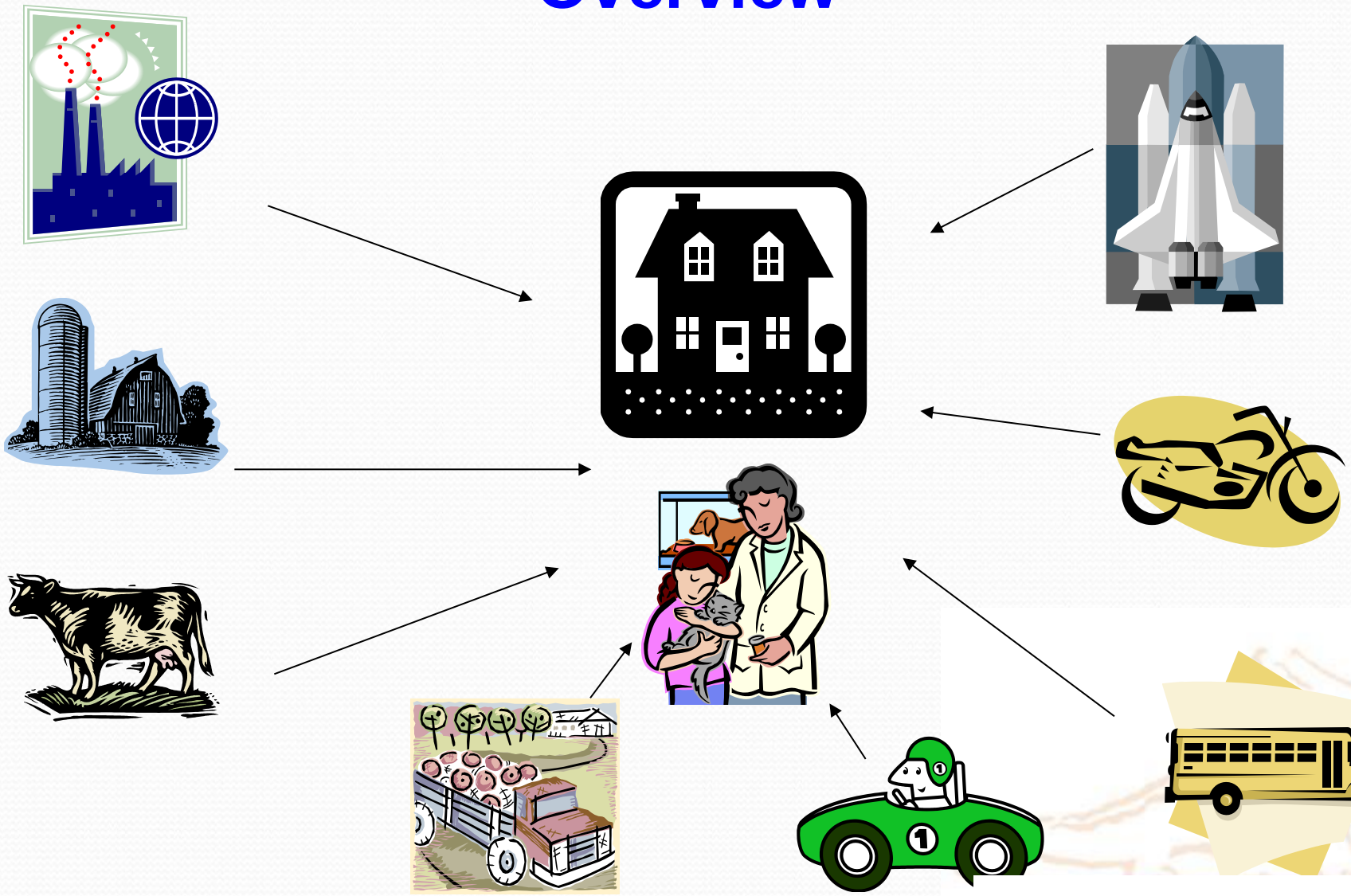
Reading: Chap 7.3

Air Quality Modeling

- Overview of AQ Models
- Gaussian Dispersion Model
- Chemical Mass Balance (CMB) Models

Overview



Overview

What is the level of my exposure to these emissions? Is my family safe? Where is safe? How about the adverse impact on the environment (plants, animals, buildings)? How to predict the impact of emissions resulting from population growth?

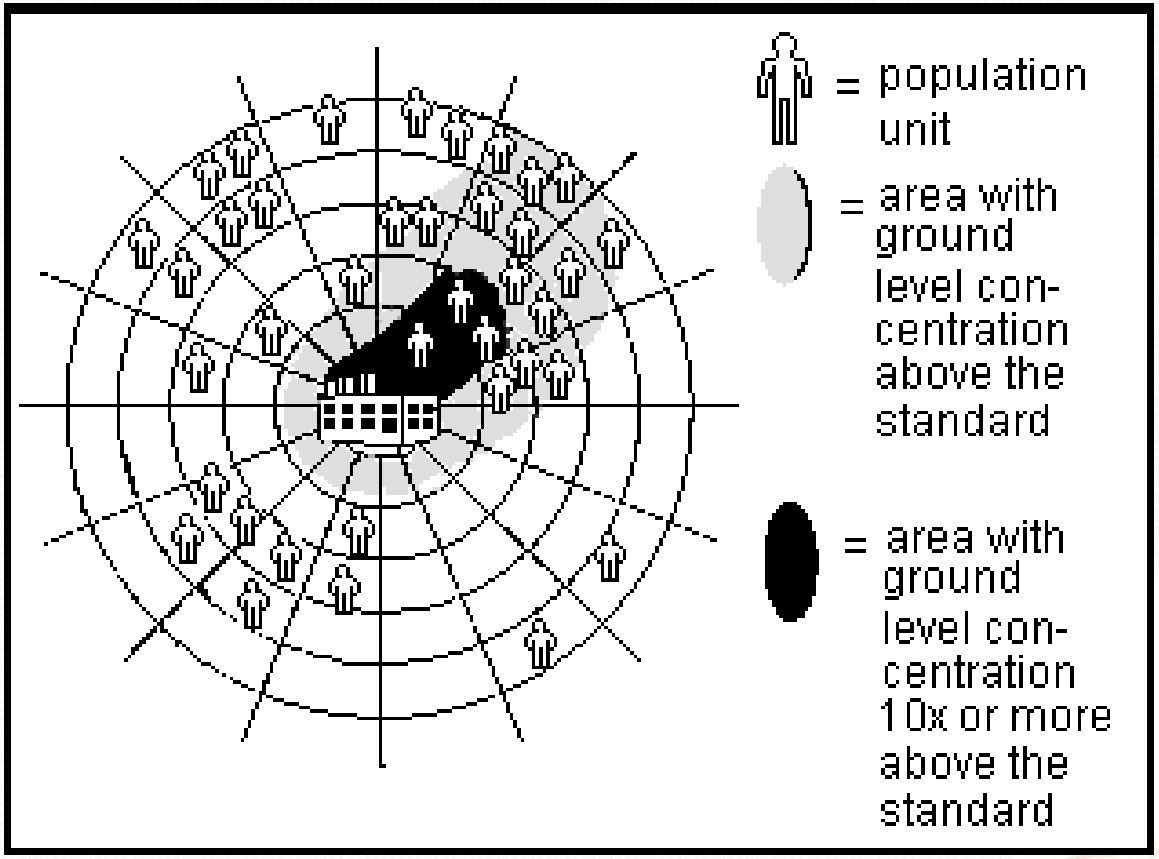
- Air Quality Models are mathematical formulations that include parameters that affect pollutant concentrations. They are used to
  - Evaluate compliance with NAAQS and other regulatory requirements
  - Determine extent of emission reductions required
  - Evaluate sources in permit applications

Air Quality Modeling (AQM)

- Predict pollutant concentrations at various locations around the source.
- Identify source contribution to air quality problems.

- Assess source impacts and design control strategies.
- Predict future pollutant concentrations from sources after implementation of new regulatory programs.

Areas Surrounding the Site of Release



Air Quality Modeling (AQM)

- Mathematical and numerical techniques are used in AQM to simulate the dispersion of air pollutants.

