Mathematical Methods in Air Pollution Studies

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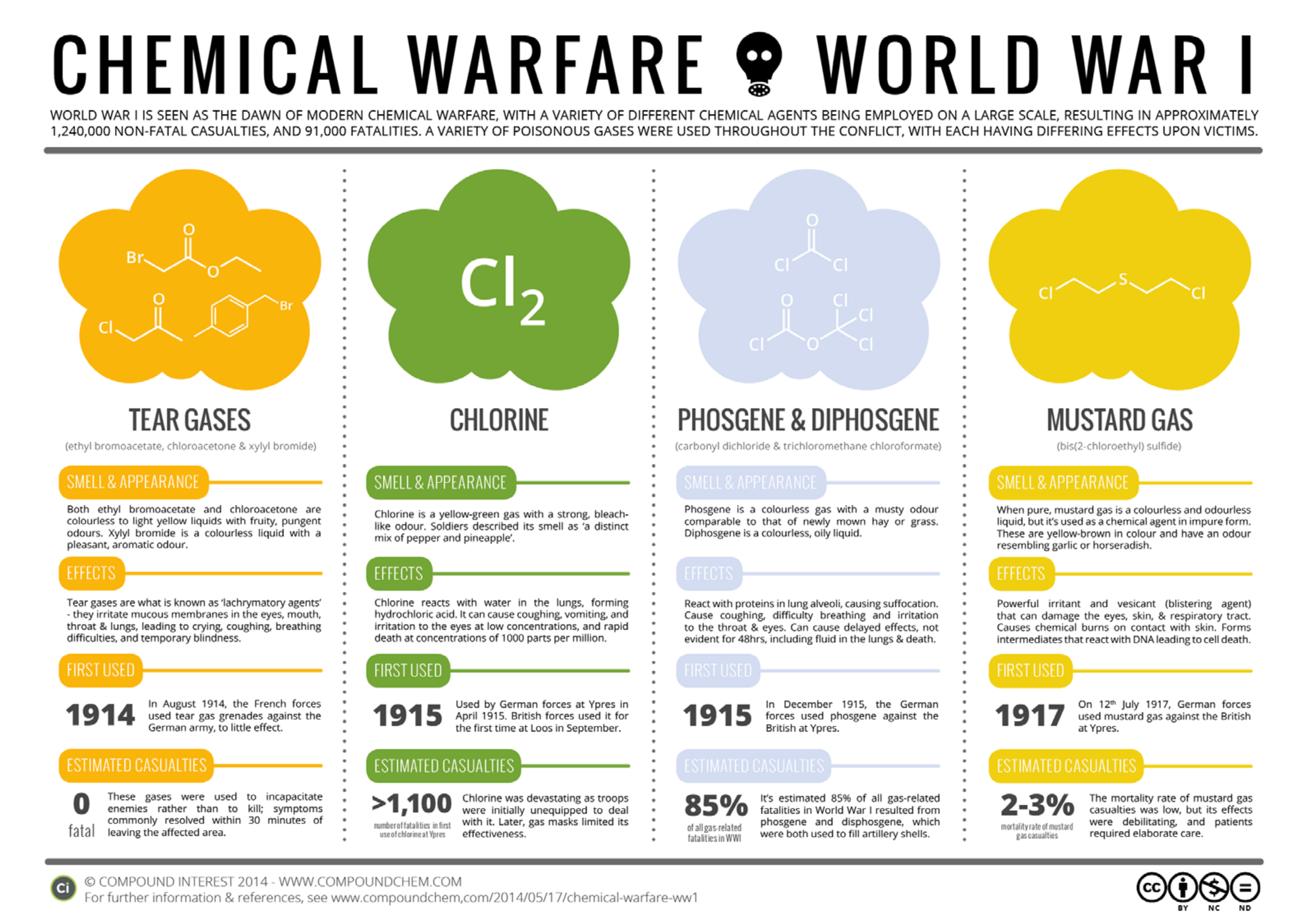
Air Pollution

- Anthropogenic emissions of gas and particulate matter (PM) causing adverse effects to humans and nature, e.g.:
  - sulfur dioxide (SO_2) from power plants
  - carbon monoxide (CO) from cars
  - carcinogenic diesel PM from trucks
  - chlorine (Cl_2) and ammonia (NH_3) gas from industrial/transportation accidents
  - elemental carbon (C) PM from fires
  - aerial drift of agricultural pesticides
  - secondary pollutants (most difficult to control), created by chemical/photochemical reactions of pollutants, e.g.,
    - NOx + RHC + hv ➔ ozone (O_3)
    - secondary PM: SO_2 ➔ sulfates ($SO_4^{=}$) ; NOx ➔ nitrates (NO_3^-) ; VOC ➔ organic particles (smaller PM is the most dangerous: PM10, PM2.5, ultrafine)

