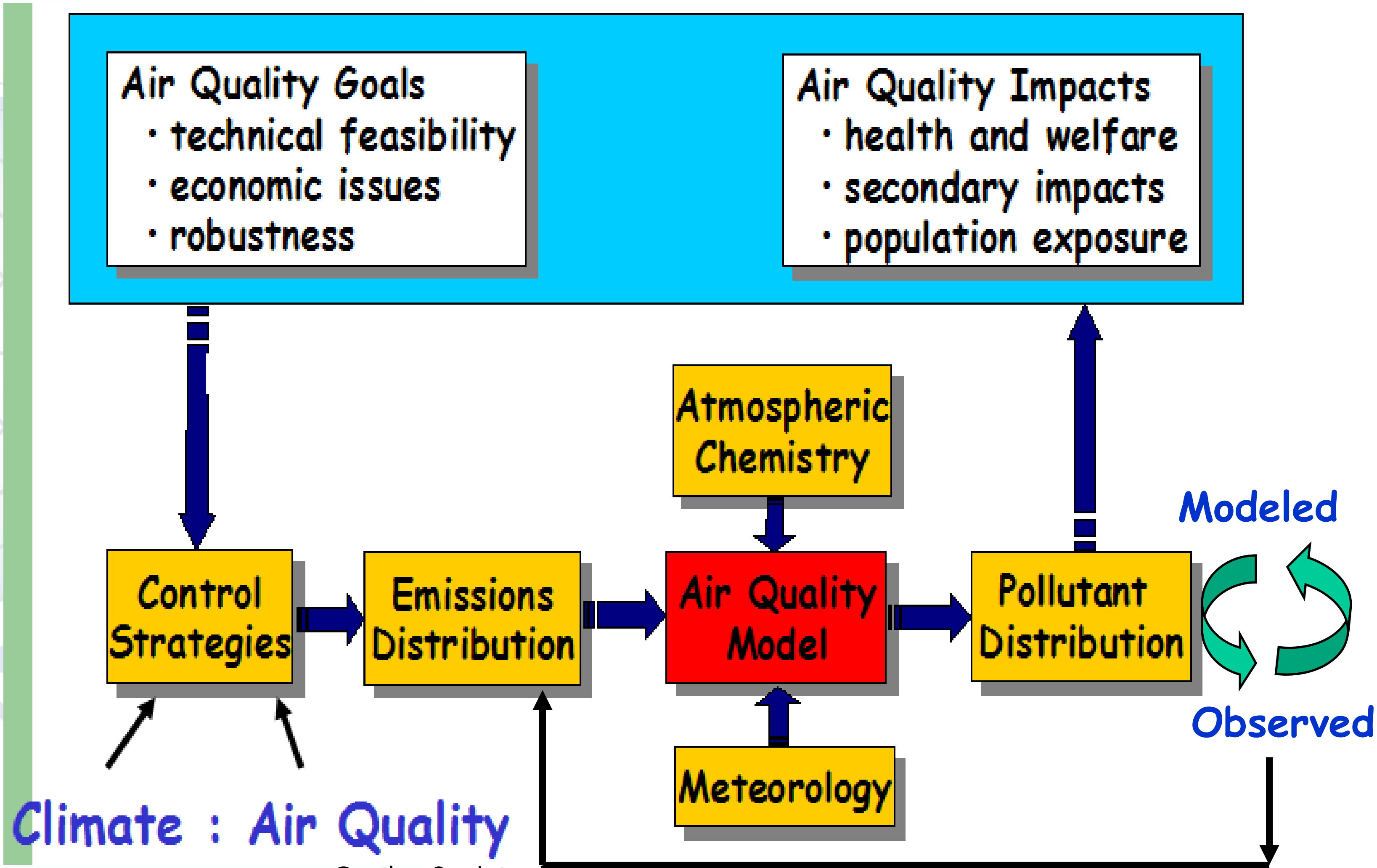
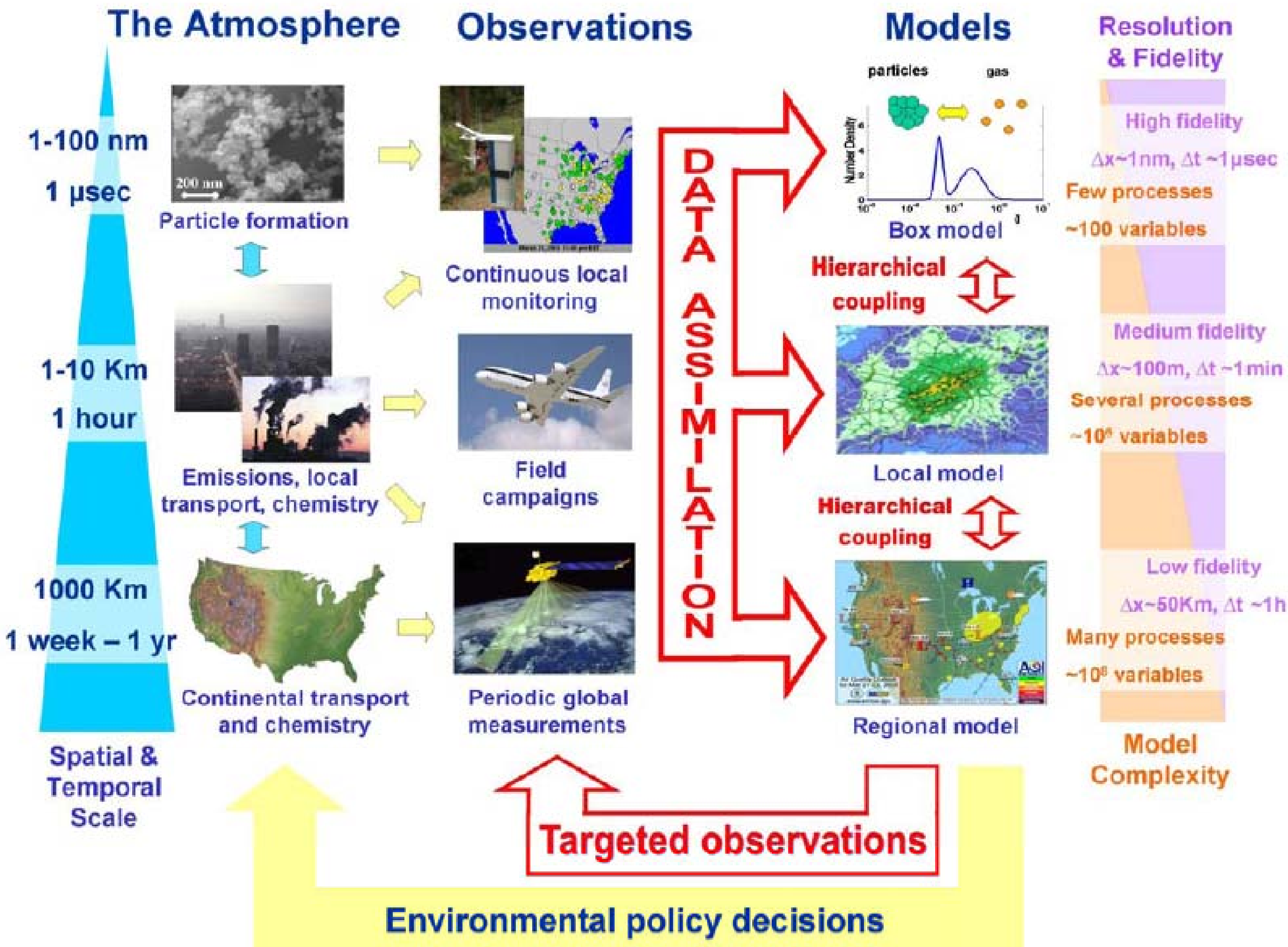
AREP
GAW