- Modeling of the dispersion of pollutants
  - Toxic and odorous substances
  - Single or multiple points
  - Point, Area, or Volume sources

- Input data required for Air Quality Modeling
  - Source characteristics
  - Meteorological conditions
  - Site and surrounding conditions

Ambient Air Concentration Modeling

- Types of Pollutant Sources
  - Point Sources
    - e.g., stacks or vents
  - Area Sources
    - e.g., landfills, ponds, storage piles
  - Volume Sources
    - e.g., conveyors, structures with multiple vents

Types of AQ Models

Meteorological Model

Emission Model

Chemical Model

Temporal and spatial emission rates
Topography
Chemical Transformation
Pollutant Transport
Equilibrium between Particles and gases
Vertical Mixing

Source Dispersion Model

Receptor Model

- **Emission Model**
  - Estimates temporal and spatial emission rates based on activity level, emission rate per unit of activity and meteorology
- **Meteorological Model**
  - Describes transport, dispersion, vertical mixing and moisture in time and space
- **Chemical Model**
  - Describes transformation of directly emitted particles and gases to secondary particles and gases; also estimates the equilibrium between gas and particles for volatile species

- **Source Dispersion Model**
  - Uses the outputs from the previous models to estimate concentrations measured at receptors; includes mathematical simulations of transport, dispersion, vertical mixing, deposition and chemical models to represent transformation.

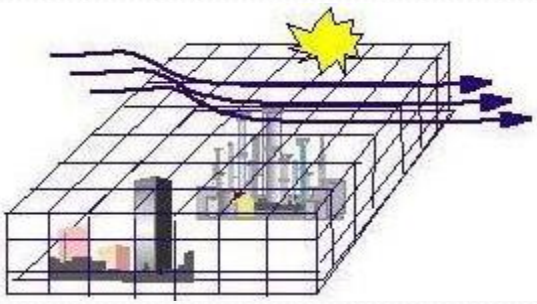
- **Receptor Model**
  - Infers contributions from different primary source emissions or precursors from multivariate measurements taken at one or more receptor sites.

Classifications of AQ Models

- Developed for a number of pollutant types and time periods
  - **Short-term** models – for a few hours to a few days; worst case episode conditions
  - **Long-term** models – to predict seasonal or annual average concentrations; health effects due to exposure
- Classified by
  - **Non-reactive** models – pollutants such as SO_2 and CO
  - **Reactive** models – pollutants such as O_3, NO_2, etc.

AQ Models

- Classified by coordinate system used
  - **Grid-based**
    - Region divided into an array of cells
    - Used to determine compliance with NAAQS
  - **Trajectory**
    - Follow plume as it moves downwind
- Classified by level of sophistication
  - **Screening**: simple estimation use preset, worst-case meteorological conditions to provide conservative estimates. **Purpose?**
  - **Refined**: more detailed treatment of physical and chemical atmospheric processes; require more detailed and precise input data. **So what?**



http://www.epa.gov/scram001/images/grid4.jpg

http://www.epa.gov/scram001/images/smokestacks.jpg

USEPA AQ models

- Screening models available at: http://www.epa.gov/scram001/dispersion_screening.htm
- Preferred models available at: http://www.epa.gov/scram001/dispersion_prefrec.htm
  - A single model found to outperform others
    - Selected on the basis of other factors such as past use, public familiarity, cost or resource requirements and availability
    - No further evaluation of a preferred model is required
- Alternative models available at: http://www.epa.gov/scram001/dispersion_alt.htm
  - Need to be evaluated from both a theoretical and a performance perspective before use
    - Compared to measured air quality data, the results indicate the alternative model performs better for the given application than a comparable preferred model
    - The preferred model is less appropriate for the specific application or there is no preferred model

USEPA AQ models

U.S. ENVIRONMENTAL PROTECTION AGENCY

Technology Transfer Network
Support Center for Regulatory Atmospheric Modeling

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Preferred/Recommended Models

You will need Adobe Acrobat Reader to view the Adobe PDF files on this page. See EPA's PDF page for more information about getting and using the free Acrobat Reader.

These refined dispersion models are listed in Appendix W and are required to be used for State Implementation Plan (SIP) revisions for existing sources and for New Source Review (NSR) and Prevention of Significant Deterioration (PSD) programs. The models in this section include the following:

AERMOD Modeling System - 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 Modeling System - 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.

Other Models - Other dispersion models including BLP, CALINE3, CAL3QHC/CAL3QHCR, CTDMPLUS, and OCD.

AERMOD Modeling System

The American Meteorological Society/Environmental Protection Agency Regulatory Model Improvement Committee (AERMIC) was formed to introduce state-of-the-art modeling concepts into the EPA's air quality models. Through AERMIC, a modeling system, AERMOD, was introduced that incorporated 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.

USEPA AQ models

Table 7.5 Preferred USEPA Air Quality Dispersion Models

Type/Terrain	Mode (Urban/Rural)	Model
Screening		
Simple	Both	SCREEN 3
Simple	Both	ISC 3
Simple	Both	TSCREEN
Simple	Urban	RAM
Complex	Rural	COMPLEX I
Complex	Urban	SHORTZ
Complex	Rural	RTDM 3.2
Complex	Rural	Valley
Complex	Both	CTScreen
Line	Both	BLP
Refined		
Simple	Urban	RAM
Simple	Both	ISC 3
Simple	Urban	CDM 2.0
Complex	Both	CTDMPLUS
Line	Both	BLP
Line	Both	CALINE-3
Ozone	Urban	UAM-V
Coastal	Both	

Gaussian Dispersion Models

- Most widely used
- Based on the assumption
  - plume spread results primarily by **molecular diffusion**
  - horizontal and vertical pollutant concentrations in the plume are normally distributed (double Gaussian distribution)
- Plume spread and shape vary in response to meteorological conditions

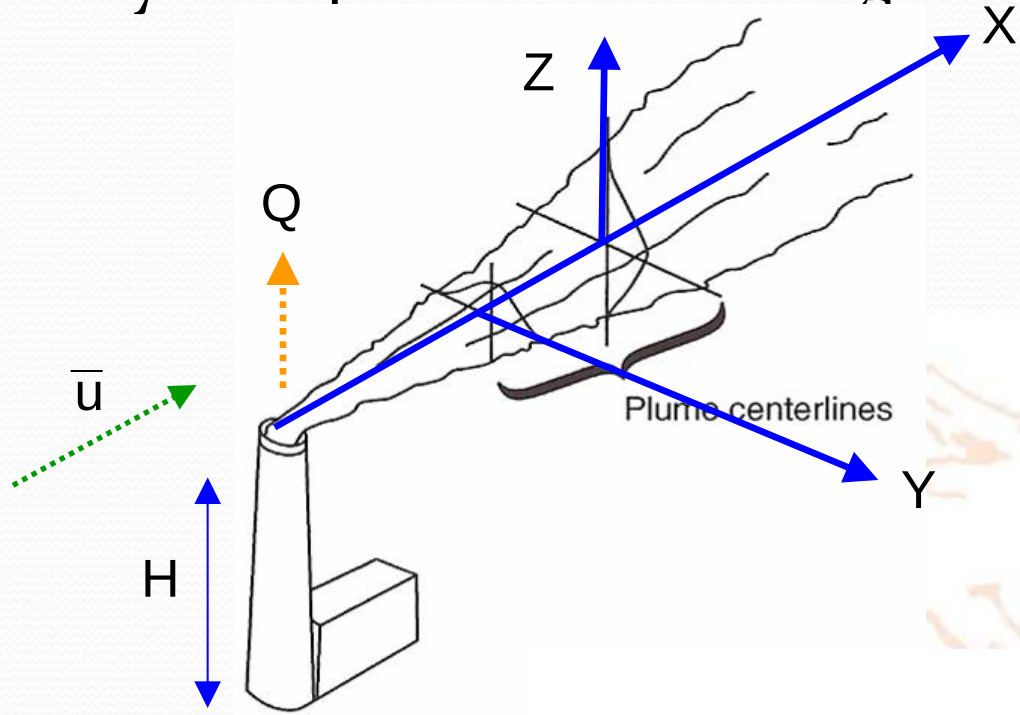


Fig 7.11

Model Assumptions

- Gaussian dispersion modeling based on a number of assumptions including
  - Steady-state conditions (constant source emission strength)
  - Wind speed, direction and diffusion characteristics of the plume are constant
  - Mass transfer due to bulk motion in the x-direction far outshadows the contribution due to mass diffusion
  - Conservation of mass, i.e. no chemical transformations take place
  - Wind speeds are $\geq$1 m/sec.
  - Limited to predicting concentrations > 50 m downwind