Meteorology-Weather-Air Pollution Studies

- Relatively new science
- Only in 1903 Vilhelm Bjerknes of Norway promulgated the idea that weather forecasting should be based on the laws of physics
- Lewis Fry Richardson in 1913-19 analyzed the equations describing the weather (pen and paper …)
- The first electronic computer (John von Neumann, 1946) included a project for weather forecasting
- Major air pollution studies started in the 1920, e.g.
  - Taylor, 1920, Diffusion by Continuous Movements http://plms.oxfordjournals.org/content/s2-20/1/196.extract

– why? -


CHEMICAL WARFARE WORLD WAR I
WORLD WAR I IS SEEN AS THE DAWN OF MODERN CHEMICAL WARFARE, WITH A VARIETY OF DIFFERENT CHEMICAL AGENTS BEING EMPLOYED ON A LARGE SCALE, RESULTING IN APPROXIMATELY 1,240,000 NON-FATAL CASUALTIES, AND 91,000 FATALITIES. A VARIETY OF POISONOUS GASES WERE USED THROUGHOUT THE CONFLICT, WITH EACH HAVING DIFFERING EFFECTS UPON VICTIMS.
Br
O
O
Cl
O
Br
TEAR GASES
(ethyl bromoacetate, chloroacetone & xylyl bromide)
SMELL & APPEARANCE
Both ethyl bromoacetate and chloroacetone are colourless to light yellow liquids with fruity, pungent odours. Xylyl bromide is a colourless liquid with a pleasant, aromatic odour.
EFFECTS
Tear gases are what is known as 'lachrymatory agents' - they irritate mucous membranes in the eyes, mouth, throat & lungs, leading to crying, coughing, breathing difficulties, and temporary blindness.
FIRST USED
1914
In August 1914, the French forces used tear gas grenades against the German army, to little effect.
ESTIMATED CASUALTIES
0
fatal
These gases were used to incapacitate enemies rather than to kill; symptoms commonly resolved within 30 minutes of leaving the affected area.
Cl2
CHLORINE
SMELL & APPEARANCE
Chlorine is a yellow-green gas with a strong, bleach-like odour. Soldiers described its smell as 'a distinct mix of pepper and pineapple'.
EFFECTS
Chlorine reacts with water in the lungs, forming hydrochloric acid. It can cause coughing, vomiting, and irritation to the eyes at low concentrations, and rapid death at concentrations of 1000 parts per million.
FIRST USED
1915
Used by German forces at Ypres in April 1915. British forces used it for the first time at Loos in September.
ESTIMATED CASUALTIES
>1,100
number of fatalities in first use of chlorine at Ypres
Chlorine was devastating as troops were initially unequipped to deal with it. Later, gas masks limited its effectiveness.
O
Cl
Cl
O
Cl
Cl
Cl
O
Cl
PHOSGENE & DIPHOSGENE
(carbonyl dichloride & trichloromethane chloroformate)
SMELL & APPEARANCE
Phosgene is a colourless gas with a musty odour comparable to that of newly mown hay or grass. Diphosgene is a colourless, oily liquid.
EFFECTS
React with proteins in lung alveoli, causing suffocation. Cause coughing, difficulty breathing and irritation to the throat & eyes. Can cause delayed effects, not evident for 48hrs, including fluid in the lungs & death.
FIRST USED
1915
In December 1915, the German forces used phosgene against the British at Ypres.
ESTIMATED CASUALTIES
85%
of all gas-related fatalities in WWI
It's estimated 85% of all gas-related fatalities in World War I resulted from phosgene and disphosgene, which were both used to fill artillery shells.
Cl
S
Cl
MUSTARD GAS
(bis(2-chloroethyl) sulfide)
SMELL & APPEARANCE
When pure, mustard gas is a colourless and odourless liquid, but it's used as a chemical agent in impure form. These are yellow-brown in colour and have an odour resembling garlic or horseradish.
EFFECTS
Powerful irritant and vesicant (blistering agent) that can damage the eyes, skin, & respiratory tract. Causes chemical burns on contact with skin. Forms intermediates that react with DNA leading to cell death.
FIRST USED
1917
On 12th July 1917, German forces used mustard gas against the British at Ypres.
ESTIMATED CASUALTIES
2-3%
mortality rate of mustard gas casualties
The mortality rate of mustard gas casualties was low, but its effects were debilitating, and patients required elaborate care.
Ci
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For further information & references, see www.compoundchem,com/2014/05/17/chemical-warfare-ww1
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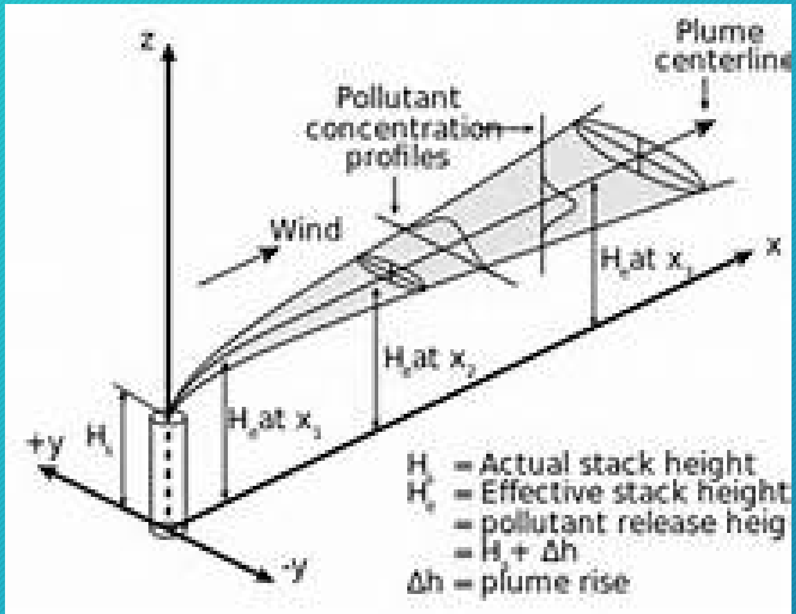
Mathematical Methods

