int_{t}^{t_0} H \, dt}{C_p \rho \left( DALR - \frac{dT}{dz} \right)} \right]^{1/2} \]
Planetary Boundary Layer

- Stable conditions
  - Mixing height

\[ h \approx 0.4 \sqrt{\frac{u_*}{f}} L \]
Surface Layer

- Fluxes of momentum, heat, and moisture remain constant
- About lower 10% of mixing layer
Surface Layer

- Monin-Obukhov length

- Monin-Obukhov length and stability classes

\[ L = -\frac{\rho C_p T u_*^3}{\rho g H} \]
Surface Layer Wind Structure

- Neutral air

\[
\bar{u} = \frac{u_*}{k_a} \ln \left( \frac{z}{z_0} \right)
\]
Surface Layer Wind Structure

- Unstable and stable air

\[ u = \frac{u_*}{k_a} \left[ \ln \left( \frac{z}{z_0} \right) - \Psi_m \left( \frac{z}{L} \right) \right] \]

For unstable air

\[ \Psi_m = 2 \ln \left( \frac{1 + x}{2} \right) + \ln \left( \frac{1 + x^2}{2} \right) - 2 \arctan(x) + \frac{\pi}{2} \]

\[ x = \left( 1 - 16 \frac{z}{L} \right)^{\frac{1}{4}} \]

For stable air

\[ \Psi_m = -5 \left( \frac{z}{L} \right) \]
Friction Velocity

\[ u_* = \frac{k_a \bar{u}}{\ln\left(\frac{z}{z_0}\right) - \Psi_m\left(\frac{z}{L}\right)} \]

- Measurements of wind speed at multiple levels can be used to determine both \( u_* \) and \( z_0 \)
Power Law for Wind Profile

- Wind profile power law
  \[
  \frac{\overline{u}}{u_m} = \left( \frac{z}{z_m} \right)^p
  \]
- Value of \( p \)
Estimation of Monin-Obukhov Length

- For unstable air
  \[ Ri = \frac{z}{L} \]

- For stable air
  \[ \frac{z}{L} = \frac{Ri}{1 - 5Ri} \]

- Bulk Richardson Number
  \[ Rb = \frac{g z^2}{T} \left( \frac{dT}{dz} + DALR \right) \]
  \[ Ri = \frac{Rb}{p^2} \]
Air Pollution Climatology

- Meteorology vs. climatology
- Meteorological measurements and surveys
- Pollution potential
  - low level inversion frequency in US
Air Pollution Climatology

- Mean maximum mixing height determined by
  - Morning temperature sounding
  - Maximum daytime temperature
  - DALR
- Stability wind rose