Gaussian Dispersion Equation

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

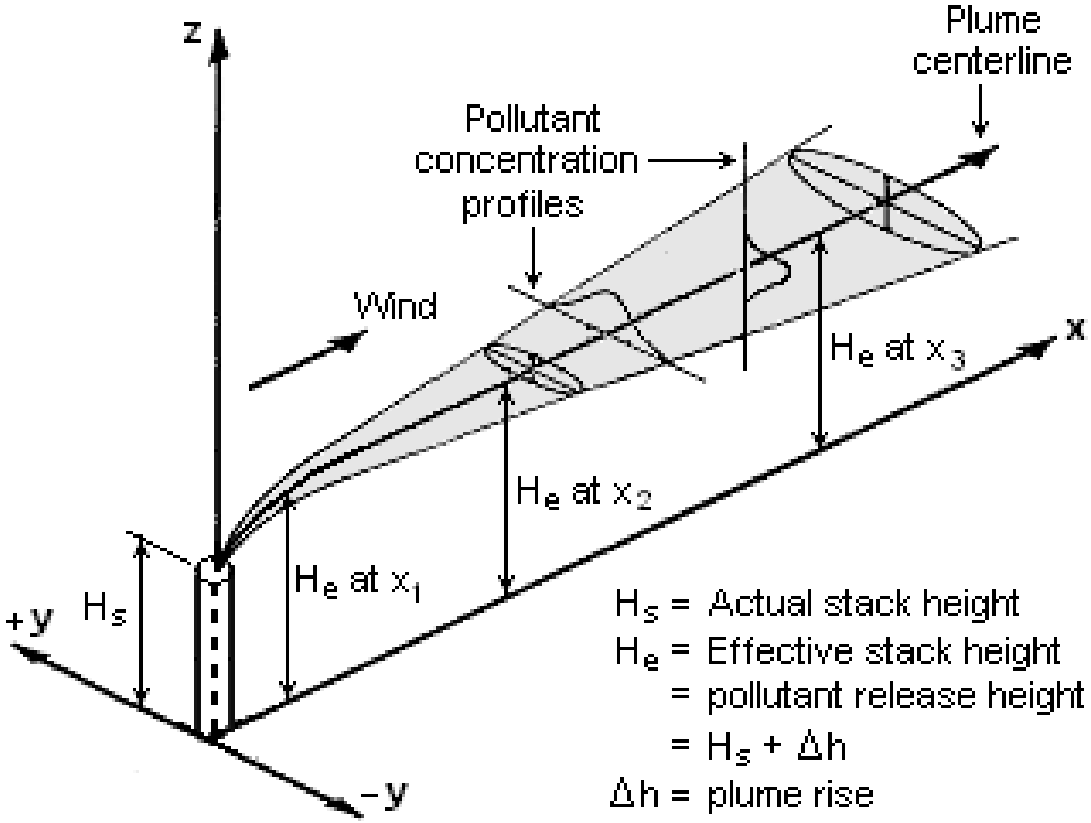
Atmospheric Stability Classes

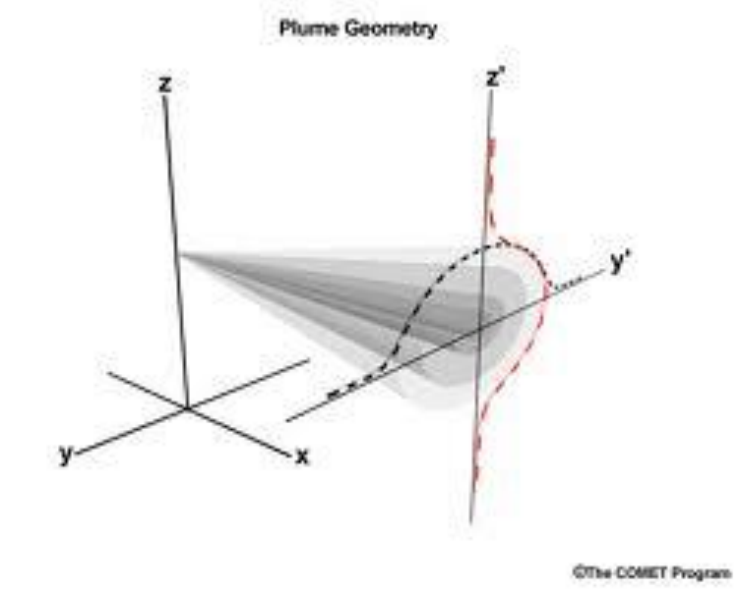
Table 7.4

Wind Speed, 10 m (m/sec)	Day: Incoming Solar Radiation			Night: Thinly Overcast	
	Strong	Moderate	Slight	>4/8 Cloud	<3/8 Cloud
<2	A	A–B	B	E	F
2–3	A–B	B	C	D	E
3–5	B	B–C	C	D	D
>6	C	D	D	D	D

مدل گوسی برای منابع آلاینده نقطه ای

- در این شکل نقطه پایه‌ی دودکش به عنوان مبدأ محور مختصات در نظر گرفته شده است(x توسعه جبهه دود به سمت پایین دست، y توسعه افقی جبهه و z توسعه عمودی جبهه و بیانگر ارتفاع ص





مدل گوسی برای منابع آلاینده نقطه ای

- معادله گوس بر ای‌ن اساس به شکل زی‌ر می باشد:

$$C(x,y,z) = \frac{Q}{2\pi U \sigma_y \sigma_z} exp \frac{-y^2}{2\sigma_y^2} \left\{ exp \frac{-(z-H)^2}{2\sigma_z^2} \right\}$$

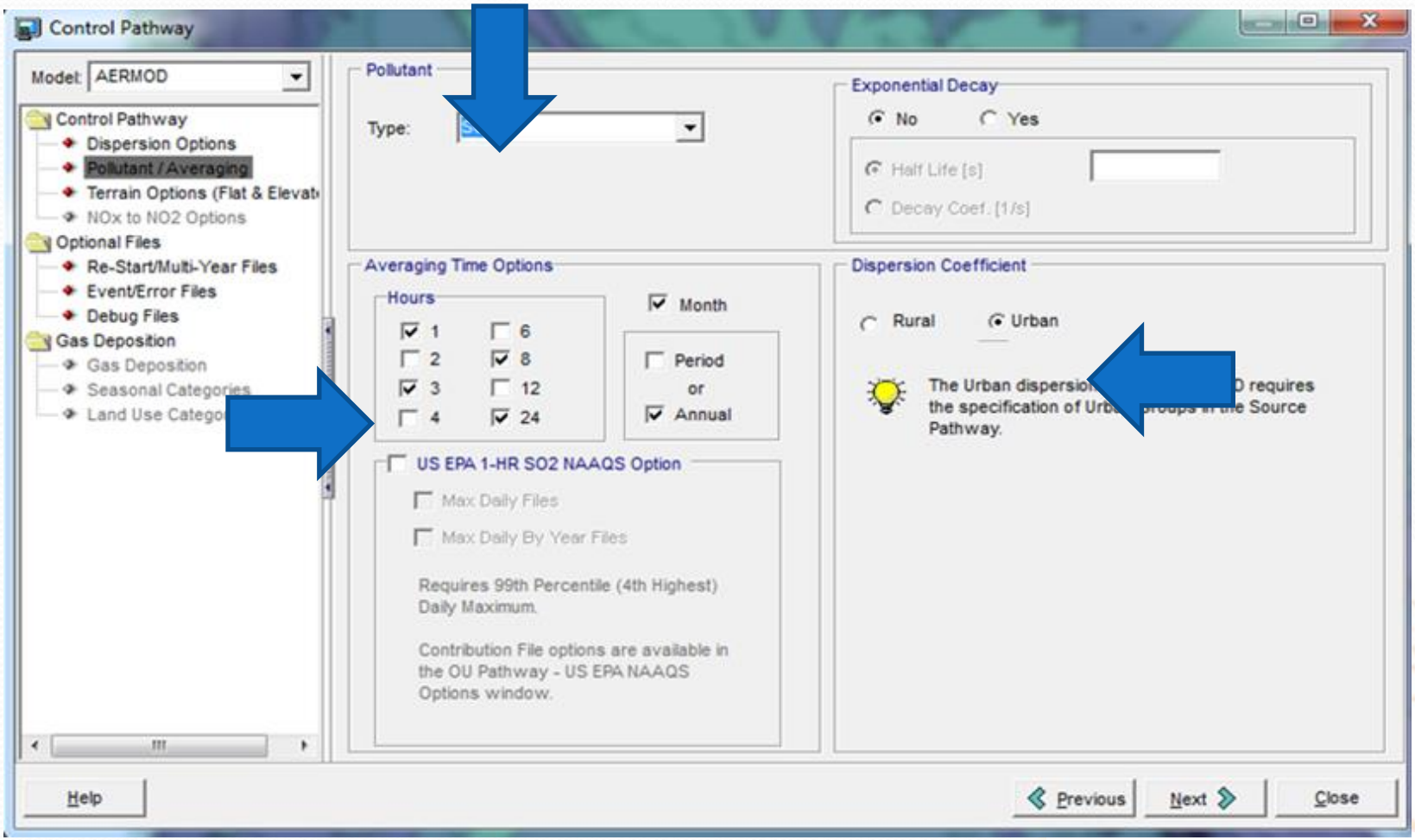
در ای‌نجا:

- ✓ C(x، y، z): غلظت مواد آلای‌نده بر حسب می‌کروگرم بر متر مکعب،
- ✓ x: مسافت در جهت پای‌ی‌ن دست بر حسب متر،
- ✓ y: فاصله افقی از محور مرکزی جبهه دود بر حسب متر،
- ✓ Q: سرعت پراکنش مواد آلای‌نده بر حسب می‌کروگرم بر ثانی‌ه،
- ✓ H: ارتفاع موثر توده بر حسب متر ($H = h + \Delta h$).
- ✓ U: سرعت متوسط باد در ارتفاع موثر صعود دود بر حسب متر بر ثانی‌ه
- ✓ σy: ضری‌ب پراکنش افقی(انحراف از استاندارد) بر حسب متر
- ✓ σx: ضری‌ب پراکنش عمودی (انحراف از استاندارد) بر حسب متر
- ✓ exp: کلمه exp اول، پراکنش افقی و کلمه exp دوم، پراکنش عمودی را توضی‌ح می دهد.

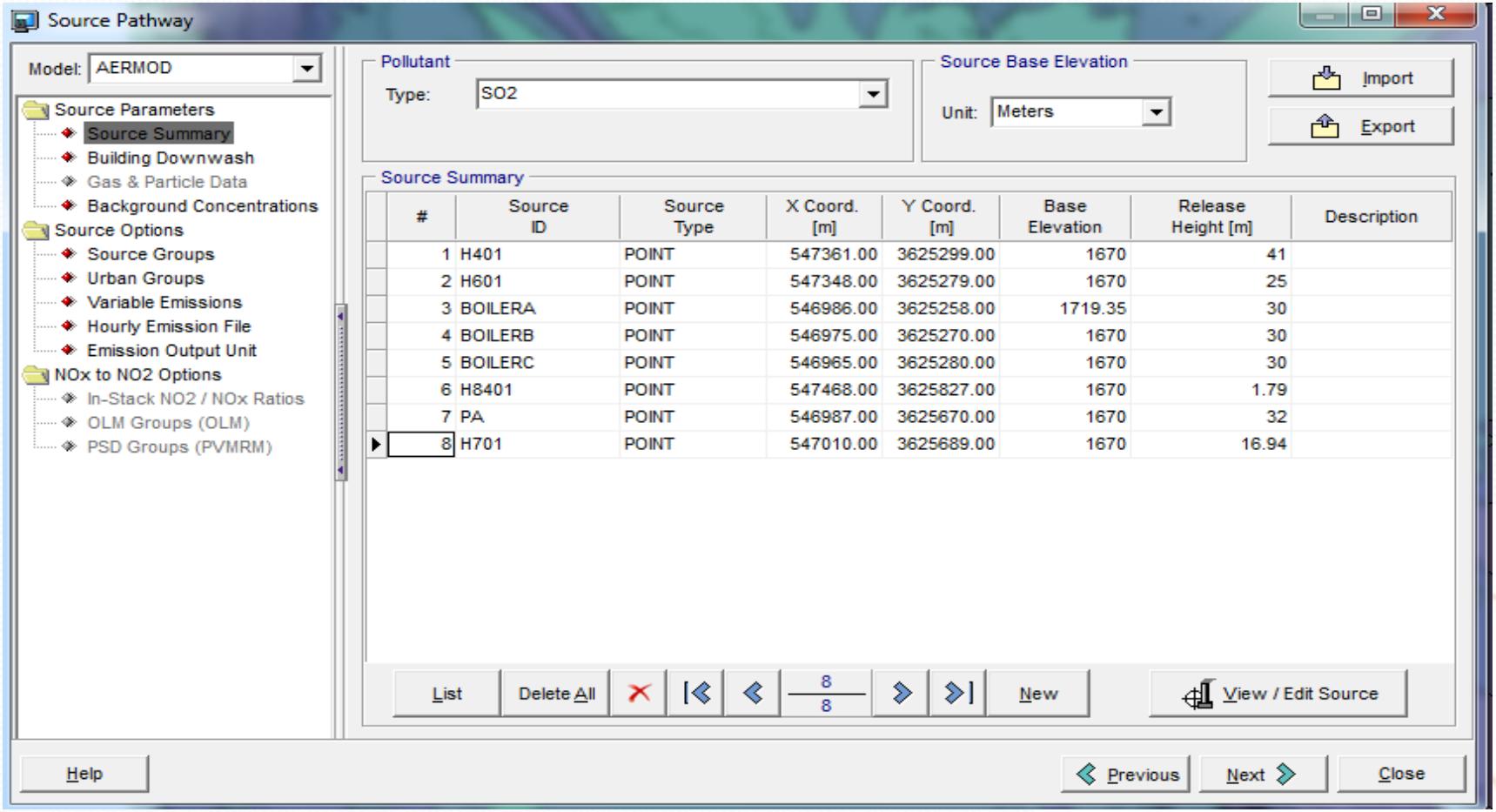
Factors Affecting Dispersion of Pollutants In The Atmosphere

- Source Characteristics
  - Emission rate of pollutant
  - Stack height
  - Exit velocity of the gas
  - Exit temperature of the gas
  - Stack diameter
- Meteorological Conditions
  - Wind velocity
  - Wind direction
  - Ambient temperature
  - Atmospheric stability

- مدل‌سازی از مسیر کنترل آغاز می‌شود. در این مسیر نام پروژه، غلظت، نوع خروجی و میانگین‌های زمانی ۱، ۳، ۸ و ۲٤ ساعته، ماهانه و سالانه، ضریب پراکنش شهری ....