Introduction and Overview of Course

WMO
OMM

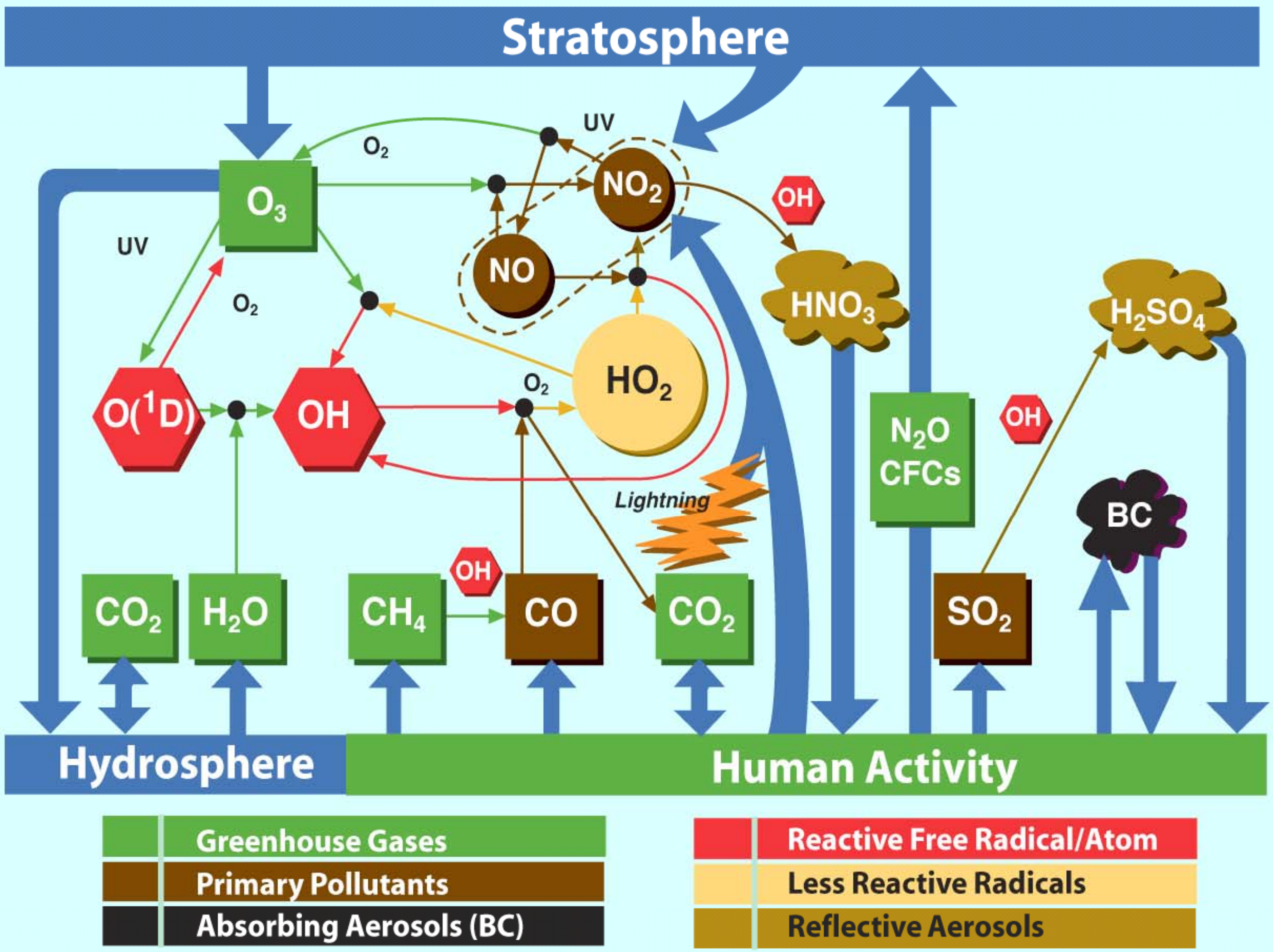
Models Play a Critical Role in Linking Emissions to Aerosol and Trace Gas Distributions and Subsequent Effects





The Atmosphere
Observations
Models
Resolution & Fidelity
1-100 nm
1 μsec
Particle formation
1-10 Km
1 hour
Emissions, local transport, chemistry
1000 Km
1 week – 1 yr
Continental transport and chemistry
Spatial & Temporal Scale
Continuous local monitoring
Field campaigns
Periodic global measurements
DATA ASSIMILATION
particles
gas
Box model
Hierarchical coupling
Local model
Hierarchical coupling
Regional model
High fidelity
Δx~1nm, Δt ~1μsec
Few processes
~100 variables
Medium fidelity
Δx~100m, Δt ~1min
Several processes
~10⁴ variables
Low fidelity
Δx~50Km, Δt ~1h
Many processes
~10⁸ variables
Model Complexity
Targeted observations
Environmental policy decisions

Interactions Between Air Pollution and Climate



Courtesy John Reilly, MIT

AREP
GAW

Chemical Transport Model

- 3D atmospheric transport-chemistry model (STEM-III)

$$\frac{\partial c_i}{\partial t} = -u \cdot \nabla c_i + \frac{1}{\rho} \nabla \cdot (\rho K \nabla c_i) + f_i(c) + E_i$$

where chemical reactions are modeled by nonlinear stiff terms

$$f_i(c) = P_i(c) - D_i(c) c_i$$

- Use operator splitting to solve CTM

$$\mathrm{M}_{[t,t+\Delta t]} = T_X^{\Delta t/2} \cdot T_Y^{\Delta t/2} \cdot T_Z^{\Delta t/2} \cdot C^{\Delta t} \cdot T_Z^{\Delta t/2} \cdot T_Y^{\Delta t/2} \cdot T_X^{\Delta t/2}$$

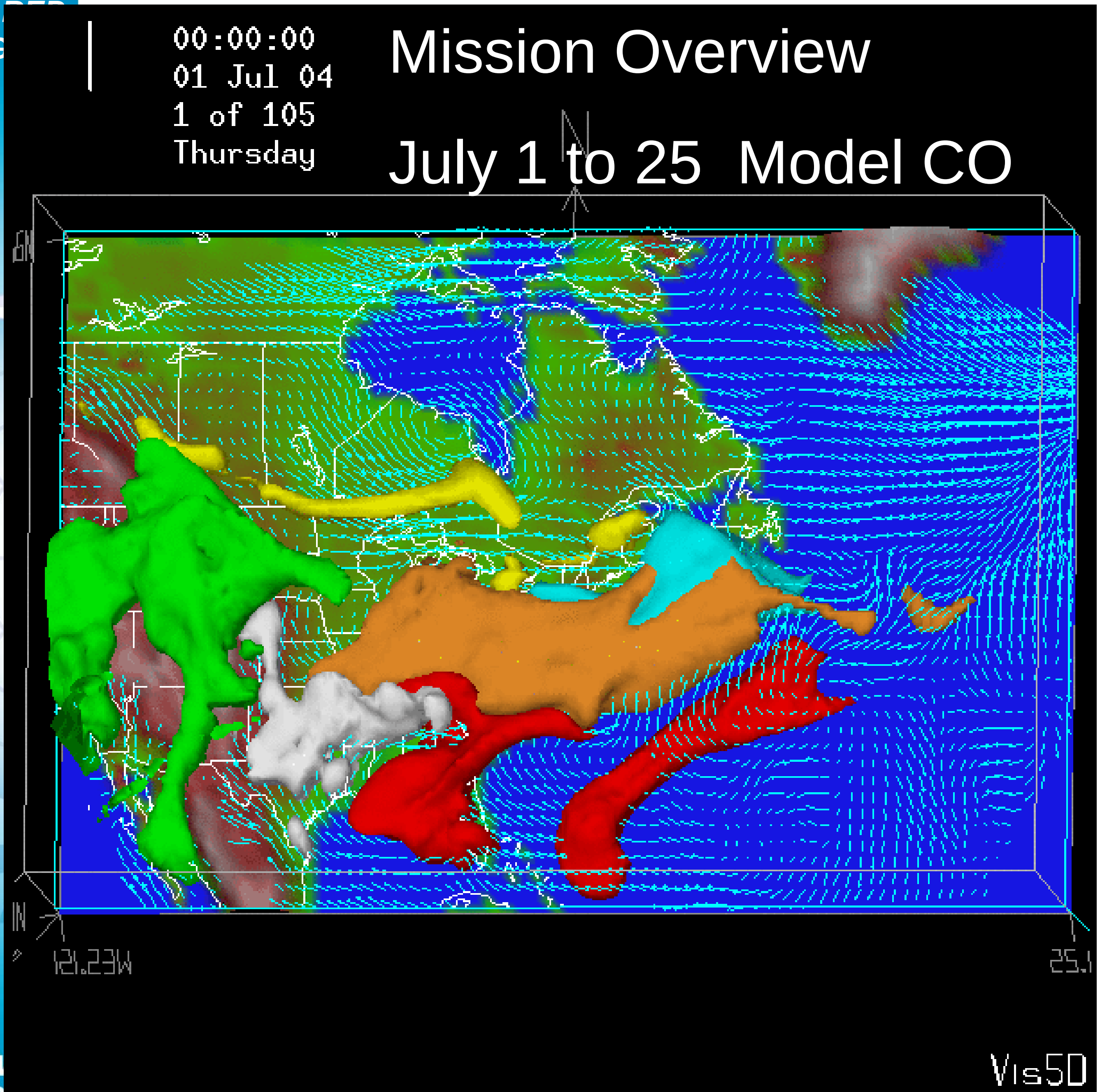
WMO
OMM

Models are an Integral Part of Air Quality Studies

- Field experiment planning
- Provide 4-Dimensional context of the observations
- Facilitate the integration of the different measurement platforms
- Evaluate processes (e.g., role of biomass burning, heterogeneous chemistry....)
- Evaluate emission estimates (bottom-up as well as top-down)
- Emission control strategies testing
- Air quality forecasting
- Measurement site selection