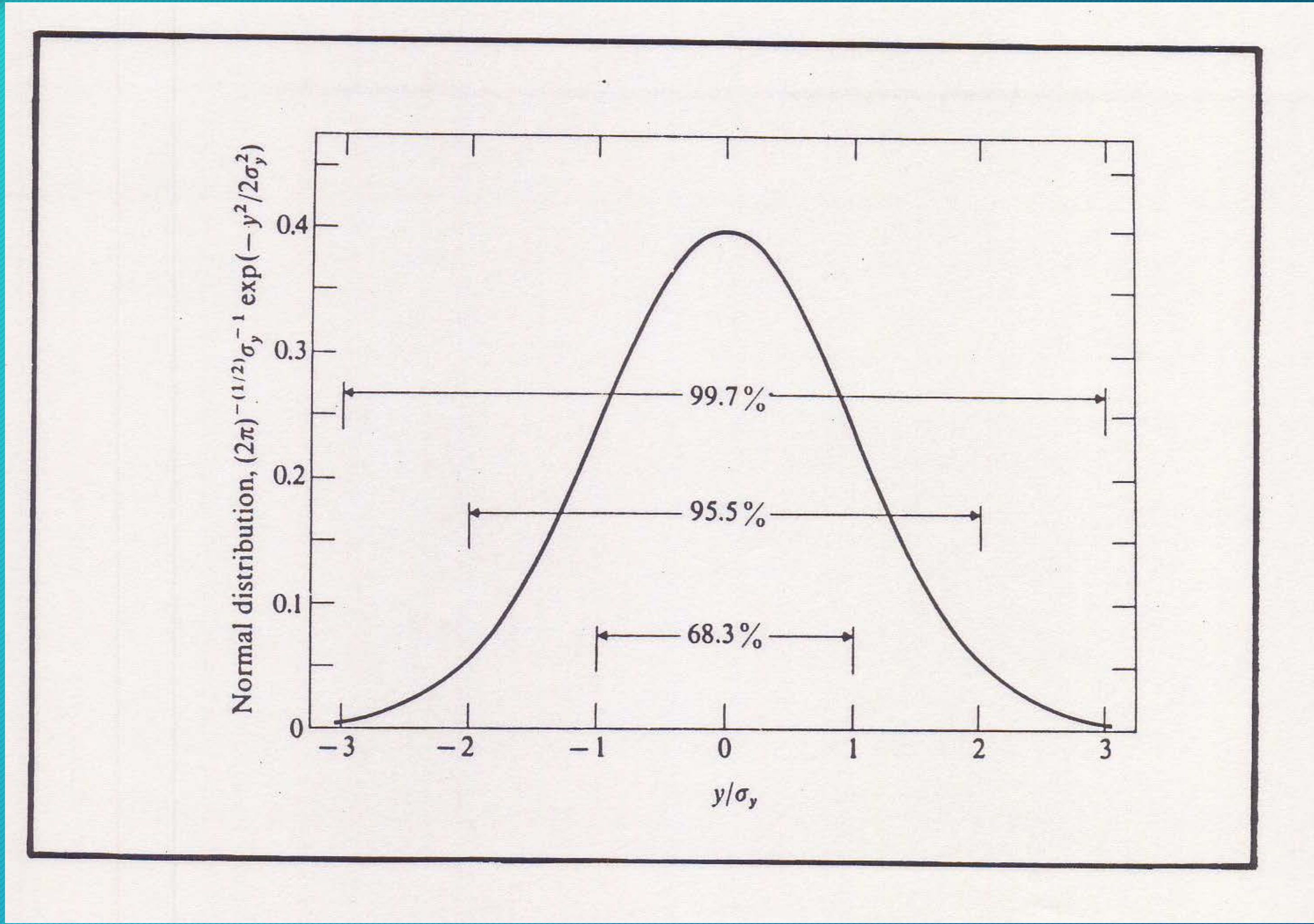
- Either very simple …
  - Empirical engineering formula (simple algebraic formulas)
  - E.g.: the Gaussian Plume Equation