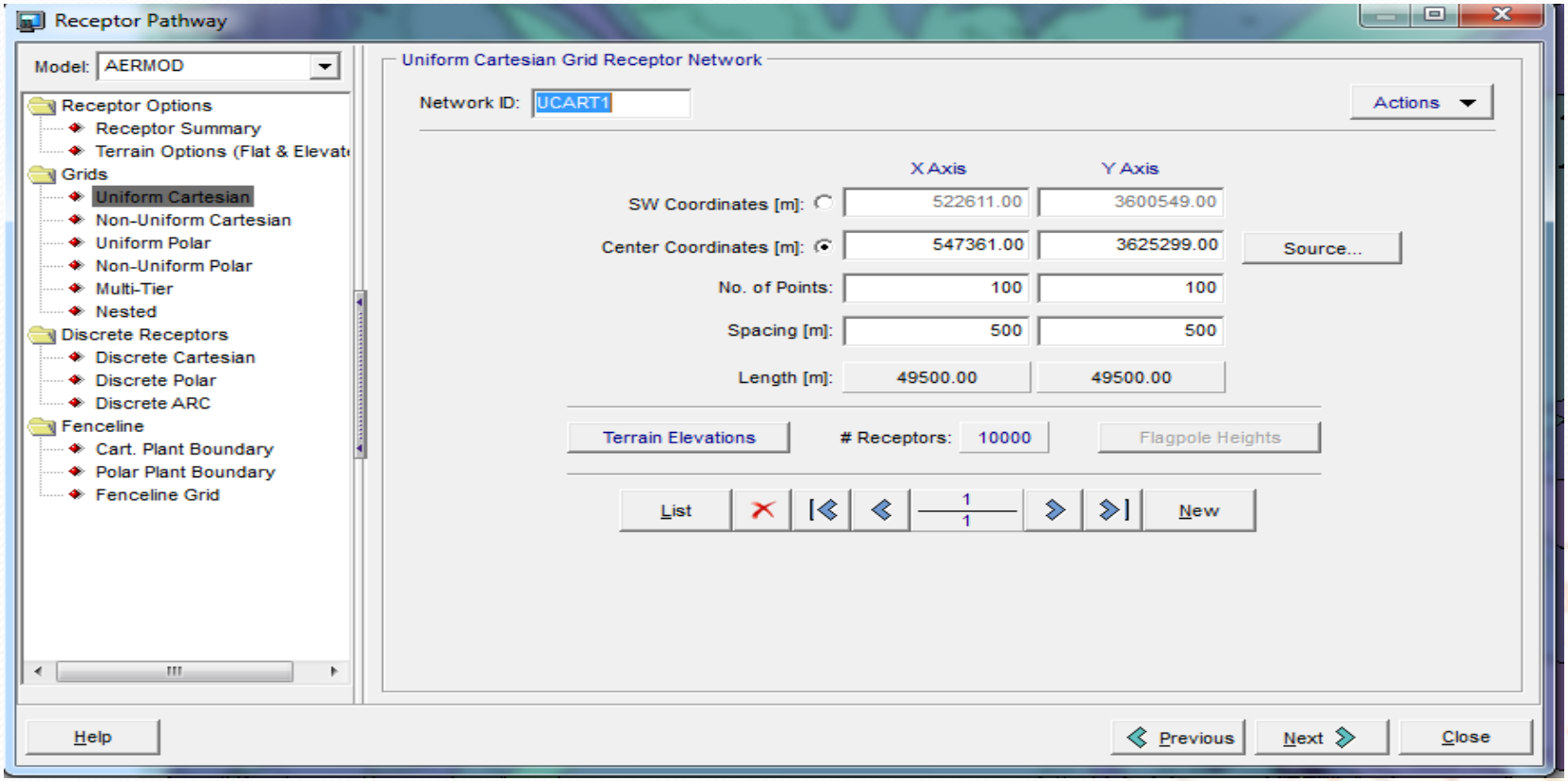


- درمسیر منبع، نوع آلاینده و نوع منبع تعیین می‌شود.

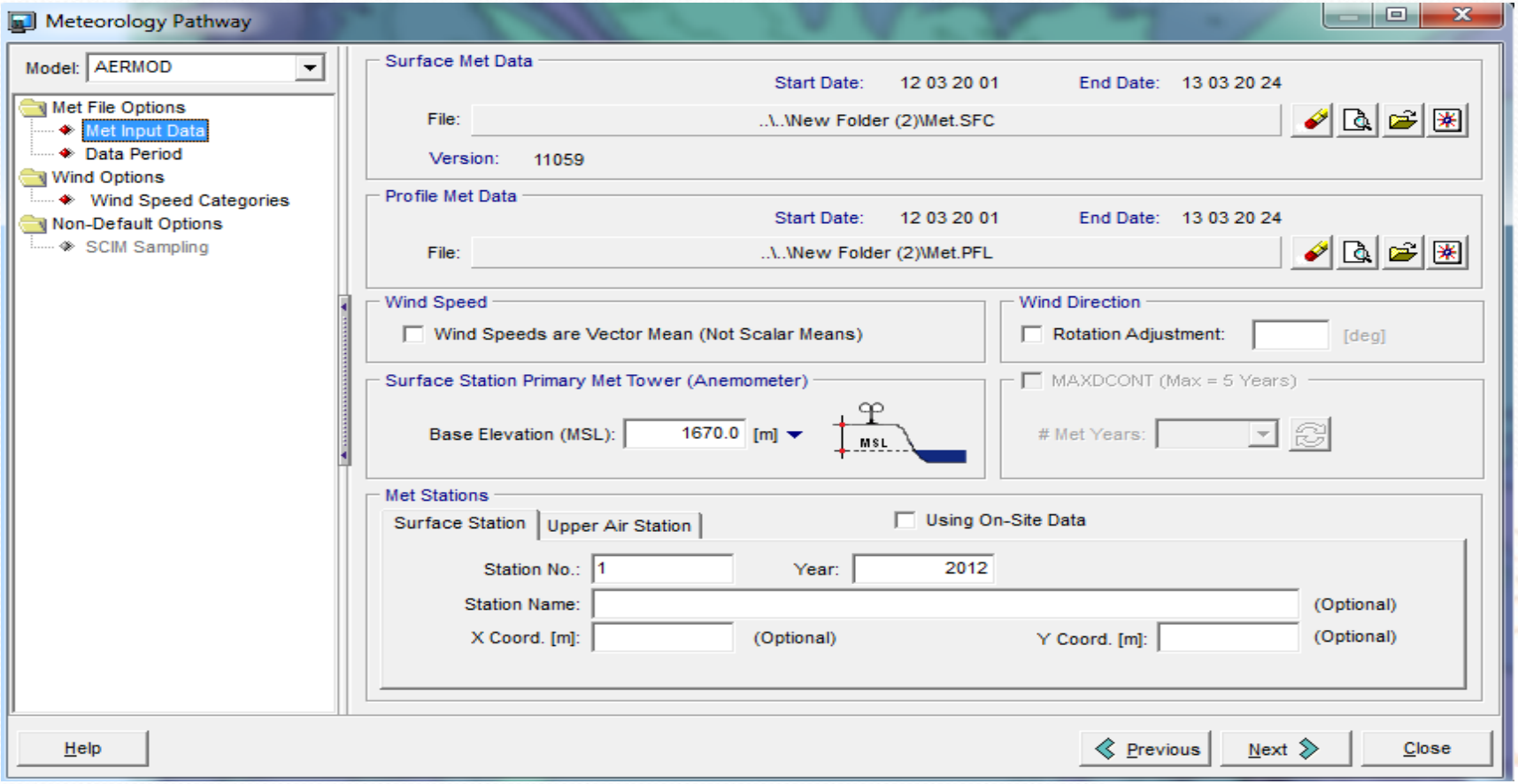


#	Source ID	Source Type	X Coord. [m]	Y Coord. [m]	Base Elevation	Release Height [m]	Description
1	H401	POINT	547361.00	3625299.00	1670	41	
2	H601	POINT	547348.00	3625279.00	1670	25	
3	BOILERA	POINT	546986.00	3625258.00	1719.35	30	
4	BOILERB	POINT	546975.00	3625270.00	1670	30	
5	BOILERC	POINT	546965.00	3625280.00	1670	30	
6	H8401	POINT	547468.00	3625827.00	1670	1.79	
7	PA	POINT	546987.00	3625670.00	1670	32	
8	H701	POINT	547010.00	3625689.00	1670	16.94	

- در مسیر گیرنده، برای هر منبع یک شبکه منظم دکارتی ۱۰۰×۱۰۰ نقطه، با فاصله نقاط ۵۰۰ مترتعریف شد. منبع مورد نظر نیز در مرکز شبکه‌ی تعریف شده قرار گرفت.