Mission Overview

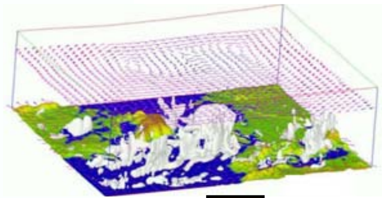
July 1 to 25 Model CO



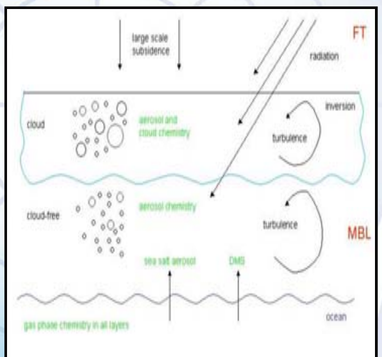
AREP
GAW

Air Quality Modeling: Improving Predictions of Air Quality (analysis and forecasting perspectives)

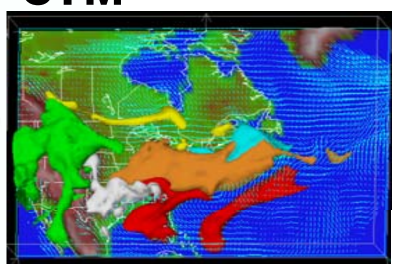
Met model



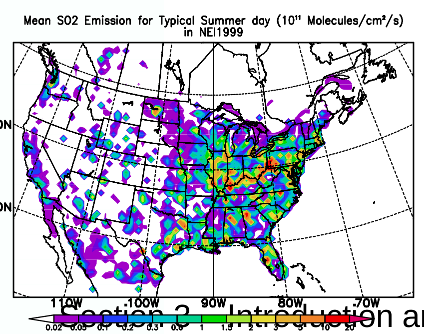
Chemical, Aerosol, Removal modules



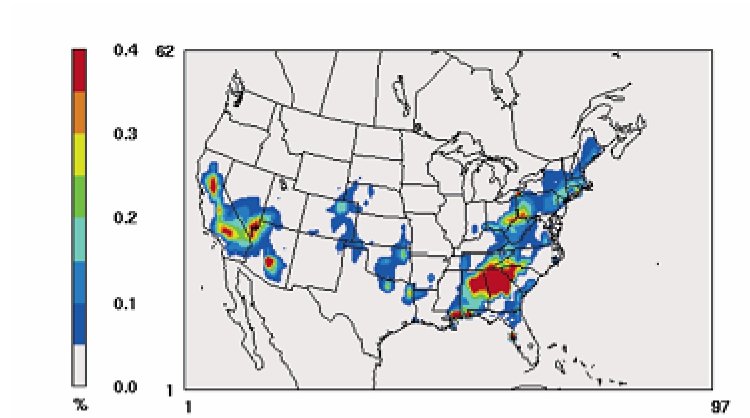
CTM



Emissions

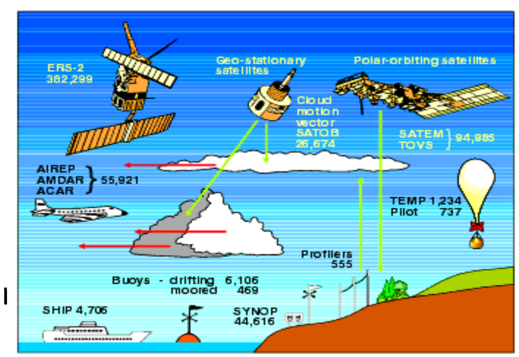


Predicted Quantity: e.g., *ozone AQ violation*



How confident are we in the models & predictions?

Observations

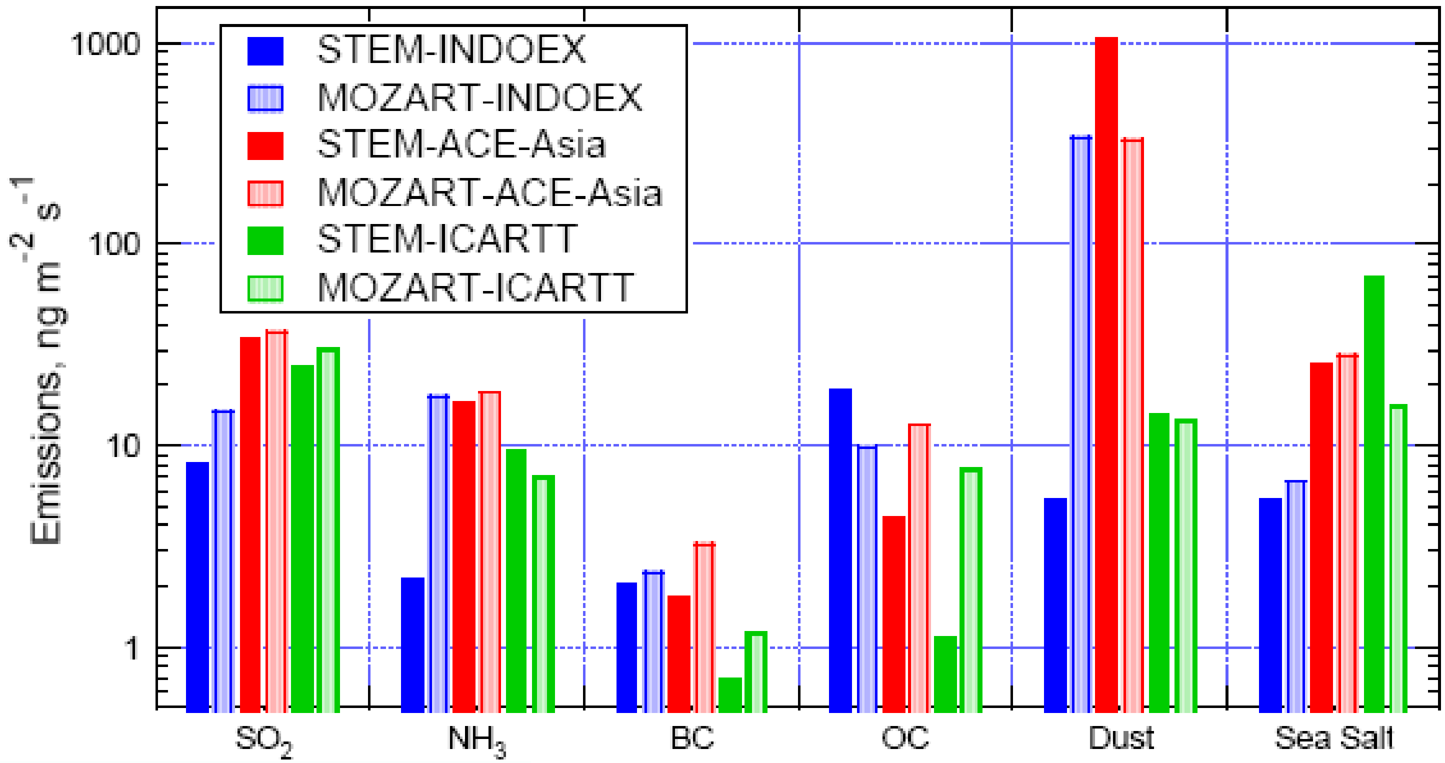


WMO
OMM

How do we build upon what is done and move beyond to improve air quality prediction?

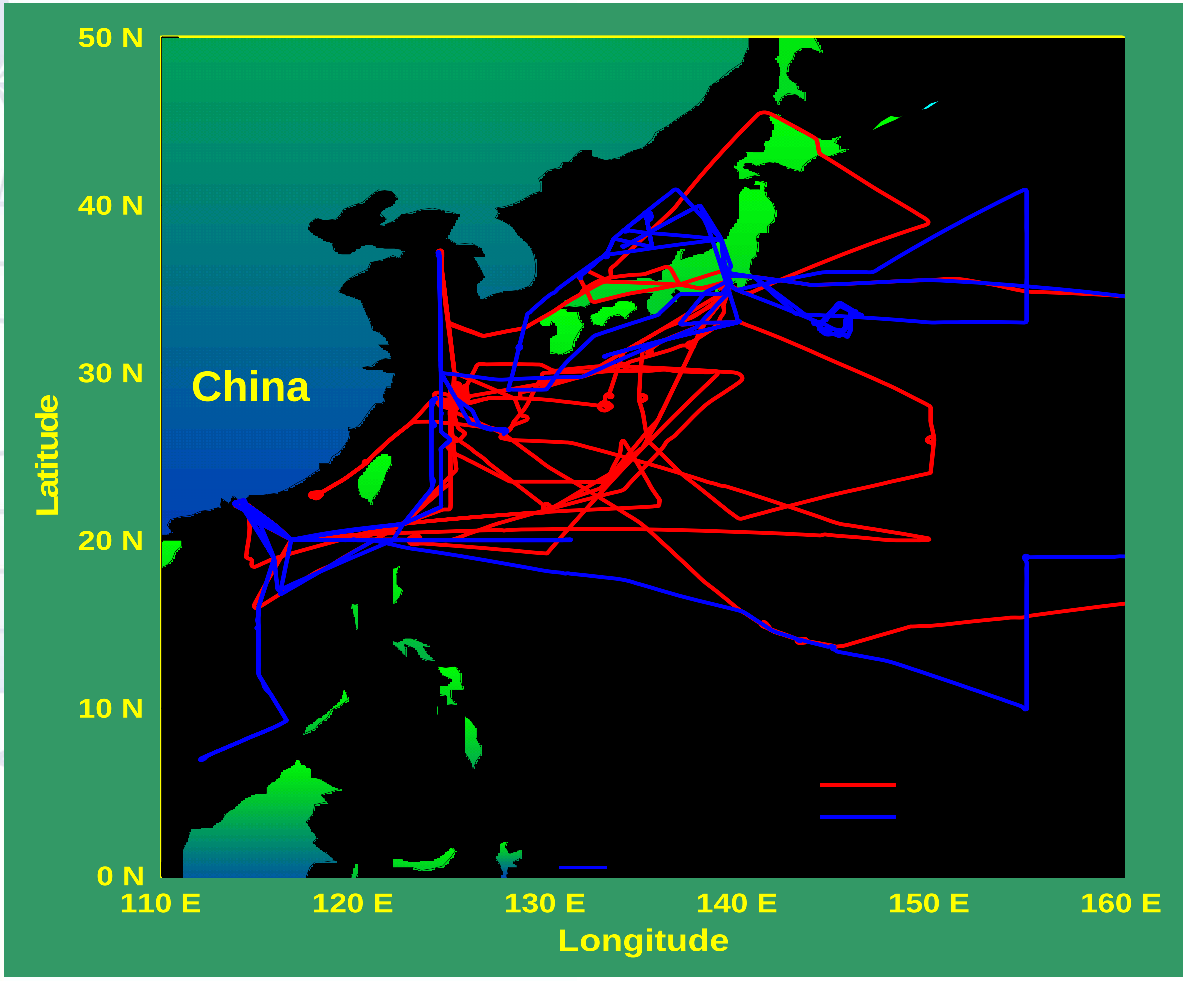
- ✓ Informed by comparisons of predictions with observations.
- ✓ Informed by process studies.
- ✓ Informed by model inter-comparison studies.