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

C = Concentration of the chemical in air. [M/L^3]
Q = Rate of chemical emission. [M/T]
u = Wind speed in x direction. [L/T]
σ_y = Standard deviation in y direction. [L]
σ_z = Standard deviation in z direction. [L]
y = Distance along a horizontal axis perpendicular to the wind. [L]
z = Distance along a vertical axis. [L]
H = Effective stack height. [L]

Gaussian Distribution



Plume Sigmas

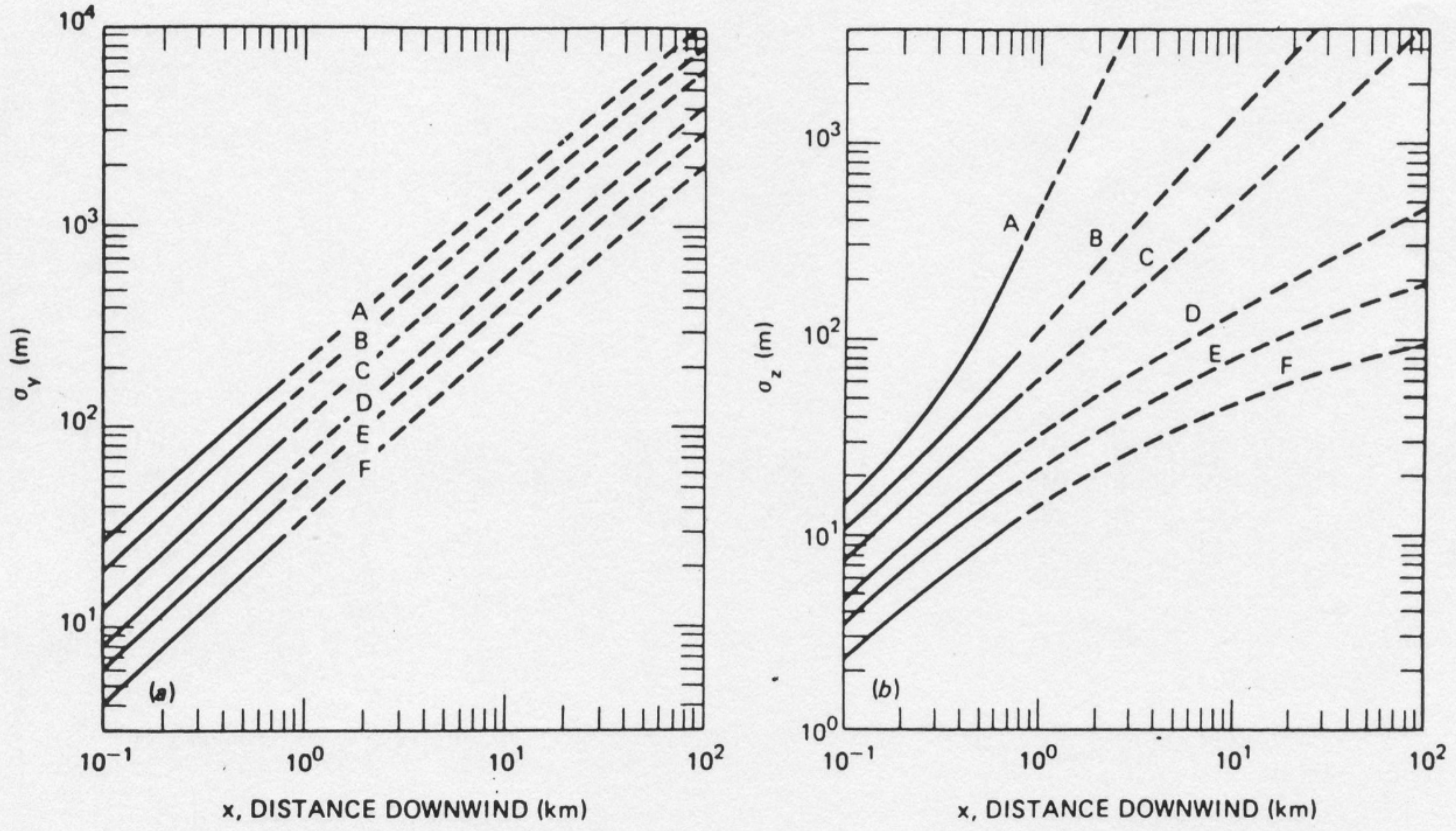
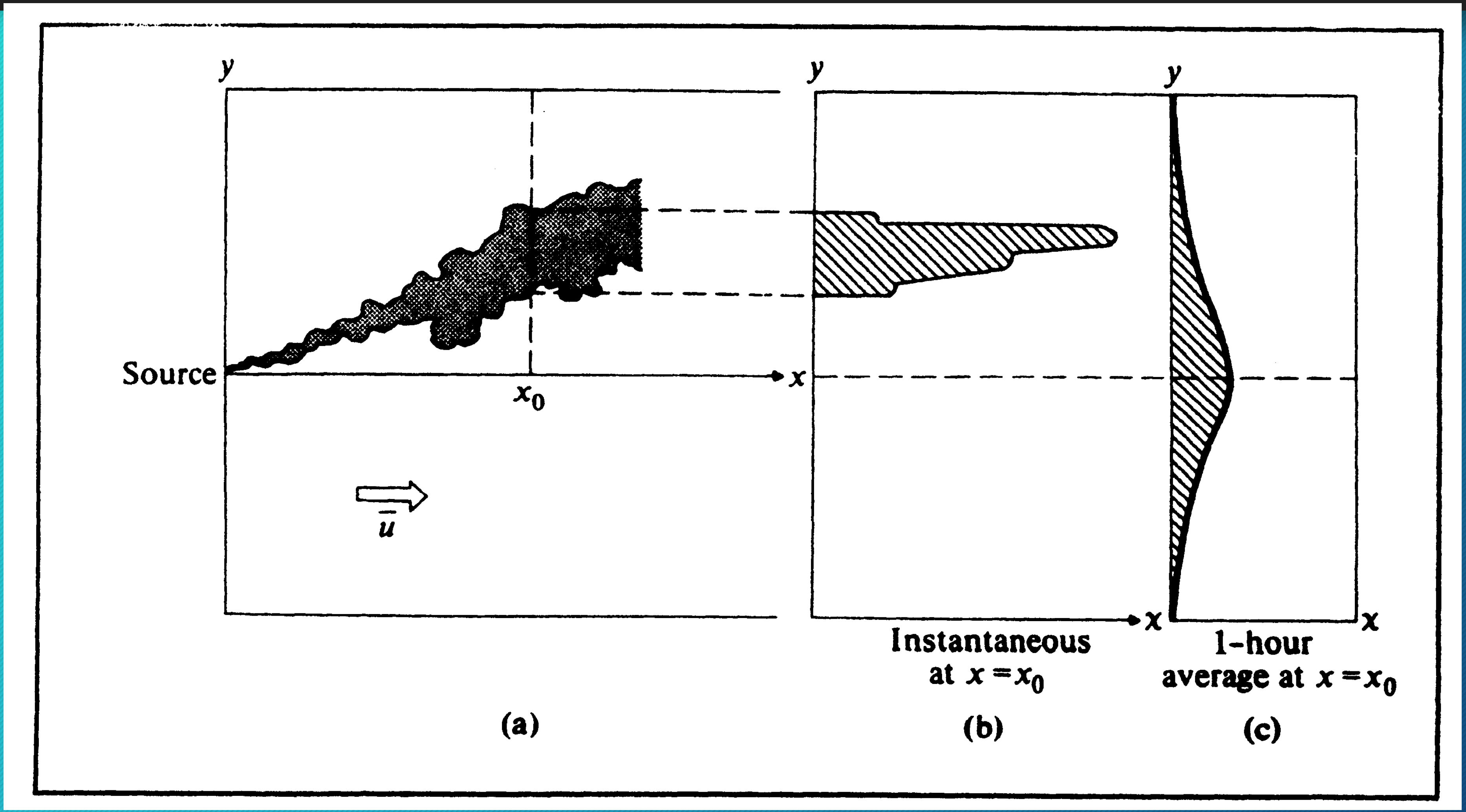
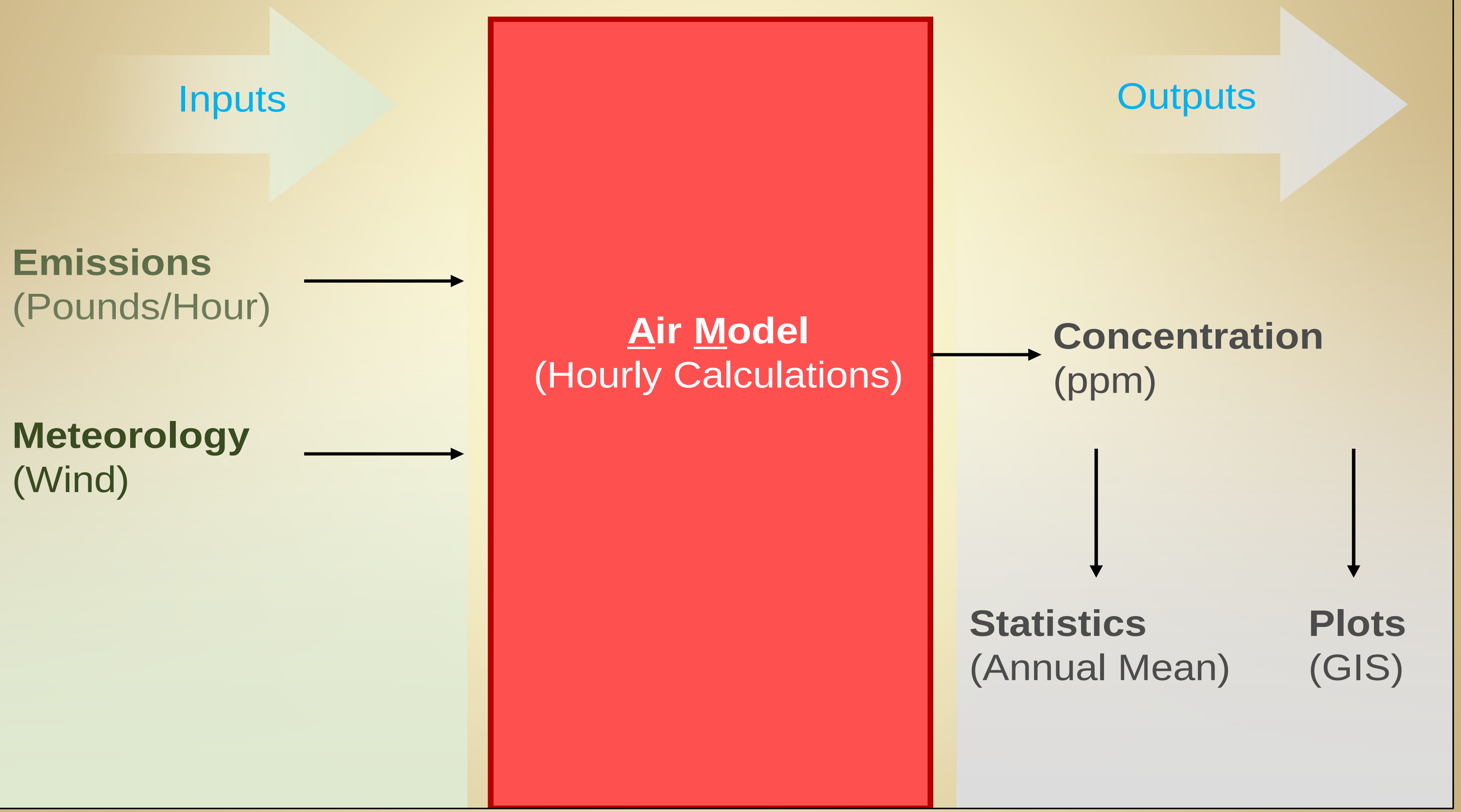