- داده‌های هواشناسی پس از پردازش در ماژول AERMET وارد مسیر هواشناسی درAERMOD میشوند. داده‌های هواشناسی یک ساله از تاریخ 2011/03/21 با فرمت SAMSON وارد AERMET می شود



- این اسلاید به بعد فقط جهت مطالعه جنبی ارائه شده است

Dispersion Coefficients: Horizontal

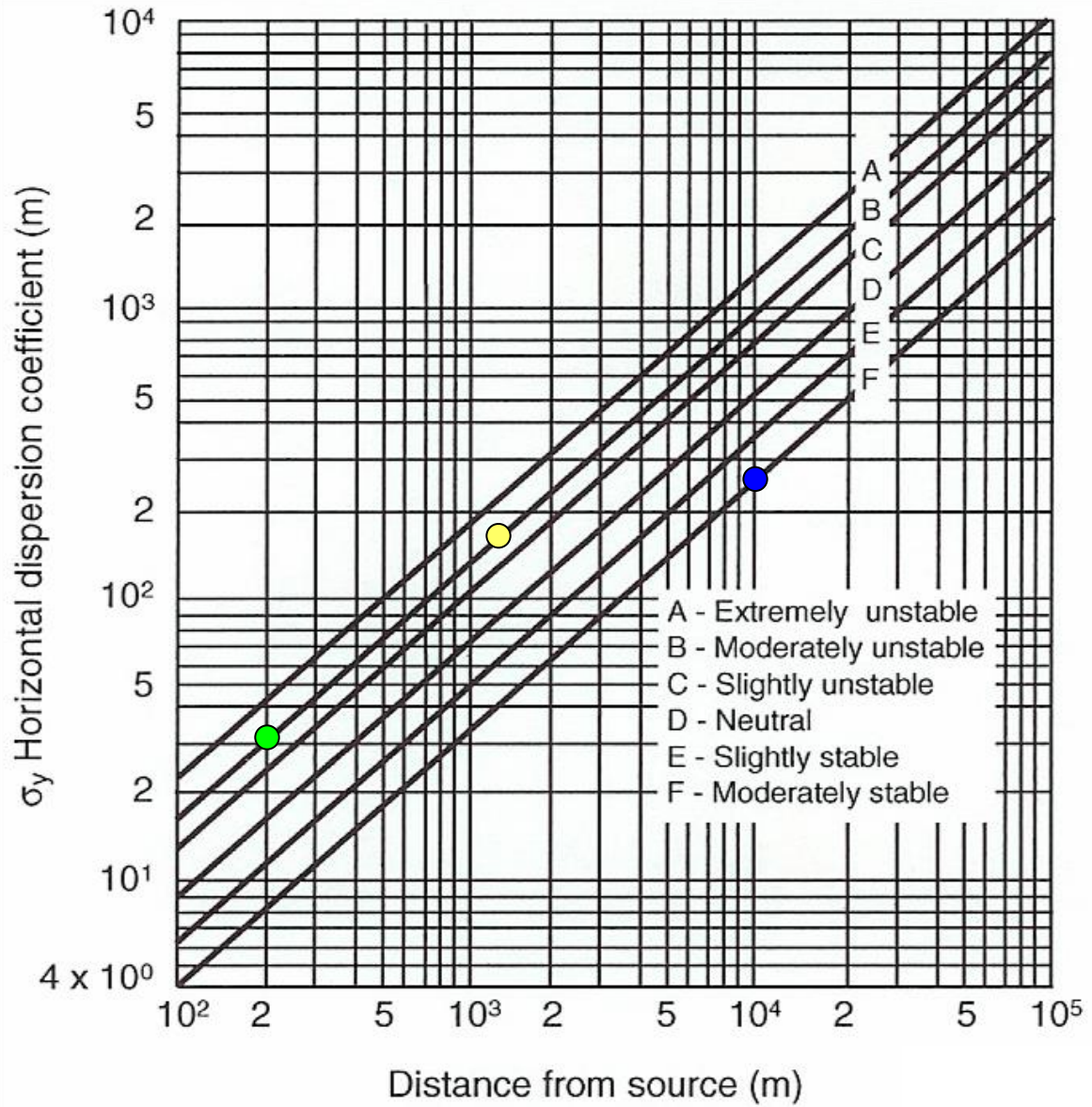


Fig 7.12

Dispersion Coefficients: Vertical

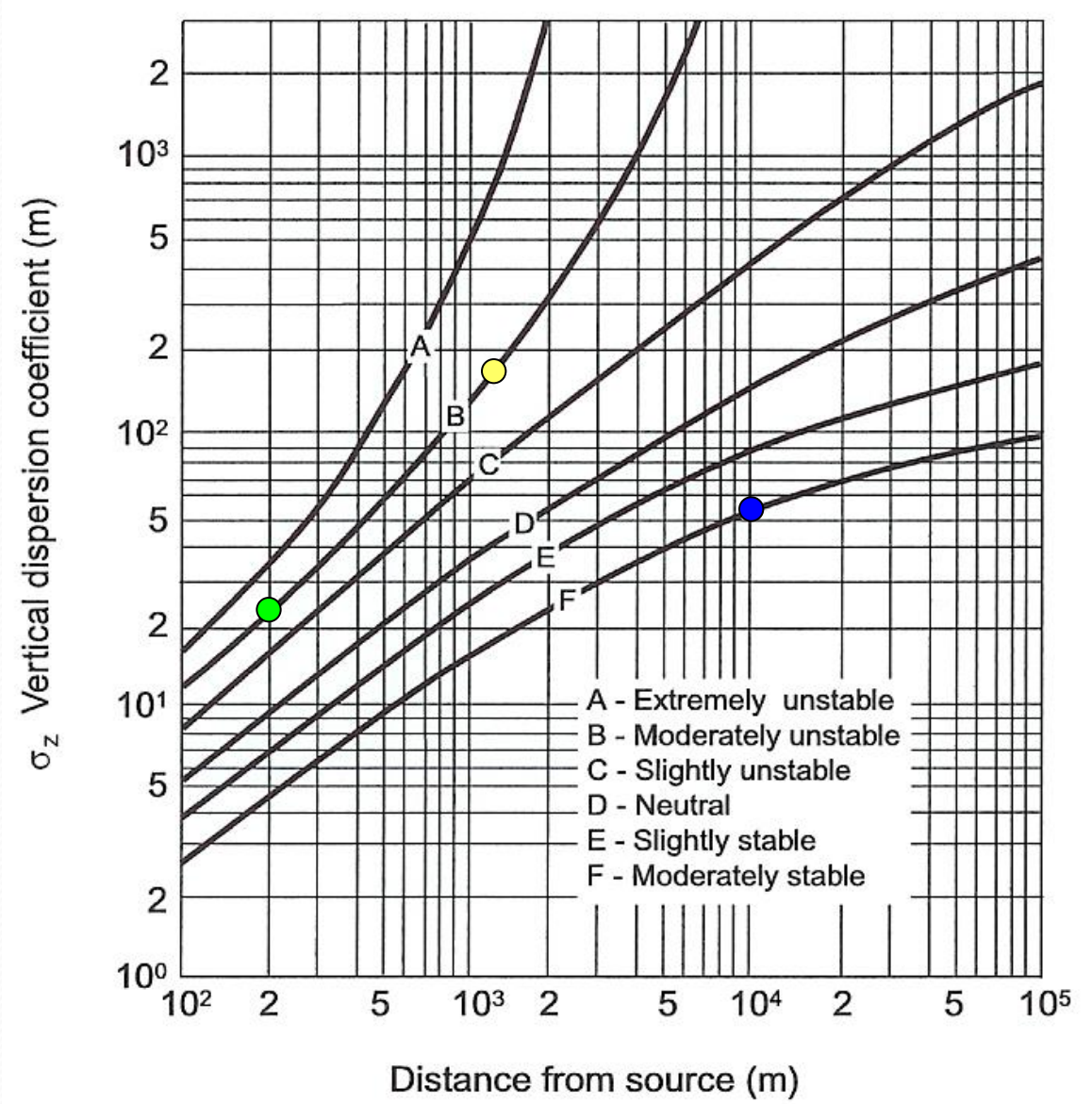


Fig 7.13

Gaussian Dispersion Equation

If the emission source is at ground level with no effective plume rise then

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

Plume Rise

- H is the sum of the physical stack height and plume rise.

$$H=\Delta h_{plume\ rise}+h_{actual\ stack}$$

Plume Rise

Buoyant plume: Initial buoyancy >> initial momentum
Forced plume: Initial buoyancy ~ initial momentum
Jet: Initial buoyancy << initial momentum