Emissions are the Largest Single Source of Uncertainty



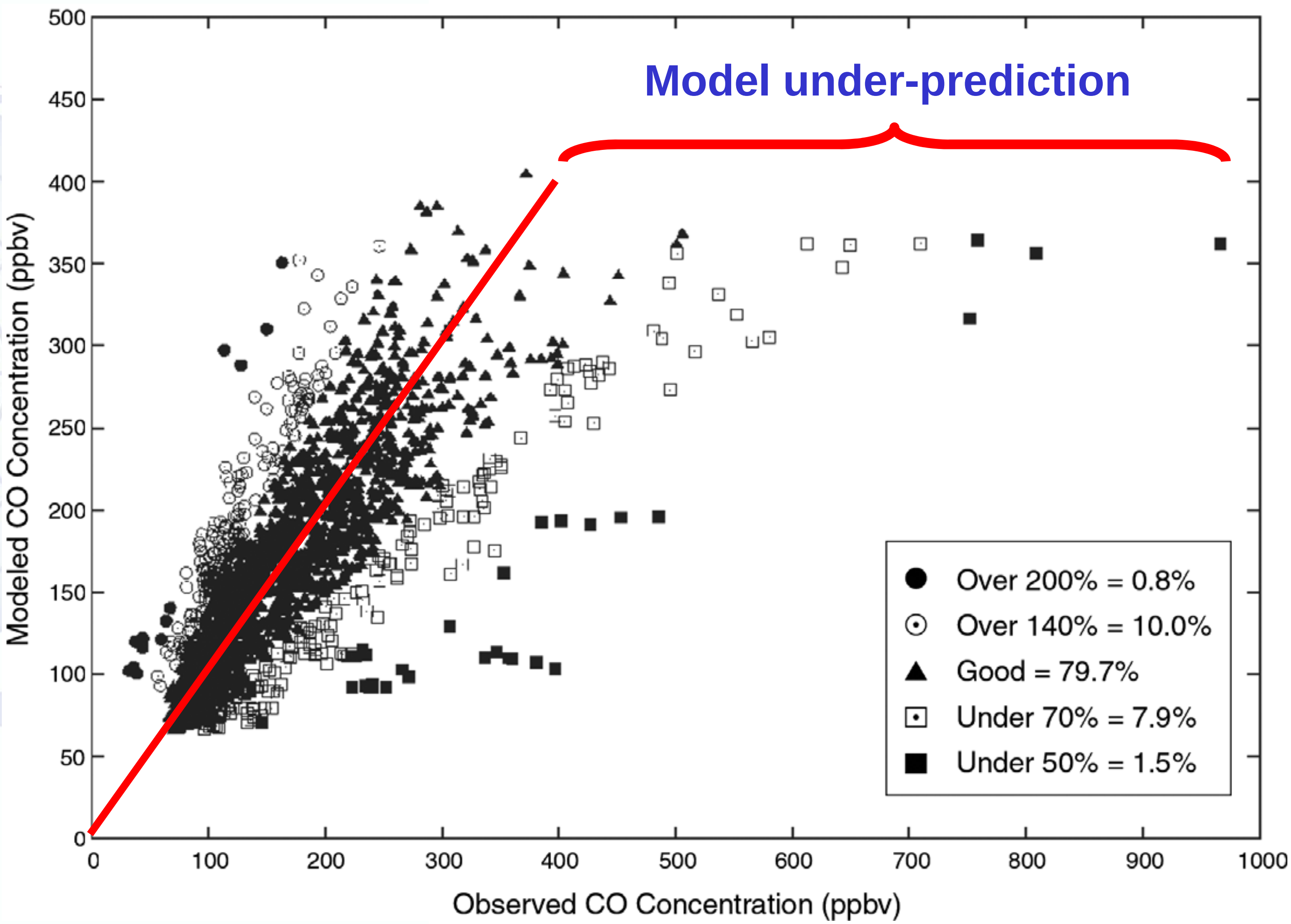
Uncertainties: SO2 <BC & OC < Dust & Sea Salt

Experiments such as TRACE-P and ACE-Asia employ mobile "Super-Sites" and study pollution outflow from source regions



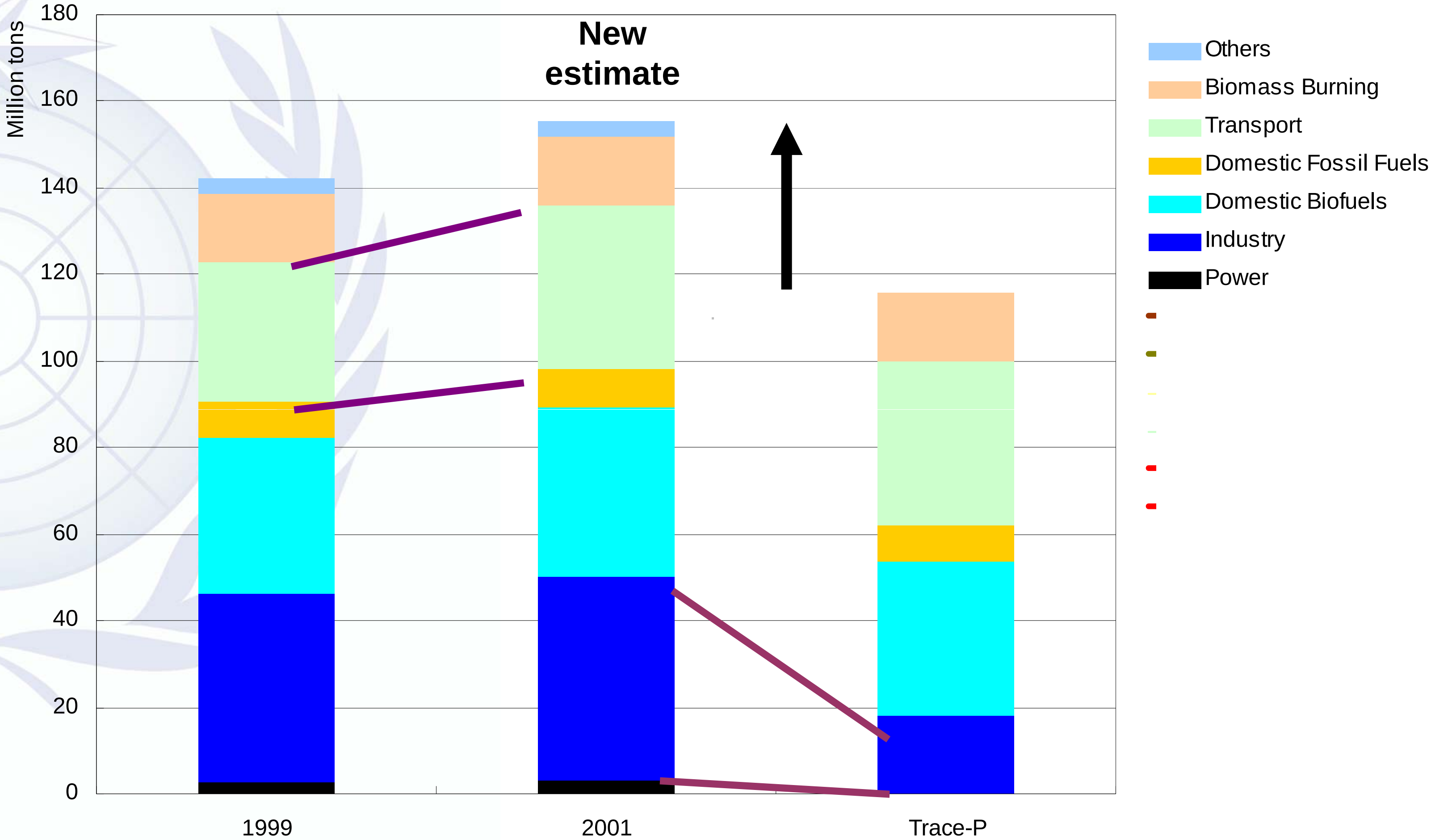
Spring 2001

Post-mission analysis has shown that the inventory seems good for most species, except for high CO and BC observations in the Yellow Sea