Fig. 19-6. Pasquill–Gifford σ_y (left) and σ_z (right). Source: From Gifford (12).

Instantaneous vs. Average Concentration



Air Modeling Methodology



Mathematical Methods (cont.)

- … Or very complex
  - Numerical solutions of partial differential equations
  - E.g.: the Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial x} + \frac{\partial \rho v}{\partial y} + \frac{\partial \rho w}{\partial z} = 0 \quad (1)$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2)}{\partial x} + \frac{\partial (\rho u v)}{\partial y} + \frac{\partial (\rho u w)}{\partial z} = -\frac{\partial p}{\partial x} + \nu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2} \right) \quad (2)$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial (\rho u v)}{\partial x} + \frac{\partial (\rho v^2)}{\partial y} + \frac{\partial (\rho v w)}{\partial z} = -\frac{\partial p}{\partial y} + \nu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} \right) \quad (3)$$

$$\frac{\partial \rho w}{\partial t} + \frac{\partial (\rho u w)}{\partial x} + \frac{\partial (\rho v w)}{\partial y} + \frac{\partial (\rho w^2)}{\partial z} = -\frac{\partial p}{\partial z} + \nu \left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2} + \frac{\partial^2 w}{\partial z^2} \right) \quad (4)$$

$$\frac{\partial \rho E}{\partial t} + \frac{\partial (\rho u E)}{\partial x} + \frac{\partial (\rho v E)}{\partial y} + \frac{\partial (\rho w E)}{\partial z} = -\frac{\partial p u}{\partial x} - \frac{\partial p v}{\partial y} - \frac{\partial p w}{\partial z} + S \quad (5)$$

where ρ is the air density, u, v, w are the components of the air's velocity, E is measure of the air's internal energy (which allows us to compute its temperature) and p is the air pressure.

Air Pollution Topics

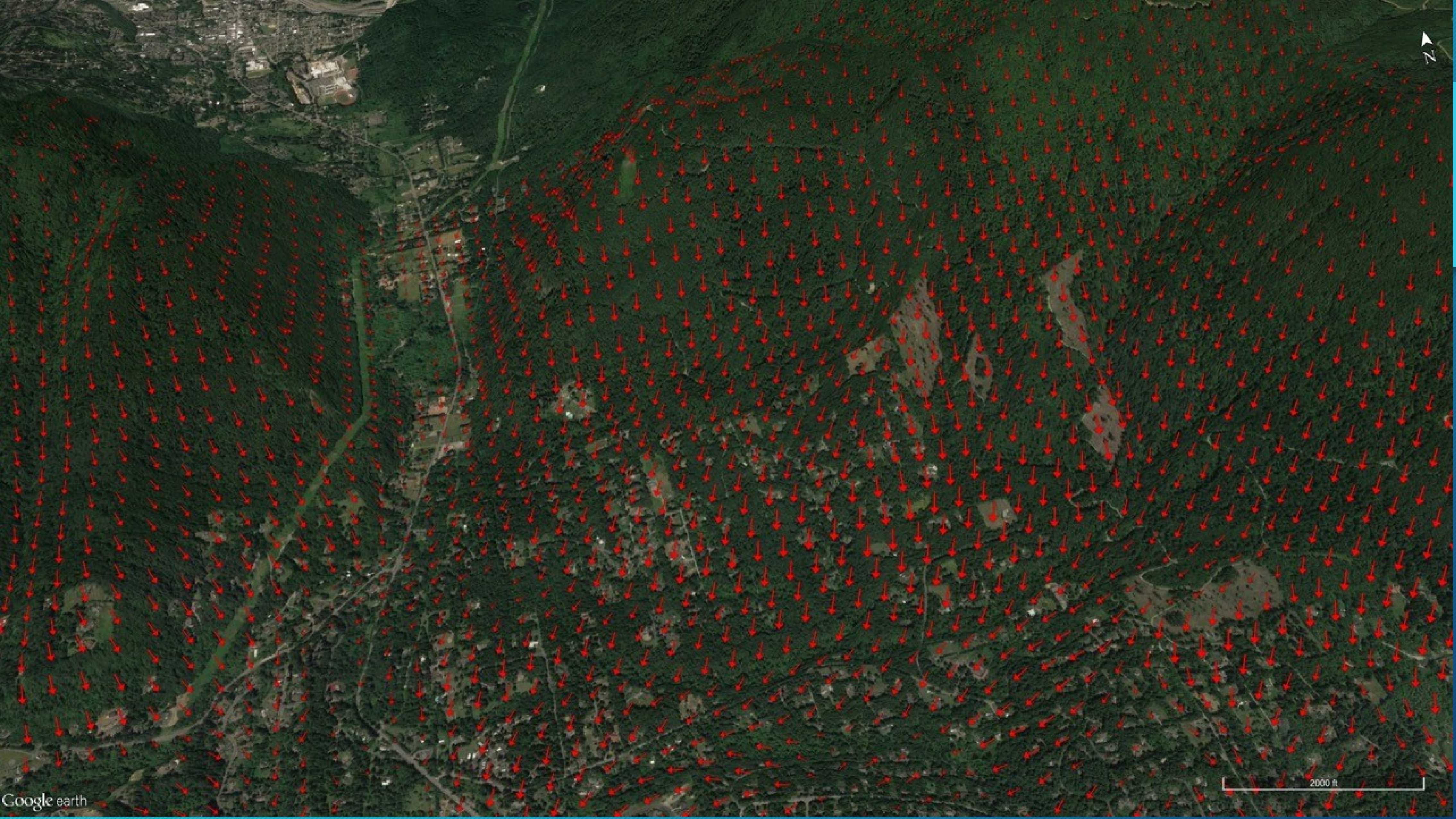
- Meteorological models
- Emission models
- Plume rise models
- Dispersion models
- Chemical/photochemical reaction models
- Deposition models
  - Dry and wet deposition
- Adverse effects models
  - Human health
    - Cancer risk, mortality, morbidity
  - Environmental/ecological damages
- Books:
  - Free: http://www.envirocomp.com/pops/airpollution.html
  - Most current: http://envirocomp.org/books/aqm.html