- For neutral and unstable atmospheric conditions, **buoyant rise** can be calculated by

$$\Delta h_{plume\ rise} = \frac{21.425F^{0.75}}{\bar{u}} \qquad (\mathrm{F} < 55\, m^4/s^3)$$

$$\Delta h_{plume\ rise} = \frac{38.71F^{0.6}}{\bar{u}} \qquad (\mathrm{F} > 55\, m^4/s^3)$$

where **buoyancy flux** is

$$F = gV_s d^2 (T_s - T_a)/4T_S$$

V_s: Stack exit velocity, m/s
d: top inside stack diameter, m
T_s: stack gas temperature, K
T_a: ambient temperature, K
g: gravity, 9.8 m

Carson and Moses: vertical momentum & thermal buoyancy, based on 615 observations involving 26 stacks.

$$\Delta h_{plume\,rise} = 3.47\frac{V_s d}{\bar{u}} + 5.15\frac{\sqrt{Q_h}}{\bar{u}} \qquad \text{(unstable)}$$

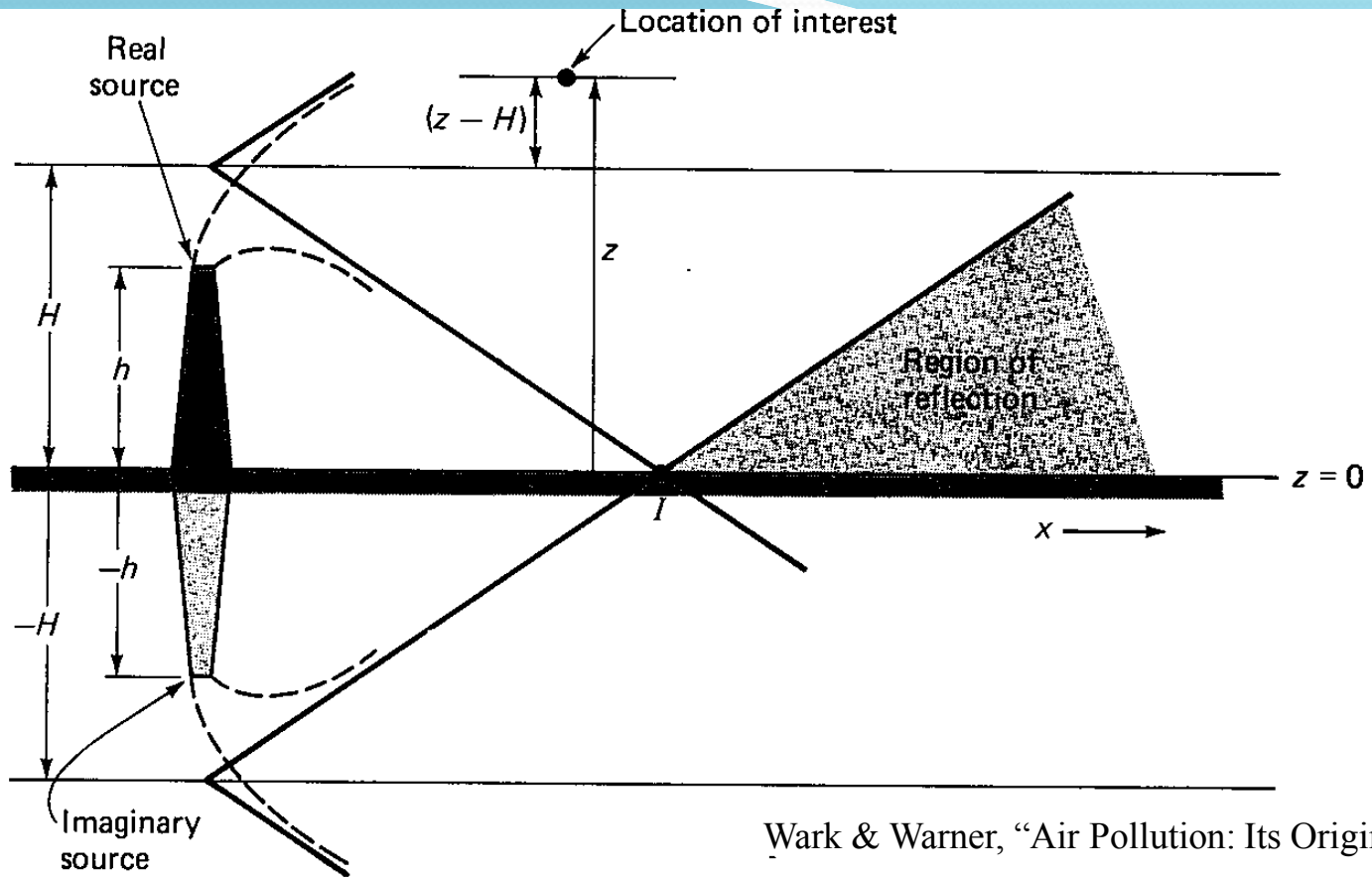
$$\Delta h_{plume\,rise} = 0.35\frac{V_s d}{\bar{u}} + 2.64\frac{\sqrt{Q_h}}{\bar{u}} \qquad \text{(neutral)}$$

$$\Delta h_{plume\,rise} = -1.04\frac{V_s d}{\bar{u}} + 2.24\frac{\sqrt{Q_h}}{\bar{u}} \qquad \text{(stable)}$$

$$Q_h = \dot{m}C_p\left(T_s - T_a\right) \qquad \text{(heat emission rate, kJ/s)}$$

$$\dot{m} = \frac{\pi d^2}{4}V_s\frac{P}{RT_s}MW \qquad \text{(stack gas mass flow rate. kg/s)}$$

When pollutants are dispersed to the ground level, how should we handle the situation?



Wark & Warner, "Air Pollution: Its Origin & Control"

Figure 4-3 Use of an imaginary source to describe mathematically gaseous reflection at surface of the earth.

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

What if the surface is absorbing?