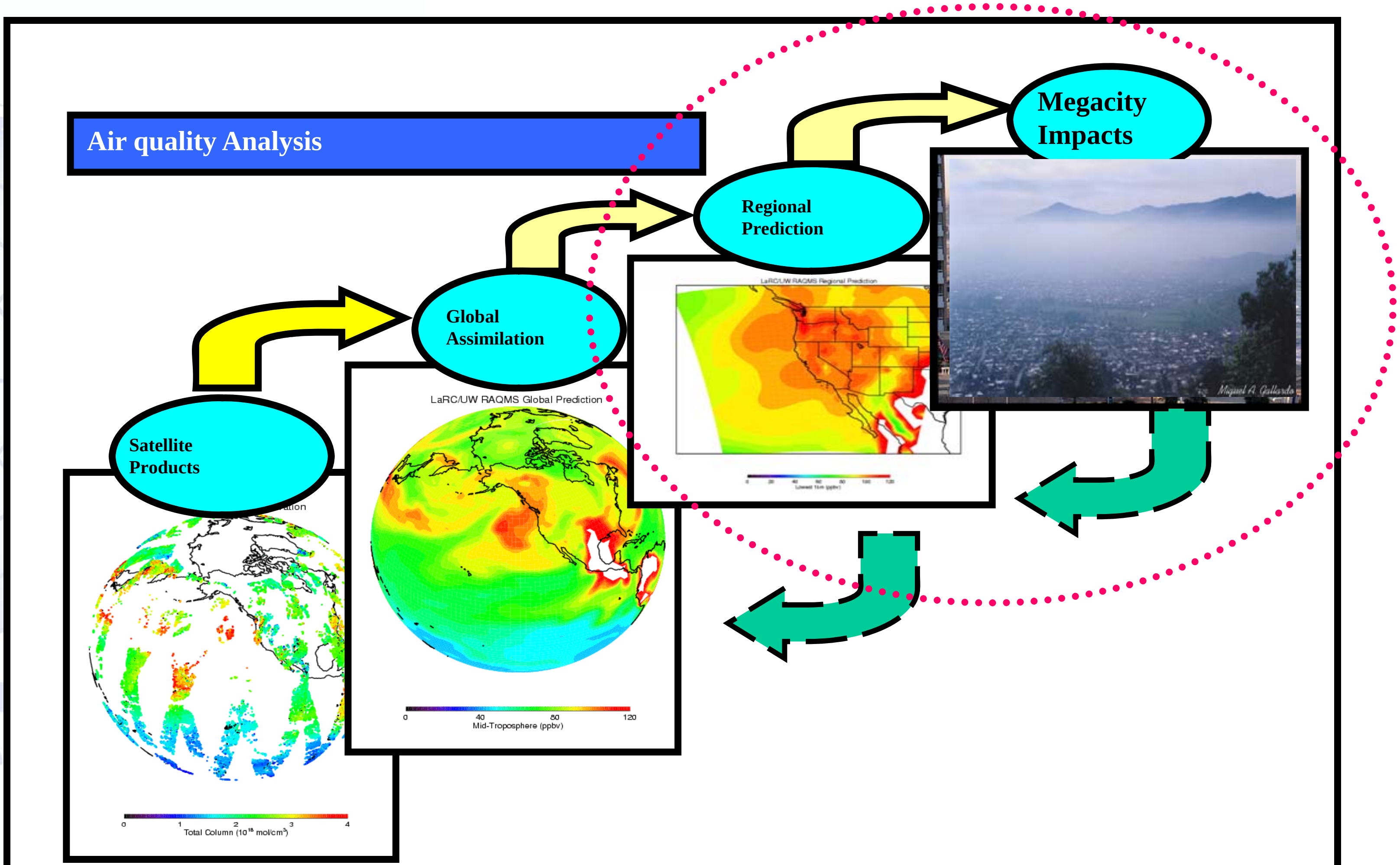
(Carmichael et al., JGR, 2003)

Comparison of New CO Inventory with Trace-P



AREP
GAW

Air Quality Prediction: A Challenge of Scales and Integration



Modified after Pierce NASA/Langley

WMO
OMM

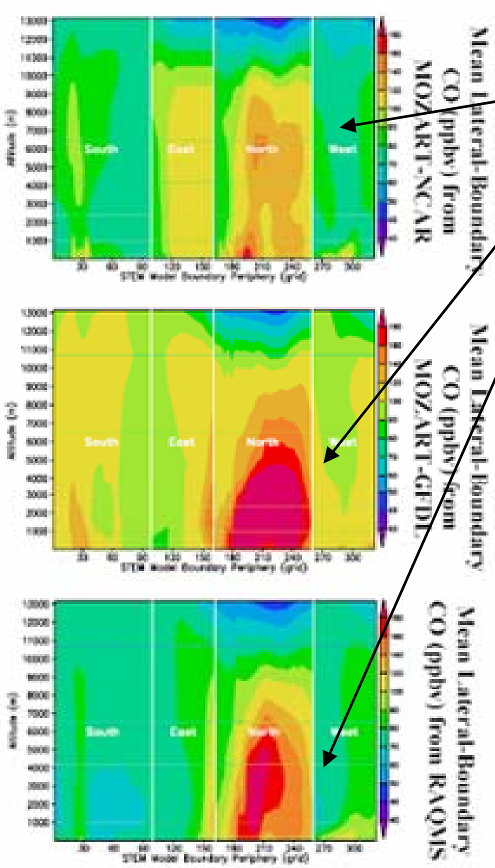
AREP GAW

Integrated Science Studies:

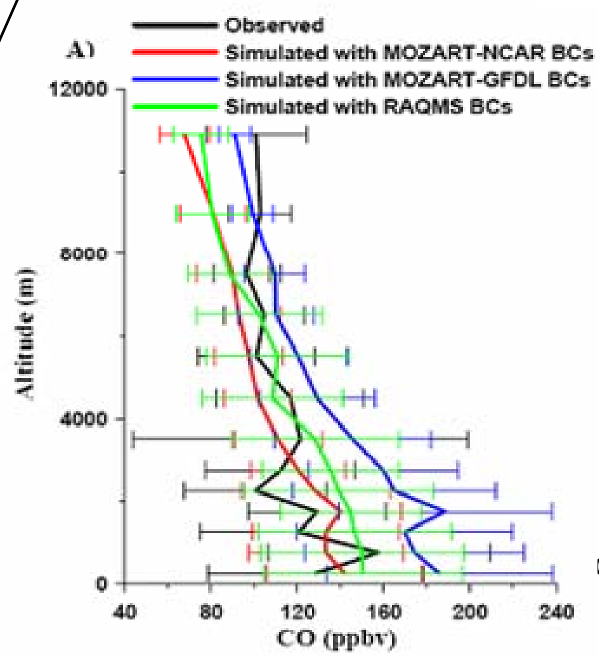
Impacts of Global Composition on Regional Air Quality

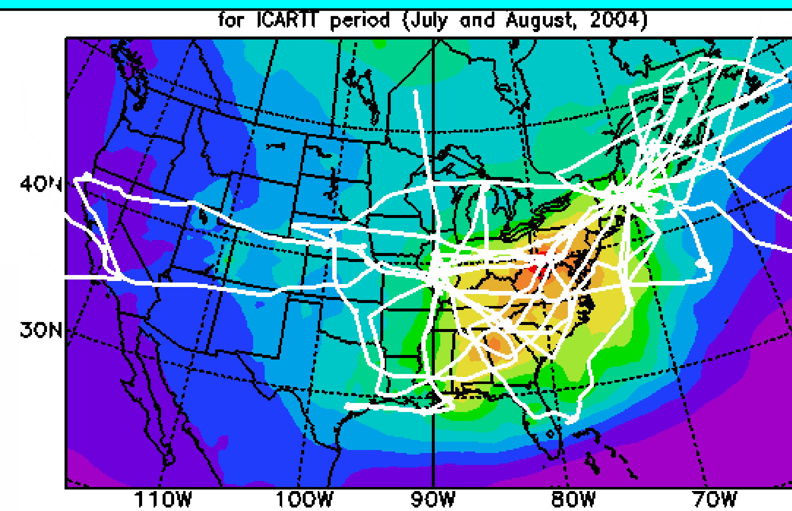
Global-Regional-Urban nesting of CTMs

Effects of Boundary Conditions are significant and improve predictions (*Tang et al., JGR 2007*).