Topic – Meteorological/Airflow Models

- Needed to calculate the meteorological parameters to run air pollution models, e.g., wind speed and direction
- Diagnostic 3D models based upon an "intelligent" interpolation/extrapolation of available measurements, e.g.:
  - CALMET http://www.src.com/calpuff/download/CALMET_UsersGuide.pdf
- Prognostic 3D models solving, e.g.
  - WRF which numerically integrates the compressible, non-hydrostatic Euler equations http://www2.mmm.ucar.edu/wrf/users/docs/arw_v3.pdf
- General CFD models, e.g.
  - FLUENT http://www.ansys.com/Products/Fluids/ANSYS-Fluent powerful computational fluid dynamics (CFD) software tool to model flow, turbulence, heat transfer, and reactions for industrial applications

Results from Meteorological Models

- Large scale:
  - The earth now: https://earth.nullschool.net/
- Small scale: ➔


N
2000 ft
Google earth


N
900 ft
Google earth

Topic – Atmospheric Dispersion

- Key role of turbulence
- Lack of complete mathematical theory
- Approximate solutions
  - Initial and boundary conditions become quickly irrelevant
  - Random effects – stochastic motion
  - Reality is only one “realization” among an infinite set of possible events

Figure 8.1: Drawing of a turbulent flow by Leonardo da Vinci (1452–1519), who recognized that turbulence involves a multitude of eddies at various scales.

van Gogh's Starry Night, 1889

MONTECARLO Methods

- “Montecarlo” methods are particularly suitable to describe turbulent phenomena
- Inclusion of computer-generated semi-random velocities
- Why Montecarlo?

Montecarlo

Montecarlo Particle Modeling

1. Pollution is represented by a large number of moving points (x,y,z), or "fictitious particles", instead of a continuous concentration function C(x,y,z,t)
2. The points are moved at every Δt according to the local wind (ux, uy, uz) PLUS a semi-random component (ux', uy', uz')
3. The semi-random component is generated using algorithms to reproduce local turbulence intensity and properties

- Theoretical foundation: Langevin stochastic equation
  - http://units.physics.uwa.edu.au/__data/page/115450/lecture3_(brownian_motion)-NF.pdf
- Example: plume animation

Discussion of Case Studies

- Large fire
  - Slides from http://www.envirocomp.com/caps/projects/biolab/
- Indoor air pollution (CFD)
  - Slides from http://www.envirocomp.com/caps/projects/ibm/
- Agricultural case
  - Slides from http://www.envirocomp.com/caps/projects/idahogrowers/
- Chronic urban exposure
  - Slides from http://www.envirocomp.com/caps/projects/bevhills/
- Industrial accidental release
  - Slides from http://www.envirocomp.com/caps/projects/monsanto/
- Other case studies →

Military Issues

- Weather forecast
- Use of obscurants in the battlefield
- Poison/radioactive gas scenarios used by enemy forces
- COMBIC - http://www.dtic.mil/cgi-bin/GetTRDoc?AD=ADA382944
  - The Combined Obscuration Model for Battlefield Induced Contaminants (COMBIC) predicts time and spatial variations in transmission through dust and debris raised by high-energy explosives and by vehicular movement; smoke from phosphorus and hexachloroethane munitions; smoke from diesel oil fires; generator-disseminated fog oil and diesel fuel; and other screening aerosols from sources defined by inputs.
  - COMBIC has been designed primarily for large scenarios where many different obscuration sources are present and where many observer-target lines of sight (LOS) must be treated simultaneously.
- Joint Urban 2003 (JU03) Tracer Field Tests

  tracer experiment held in Oklahoma City during July of 2003

  http://www.noaa.inel.gov/projects/ju03/ju03.htm
- Other atmospheric software: http://www.ontar.com/Software/ProductDetails.aspx?item=products

End of Presentation

Thank you!

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