How should the concentration profile look

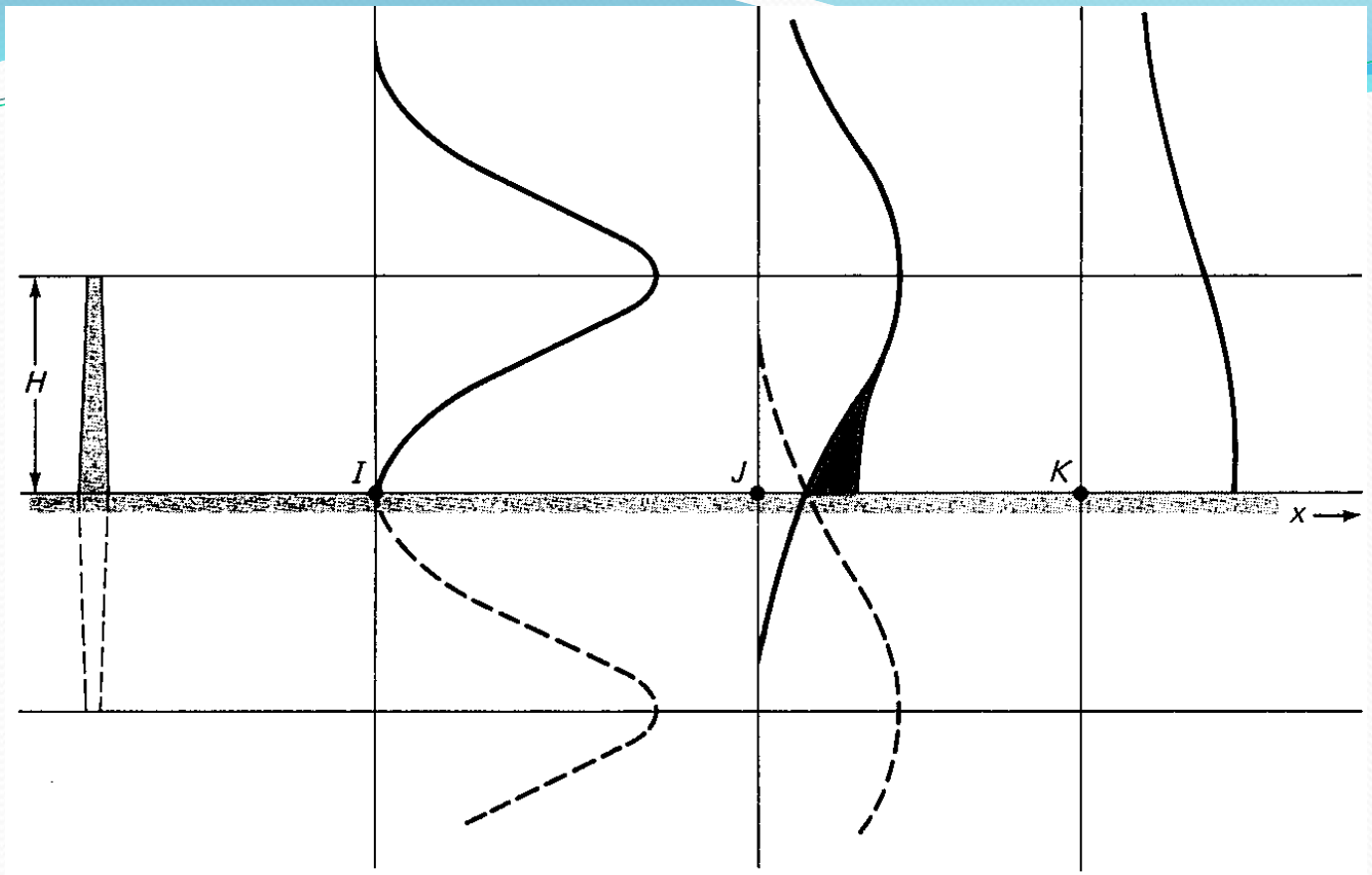


Figure 4-4 Effect of ground reflection on pollutant concentration downwind.

Ground level concentration

$$C = \frac{Q}{\pi \sigma_y \sigma_z \bar{u}} \exp\left[-\frac{y^2}{2\sigma_y^2}\right] \exp\left[-\frac{H^2}{2\sigma_z^2}\right]$$

Maximum Ground Level Concentration

Under moderately stable to near neutral conditions,

$$\sigma_y = k_1 \sigma_z$$

The ground level concentration at the center line is

$$C(x,0,0) = \frac{Q}{\pi k_1 \sigma_z^2 u} \exp\left[-\frac{H^2}{2\sigma_z^2}\right]$$

The maximum occurs at

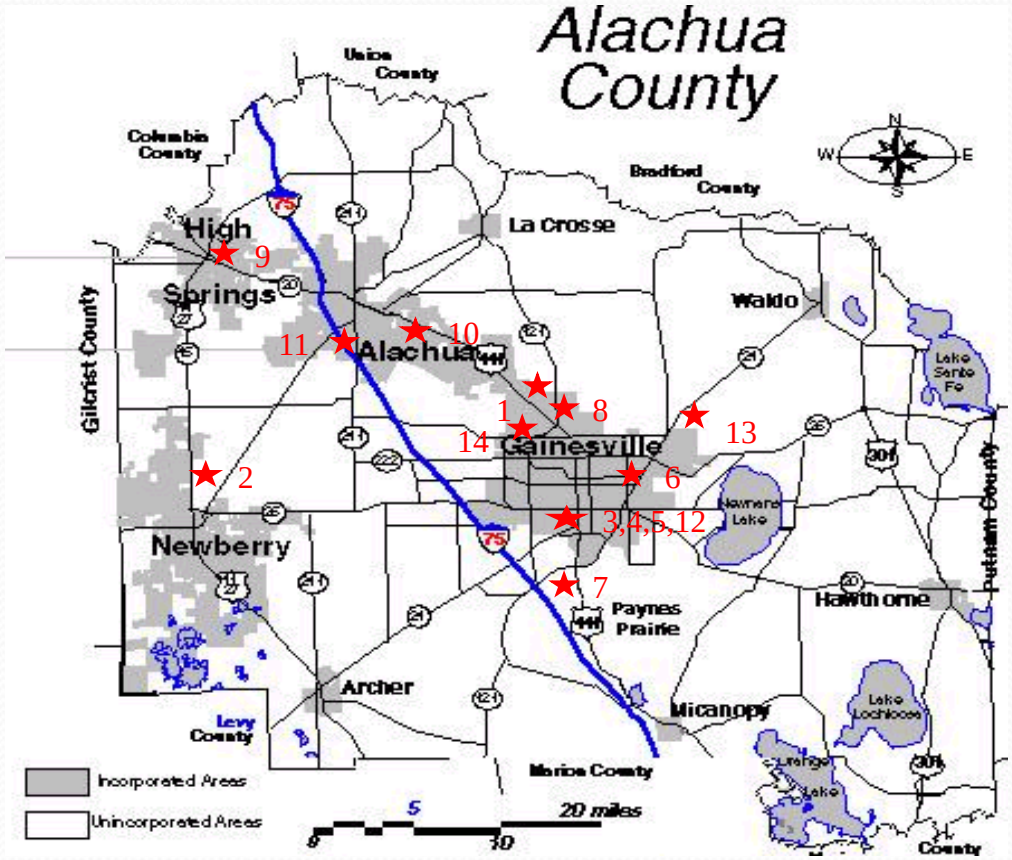
$$dC/d\sigma_z = 0 \quad \Rightarrow \sigma_z = \frac{H}{\sqrt{2}}$$

Once σ_z is determined, x can be known and subsequently C.

$$C(x,0,0) = \frac{Q}{\pi \sigma_y \sigma_z u} \exp[-1] = 0.1171 \frac{Q}{\sigma_y \sigma_z u}$$

Chemical Mass Balance Model

- A receptor model for assessing source apportionment using ambient data and source profile data.
- Available at EPA Support Center for Regulatory Air Models - http://www.epa.gov/scram001/tt23.htm



PM_{10} **emissions from permitted sources** in Alachua County (tons) (ACQ,2002)

2000 Values

1. GRU Deerhaven 144.2
2. Florida Rock cement plant 34.35
3. Florida Power UF cogen. plant 3.19

1997 Values

4. VA Medical Center incinerator 0.2
5. UF Vet. School incinerator 0.2
6. GRU Kelly 1.9
7. Bear Archery 9.5
8. VE Whitehurst asphalt plant 4.9
9. White Construction asphalt plant 0.7
10. Hipp Construction asphalt plant 0.3
11. Driltech equipment manufacturing 0.2

Receptor Sites

12. University of Florida
13. Gainesville Regional Airport
14. Gainesville Regional Utilities (MillHopper)

Principles

- Mass at a receptor site is a linear combination of the mass contributed from each of a number of individual sources;
- Mass and chemical compositions of source emissions are conserved from the time of emission to the time the sample is taken.

$$C_{ij} = \Sigma(a_{ik} \times S_{kj})$$

- C_{ij} is the concentration of species i_{th} in the sample j_{th} measured at the receptor site:
- a_{ik} is the mass fraction of the species in the emission from source k_{th}, and
- S_{kj} is the total mass contribution from source k_{th} in the j_{th} sample at the receptor site.

Example

- Total Pb concentration (ng/m³) measured at the site: a linear sum of contributions from independent source types such as motor vehicles, incinerators, smelters, etc

  $Pb_T = Pb_{auto} + Pb_{incin.} + Pb_{smelter} + \ldots$
- Next consider further the concentration of airborne lead contributed by a specific source. For example, from automobiles in ng/m³, Pb_{auto}, is the product of two cofactors: the mass fraction (ng/mg) of lead in automotive particulate emissions, $a_{Pb,\ auto}$, and the total mass concentration (mg/m³) of automotive emission to the atmosphere, S_{auto}
- $Pb_{auto} = a_{auto}\ (ng/mg) \times S_{auto}\ (mg/m^3{}_{air})$

Assumptions

- Composition of source emissions is constant over period of time,
- Chemicals do not react with each other,
- All sources have been identified and have had their emission characterized, including linearly independent of each other,
- The number of source category (j) is less than or equal to the number of chemical species (i) for a unique solution to these equations, and
- The measurement uncertainties are random, uncorrelated, and normally distributed (EPA, 1990).