Alaskan BB Impacts Northern Boundary



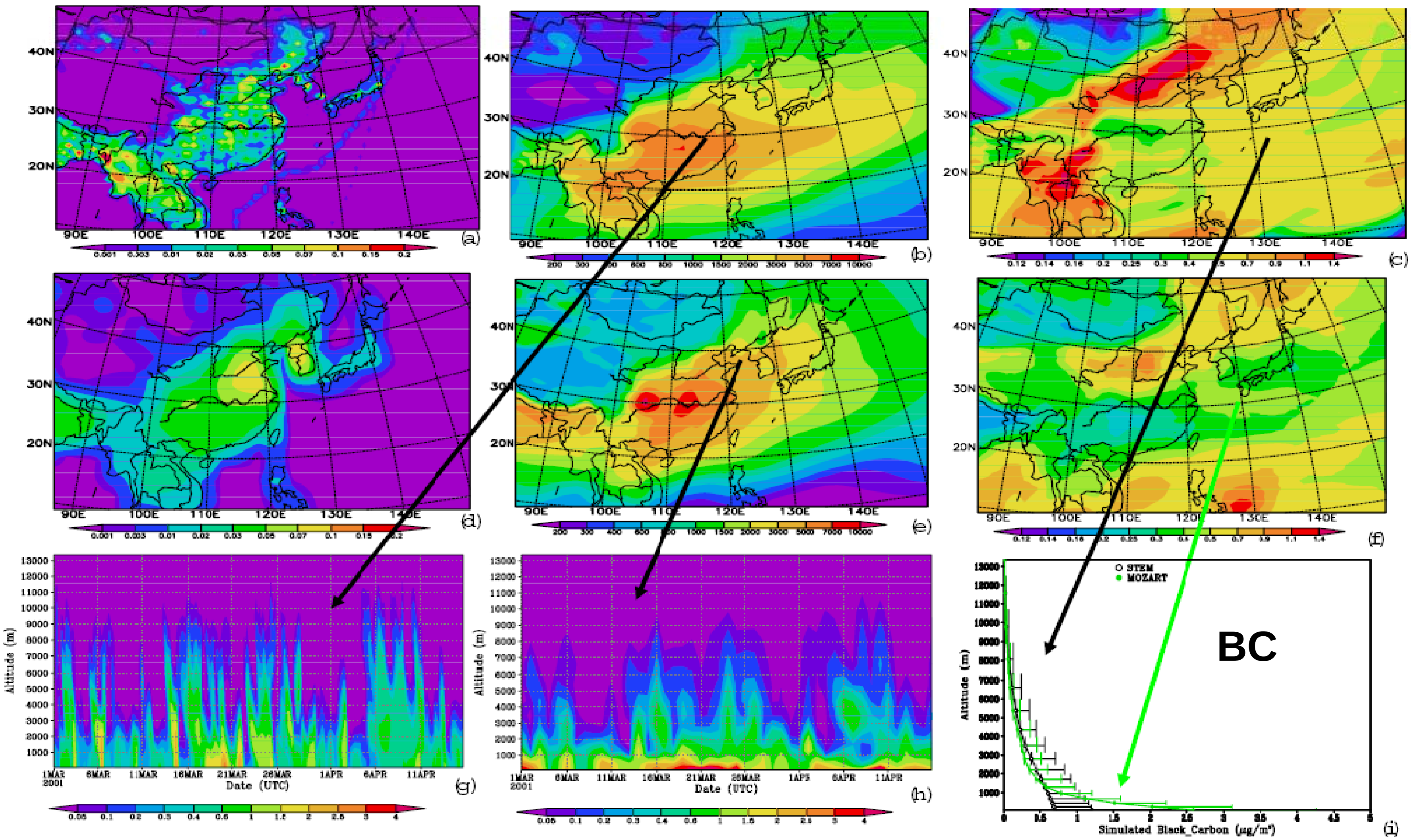


Assessment of continental inflow/outflow requires unified modeling/measurement strategy to accurately characterize coupling between the continental boundary layer, free troposphere, and long-range transport.

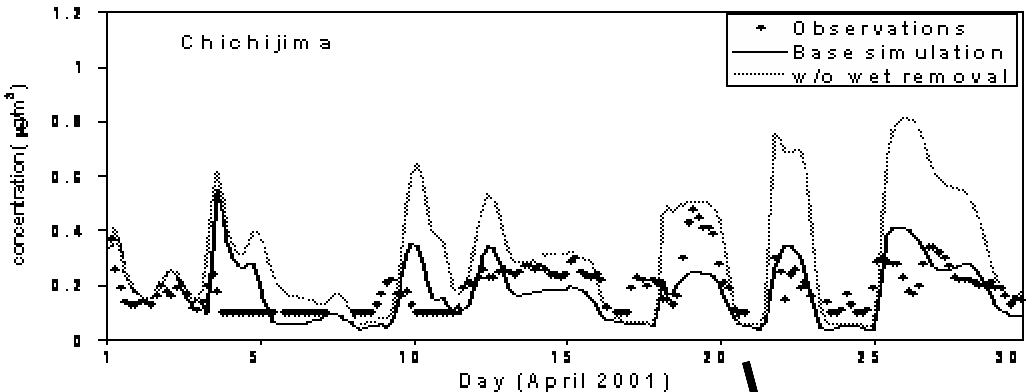
AREP
GAW

Model Resolution, Transport and Removal also Contribute to Differences

Emissions *Monthly mean concentrations* *Temporal variation in concentrations*



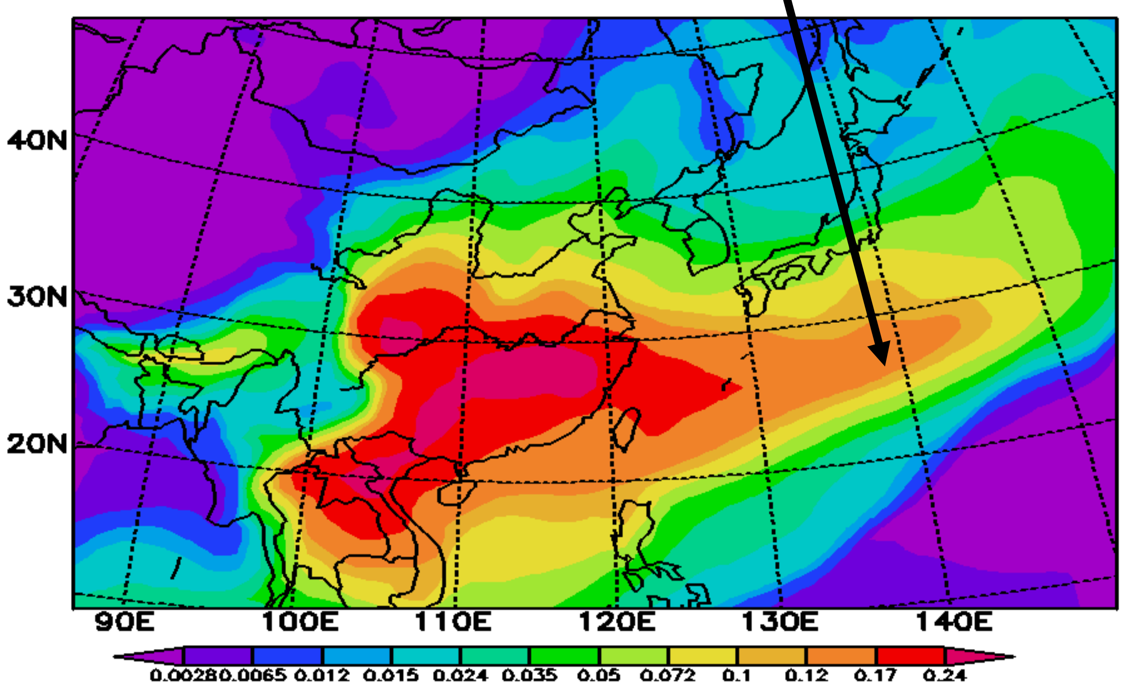
Removal Processes Remain Poorly Characterized in Models

