UNDERSTANDING AIR POLLUTION

The Past and the Future

Akula Venkatram

- 'Understanding'
- Air pollution problems
 - Acid deposition
 - Urban pollution
- The future



Air Pollution in the News



Empty skies proved that airports cause pollution, say researchers By Michael McCarthy, Environment Editor and Phil Boucher

Eyja*fjalla*jokull

Islandmountainglacier

Understanding



Acid Deposition

- Deposition of acidifying pollutants became a concern in the 1970s
- Acid deposition believed to be damaging lake and forest ecosystems in Scandinavia





Acid Deposition



Acid Deposition

The early models were semi-empirical: Lagrangian trajectory models, statistical models for long-term concentrations

- Bolin and Persson, 1975
- Eliassen and Saltbones, 1975
- Fisher, 1975
- Venkatram et al., 1982

Semi-Empirical Models

- Parameters for chemistry, dry deposition, wet deposition
- Transport modeled using trajectories or 'wind roses'





Comparison of model predictions with observations of sulfur concentrations in rain averaged over 1982-1985. Venkatram et al. 1990

Issues with Semi-empirical Models

- Difficult to incorporate fundamental understanding into parameter values
 - Chemistry is generally simple
 - Transport does not account for wind shear

Comprehensive Models

- Designed to incorporate processes in as much detail as possible
- Designed to serve as numerical surrogates of governing system once it has been evaluated with observations
 - Used to conduct experiments that would be impossible in the real world

Comprehensive Models – Acid Deposition and Oxidant Model



Acid Deposition - Gas Phase Chemistry

$SO_{2} + OH \rightarrow HOSO_{2} + O_{2} \rightarrow SO_{3} + HO_{2}$ $SO_{3} + H_{2}O \rightarrow H_{2}SO_{4}$

$NO_2 + OH \rightarrow HNO_3$

 $O_3 + h\nu \rightarrow O_2 + O$ $O + H_2O \rightarrow 2OH$

Acid Deposition - Aqueous Phase Chemistry

 $SO_2 + H_2O \Leftrightarrow H_2O.SO_2$ $H_2O.SO_2 \Leftrightarrow HSO_3^- + H^+$ $HSO_{3}^{-} + H_{2}O_{2} + H^{+} \rightarrow SO_{4}^{-} + 2H^{+} + H_{2}O_{3}$



 $HO_2 + HO_2 \rightarrow H_2O_2 + O_2$

Role of H_2O_2

- Hydrogen peroxide oxidizes SO₂ in cloud water: wet removal of SO₂ is more efficient than that suggested by dissolution of SO₂
- Scavenging by rain is limited by the concentration of H_2O_2





*Fractional change in cumulative wet-sulfur deposition for April 12, 1981, as a result of a 50% reduction in SO, emissions.

Role of H_2O_2

Revealed in long-term concentrations



Without oxidant limitation

Role of Non-precipitating Clouds

Simulation of a 12 day period in 1998 showed that

- Sulfur in rain was estimated well
- Total ambient sulfur estimated well
- Sulfate in air underpredicted
- SO_2 in air overpredicted

Hypothesis

Oxidation in cloud results in ambient sulfate when the cloud evaporates

Role of Non-precipitating Clouds – results from Karamchandani and Venkatram, 1992



Role of Non-precipitating Clouds - results



Models are used to estimate the contributions of pollution sources to visibility reduction



Visibility is reduced by scattering of light by aerosols



Results from simulations

 Established culpability of different sources to acid deposition

| Receptor Source | US | Canad a |
|--------------------|------------|------------|
| US | 70% | 70% |
| Canada | 30% | 30% |

 Showed the importance of sulfate formation in non-precipitating clouds

Urban Air Pollution Modeling

- Non-uniform surface characteristics and buildings
- Complex flow and turbulent fields
 Use flat-terrain models with modifications in plume spread



