Session 2 –

Present state of Air Quality Modeling research and the issues

1. Role and Importance of Air Quality Simulation Model

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Local and roadside air pollution
10m~10km

Trans boundary air pollution
500~3000km

Long range transport of air pollution

Wide scale and urban air pollution
10km~500km

Local and roadside air pollution
10m~10km

stratosphere
troposphere
Upper general wind

Sea and Land breeze circulation

Lower general wind

Urban area

Rural area

Mountainous area

Urban Air Pollution

Stratospheric ozone

UV

Diffusion in the mixed layer

Scavenging to the cloud

SO$_4^{2-}$

Wet and Dry deposition

CO

SO$_2$

VOC

NO

NO$_2$

O$_3$

NO$_3$

PAN

HNO$_3$

SO$_4^{2-}$

(Carbon Species)

(inorganic aerosols)

(organic aerosols)

Ce

Co

Scavenging to the cloud

Urban Area Pollution

Primary pollutants:

- NO
- SO$_2$
- CO
- VOC

Secondary pollutants:

- NO$_2$
- O$_3$
- Secondary aerosol

Conc.

Distance from shore line
Air pollution from large city may cause the forest to die.

Died forest located on ridge line near the top of Mt. Shirane in Nikko
Altitude=2200m
Peak conc. coincides with that of ozone. The air pollution is clearly considered as generated in urban area.

3 dimensional distribution of air pollutants by aerial observation July, 31, 1995 3:00-4:00 p.m.

Upper of peak Sasago (2300m) Upper of Kofu City (1600m)
Emission of NMHC

Emission of NOx
Calculation of air quality

Meteorological model
- advection, diffusion, radiation process, land surface process, condensation, cumulus cloud

Air quality model
- advection, diffusion, cumulus convection, gas-/aqueous-phase reaction, aerosol, wet/dry depositions

- Meteorological objective analysis data
- topographical data, land surface data
- Met. data
- wind, temperature, pressure, water vapor, precipitation, cloud water, soil water
- emissions

- emissions
Models-3/CMAQ? What’s Models-3/CMAQ?

Third generation air quality modeling system developed by US/EPA

Features of third generation models:
“One atmosphere” concept
- Multi purpose: Sulfates, nitrates, ozone, PM, toxics, and so on.
- Multi Physical chemistry process: advection, diffusion, chemical reaction, dry deposition, and so on.
- Multi scale: Urban, Regional to continental scale
Structure of air quality modeling system

- Met. model
  - Objective analysis data
  - land use data
  - soil index data
  - met.-chem. interface

- RAMS
- Emission
  - emis.-chem. interface

- Initial/boundary conditions
  - solar radiation
  - advection
  - chemistry
  - depositions
  - cloud, precipitation
  - aerosols

- CMAQ
## Substance required to provide emission inventory data

### CB-IV gas phase chemistry

<table>
<thead>
<tr>
<th>Nitrogen Species</th>
<th>Atomic Species</th>
<th>Hydrocarbons</th>
<th>Operators</th>
<th>For transfer to liquid phase reaction</th>
<th>For transfer to aerosol simulation</th>
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</table>

**Carbon oxides**
- CO

**Odd Hydrogen Species**
- OH

**Organic nitrogen**
- PAN

**Organic Radicals**
- FORM
- ALD2
- MGLY
- CRES

**Oxidants**
- PAR
- ETH
- OLE
- TOL
- XYL

**Hydrocarbons**
- TO2
- OPEN
- ISPD

**Products of organics**
- XO2
- XO2N

**Ammonia**
- NH3

**For transfer to liquid phase reaction**
- FACD
- AACD
- PACD
- UMHP

**For transfer to aerosol simulation**
- SULAER
- TOLAER
- Xylaer
- CSLAER
- TERAER
- TERP
Aerosols

Aitken (0.1µm)
Accumulation (0.1µm through 2.5µm)
Coarse (2.5µm through 10µm)

Sulfate
Ammonium
Nitrate
Primary organic
Anthropogenic secondary organic
Biogenic secondary organic
Elemental carbon

Unspecified anthropogenic
Sea salt

Soil

Shown as log-normal distribution maximum 3 modes
Simulated results for sulfate aerosols
Simulated monthly average ozone concentration

Result using VOC emission inventory data in China

Difference between result calculated with 50% reduced VOC emission inventory and that of whole VOC data in China (Max. difference is around 5ppb)
Air pollutant transportation from continental is considered as a wider scale problem.

Oxidant annual average variation per year at national monitoring station of Matsue. Observation was held at the place of little affected by anthropogenic activities in Japan.

This kind of trend is recognized at other regions in Japan. The trend is considered to occur due to increase of NOx emissions, an causative substance of photochemical ozone, in continental. SPM emissions is also considered to affect the trend.

Air pollution transported over trans boundary will affect more seriously on urban air quality.

Increase in annual ozone concentration

Results of Shimane institute of environment and NIES
Data for NO2 mol/s
1998/01/01 12:00:00

[Map showing distribution of NO2 concentrations]
Model domains for three-stage nesting
Vortex generated in street canyon interferes diffusion of air pollutants, and generates high concentration area on the ground in windward. Such phenomenon is quite difficult to reproduce with Simulation.

Take in Ozone from upper air Accelerate chemical reaction in street canyon

High concentration
Wind tunnel study is applicable to analysis of air pollution behavior in urban area with complicated building shape or meteorological conditions, and also to establishment of prediction method of urban air pollution concentration using computer.

Actual emission source is reproduced with C$_2$H$_6$ gas, and measure the concentration distribution.

Large-scale temperature stratification wind tunnel

Miniature of urban area settled in the wind tunnel

Wind tunnel study in NIES
(1) Establishment of total model system for Continental, Regional, Urban, Street complex, Road side and Room environments.

(2) Model application for short term and long term exposure.

(3) Model prediction not only for weights but also for number and chemical composition of aerosols.

(4) Continuous efforts for obtaining real and exact emission information including anthropogenic and biogenic sources.