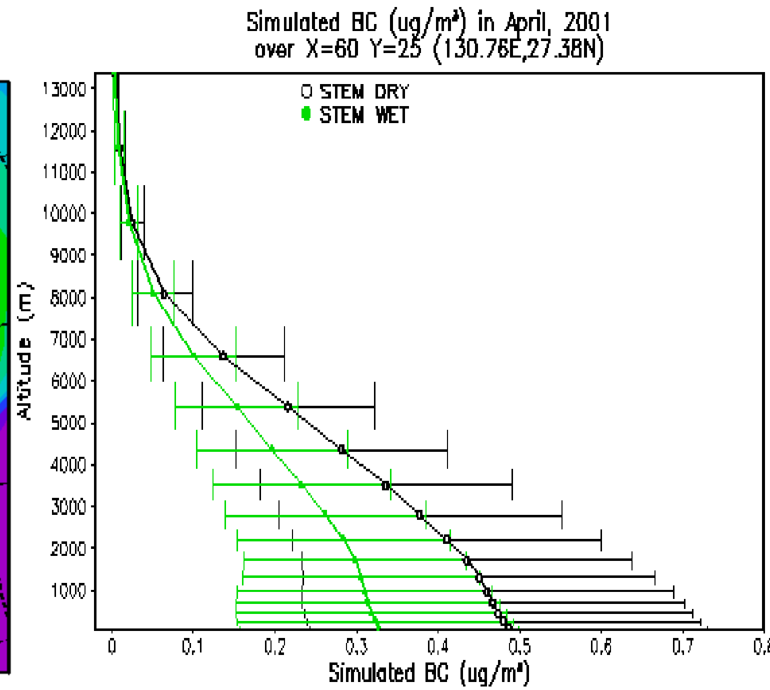


Impact of Wet Removal on Predicted BC

Progress limited by lack of understanding and observations

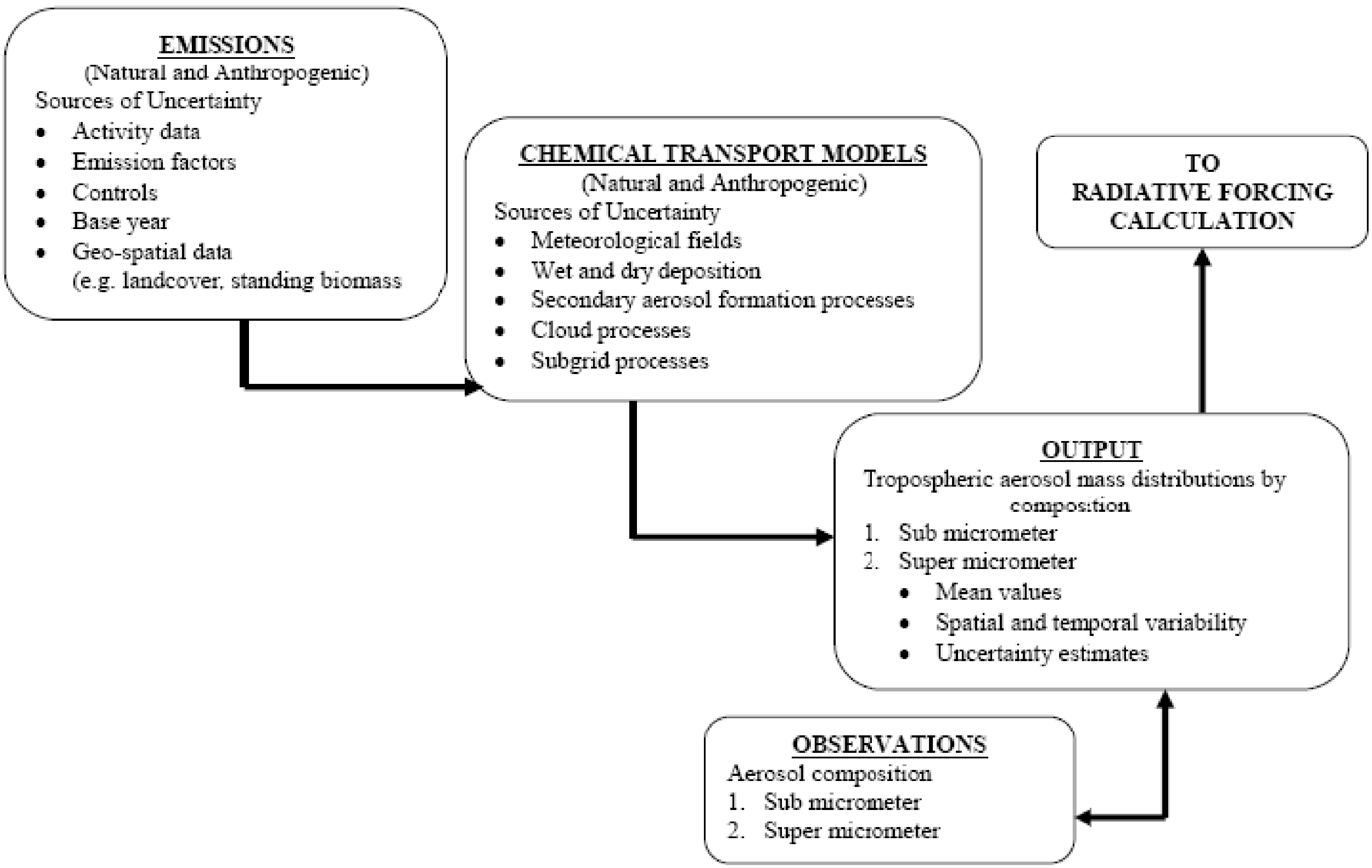
Mean BC Difference (dry−wet) (ug/m³) in the 1km Layer





AREP GAW

Schematic of the Calculation Chain Linking Emissions to Aerosol Distributions



WMO OMM

Summary of Major Sources of Uncertainty in the Calculations

Multiplicative Uncertainties

Indoex					
	Emissions	Wet removal	Vertical Transport	Chemical Formation	Total Uncertainty
nss SO4	1.3	1.3	1.5	1.3	1.8
BC	3	2	1.5	--	3.9
OC	3.5	2	1.5	3	6.4
Dust	5	2	1.5	--	6.0
Sea Salt	5	1.3	1.5	--	5.4

sub

Super micron

Note: for analysis of specific points some of these terms are larger…

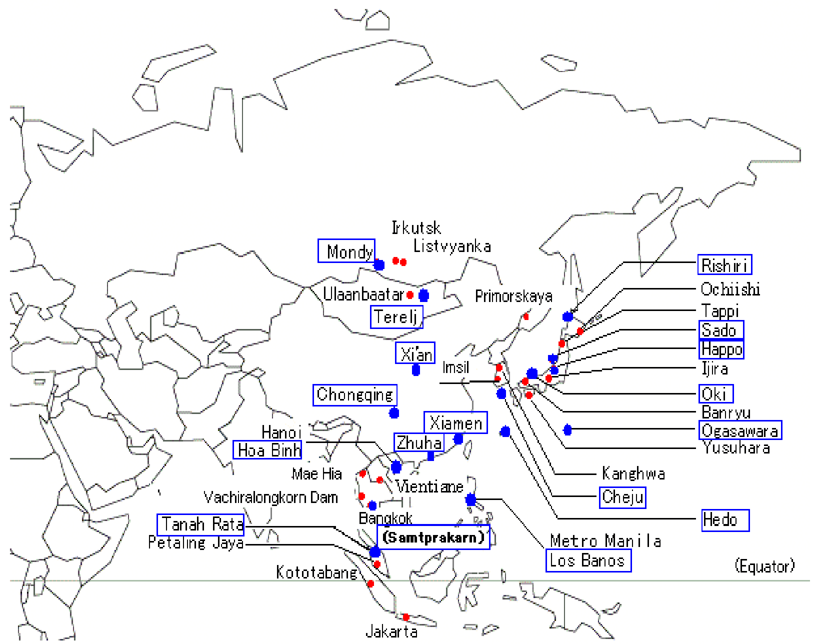
MICS-Asia < *M*odel *I*nter*C*omparison *S*tudy in *Asia* >

Main goal on of model performance to make an international common understanding and improve for air pollution modeling in East Asia

Nine different regional models

Observations:

- EANET (47 sites) (gas, aerosol, deposition)
- Ozonesondes
- Trace-P Obs.
- Special obs. (aerosols)
- Met obs (sondes and surface)
- (daily & monthly analysis)
- Special Section of *Atmospheric Environment (8 papers)*