St Louis Experiment

- Conducted in 1963-65
- Zinc Cadmium Sulfide particles released close to the surface
- Doses sampled at 30-50 locations on arcs ranging from 800 m to 16 km from the source along the estimated plume centerline
- Meteorology measured at three surface stations and an instrumented TV tower in the middle of the city
- Resulted in 26 daytime and 16 evening hour-long experiments

Analysis of Data

- McElroy and Pooler derived horizontal spreads from arc doses, and vertical spreads from maximum ground-level concentrations
- They presented these spreads as functions of stability parameters
- Briggs (1973) presented analytical forms that fit the data
- Used in ISC model as urban dispersion curves

St Louis Model Performance Briggs Curves



Current Urban Pollution Problems

Environmental Justice Freeways through neighborhoods



Sources Near Residents



Urban Field Experiments

Tracer studies designed to study dispersion at scales of meters to kilometers in urban areas.

- CE-CERT parking lot study, April-May 2001
- Dugway Proving Grounds Model Study- July 2001
- Summer and winter Barrio Logan field studies-August and December 2001
- Wilmington shoreline study- September 2003, 2004

Funded by CEC and ARB to examine Environmental Justice Issues

Dugway Experiment



CE-CERT Parking Lot



Meteorological Measurements









Sampling Sites

74 sites





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Model Results using Boundary Layer Information and Initial Spread



Model Results - Highway Modeling



Freeway concentration contributions



1-3 Butadiene Concentrations

Simple models work well

BUT...

 Simple models for dispersion provide adequate concentration estimates if mean wind and turbulence velocities are known

Point sources:

$$C \sim \frac{Q}{u_{dil}x^2}$$
$$u_{dil} = \frac{\sigma_w \sigma_v}{U}$$

Estimating model inputs from urban routine measurements



One or two level measurements of winds and σ_T can be used to estimate urban parameters.

Results-Stable Conditions

$$u_{*} = C_{D} u \P_{r} \left\{ \frac{1}{2} + \frac{1}{2} \left[1 - \left(\frac{2u_{0}}{C_{D}^{\frac{1}{2}} u} \right)^{2} \right]^{\frac{1}{2}} \right\}$$
$$\sigma_{w} = 1.6u_{*}$$

Wilmington: SU Observed vs. predicted σ_w on u_{\star} with θ_{\star} on σ_{θ} - Stable



$$\sigma_v = 1.9u_*$$

Wilmington: SU Observed ivs. predicted σ_{v} with θ_{\star} constant - Stable



Results-Unstable Conditions



Dispersion Models

- Simpler models are not appropriate for estimating concentrations within a kilometer from source when plume is still in the urban canopy
- Need numerical and/or physical models



Impact of distributed generators



Laboratory modeling



From Simple to Complex



Is Urban Canopy Layer "Convective"?



Impact of individual buildings



Flow behind a distributed generator

Chimney effect of a tall building

Performance of Numerical Models



Summary

Understanding of air pollution problems is gained through

- Basic science
- Field studies and laboratory experiments
- Modeling/Simulation

How is this going to change in the future?

Past and Future



The Future

- Measurement techniques will become more sophisticated and perhaps less/more expensive
- Models will become more comprehensive and output will be more realistic with increase in computational power







On Using Comprehensive Models

- Inevitable errors in numerous model inputs make model evaluation a difficult exercise
- Numerical errors
- Finite grid sizes create false effects-mixing and chemistry
- Responses of the complex model are very difficult to interpret
 - Need to draw generalizations based on model results that are "messy" as reality

Future of Modeling

- Need both comprehensive as well as simpler semi-empirical models
- Simple models provide insight that is more difficult to obtain from complex models
- Might need simple models to interpret results from complex models

Acknowledgements

- Collaborators over the past 30 (?) years
 - Prakash Karamchandani, Marko Princevac, David Pankratz, Dennis Fitz
- Students- Jing Yuan, Tao Zhan, Wenjun Qian, Qiguo Jing, Si Tan, Karim Alizad, Sam Pournazeri
- EPRI, USEPA, CEC, CARB, NSF, Ontario
 Environment, Umweltbundesamt

Model Performance



Field study next to major highway in Raleigh, North Carolina,