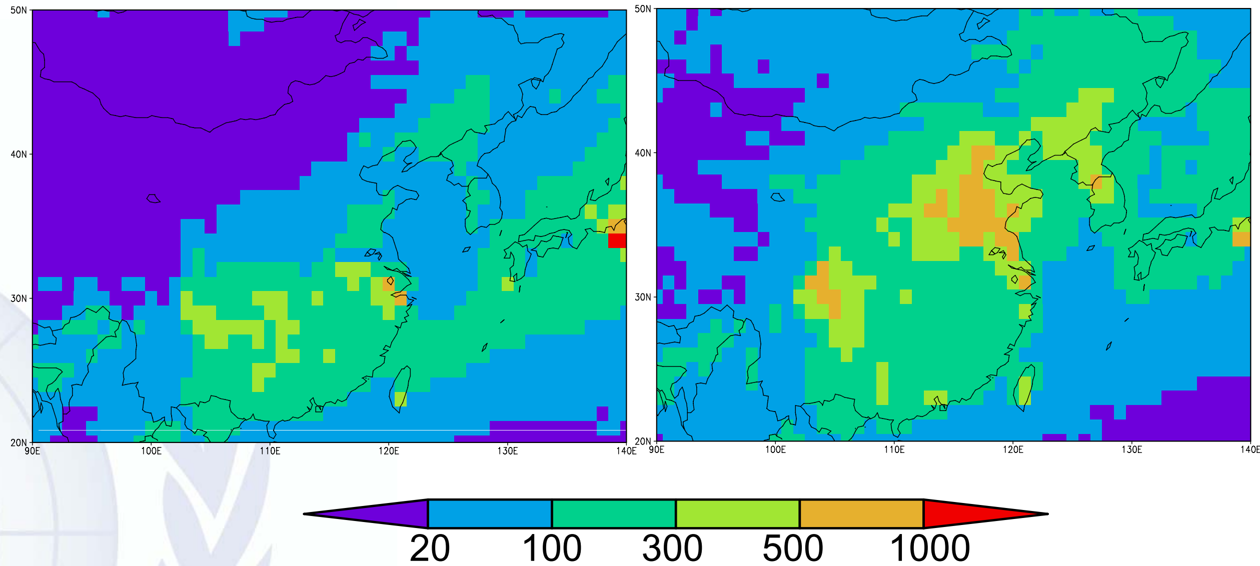


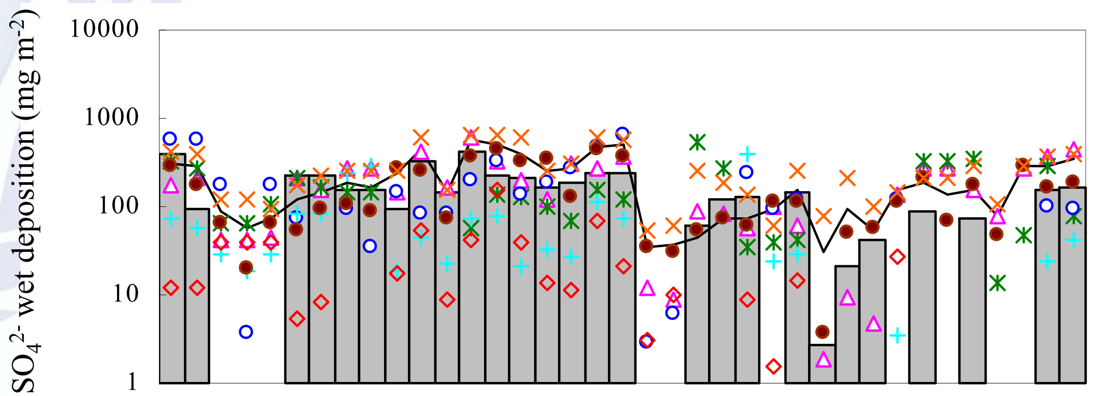
MICS-III Will look also at megacities

AREP
GAW

The ensemble mean near surface monthly mean total sulfur deposition amounts (as sulfate) for the different seasons.

March 2001 July 2001





(mg m^{-2})

Nitrate quantities typically underestimated.

AREP
GAW

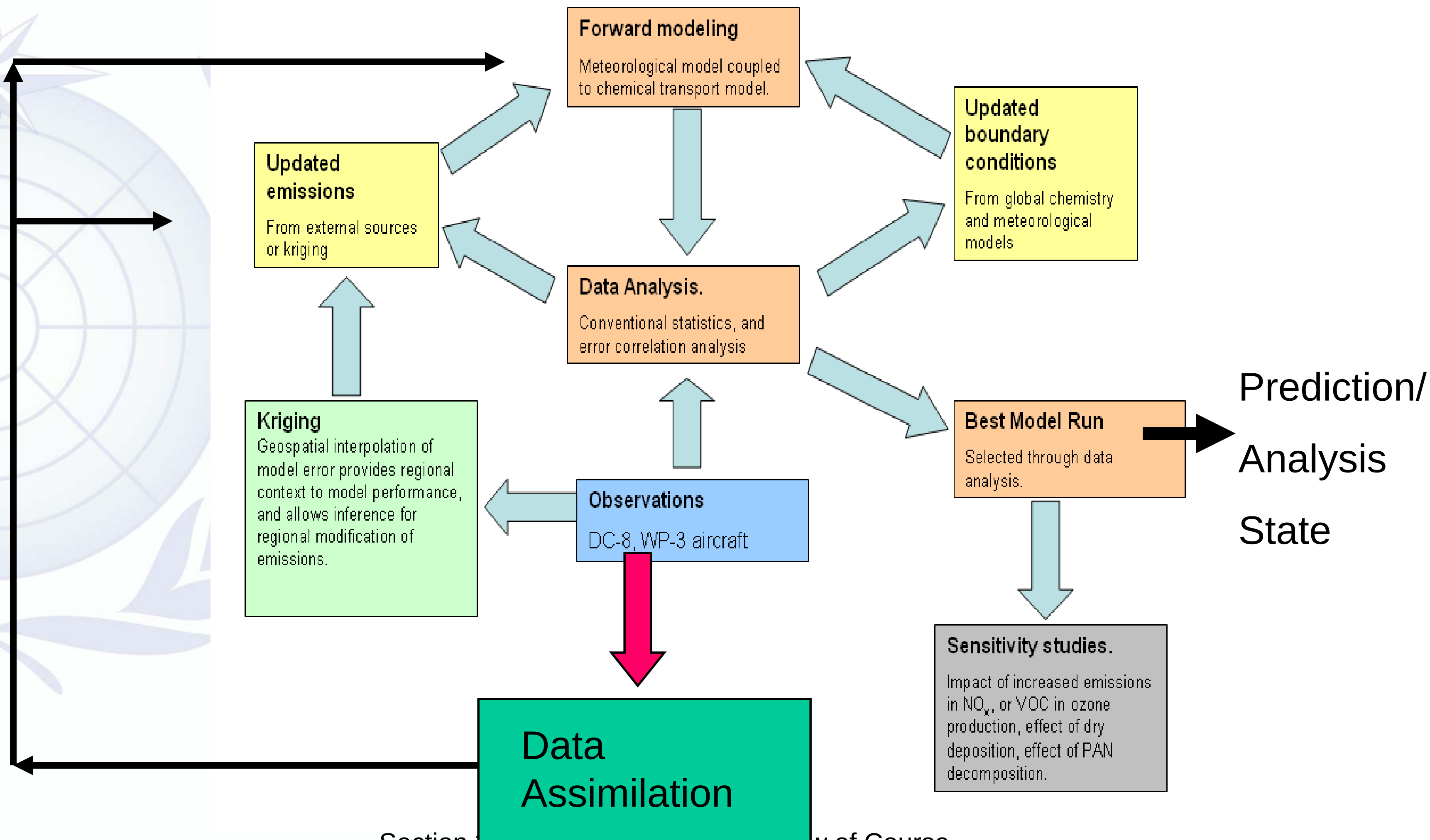
Special Section Atmospheric Environment

- The Model Intercomparison Study for Asia Phase II, Methodology and Overview of Findings
- Model Intercomparison and Evaluation of Ozone and Relevant Species
- Model Intercomparison and Evaluation of Particulate Sulfate, Nitrate and Ammonium
- Impact of Global Emissions on Regional Air Quality in Asia
- An intercomparison study of emission inventories for the Japan region.
- Sensitivity analysis of predicted aerosol composition to the aerosol module formulation.
- Model Intercomparison and Evaluation of Acid Deposition
- Evaluating Gaseous Pollutants in East Asia Using An Advanced Modeling System: Models-3/CMAQ System

WMO
OMM

AREP
GAW

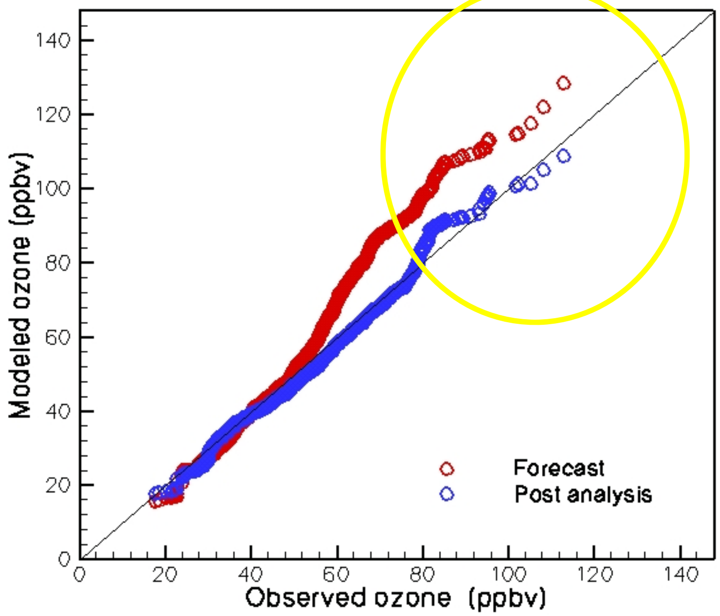
Our Analysis Approach

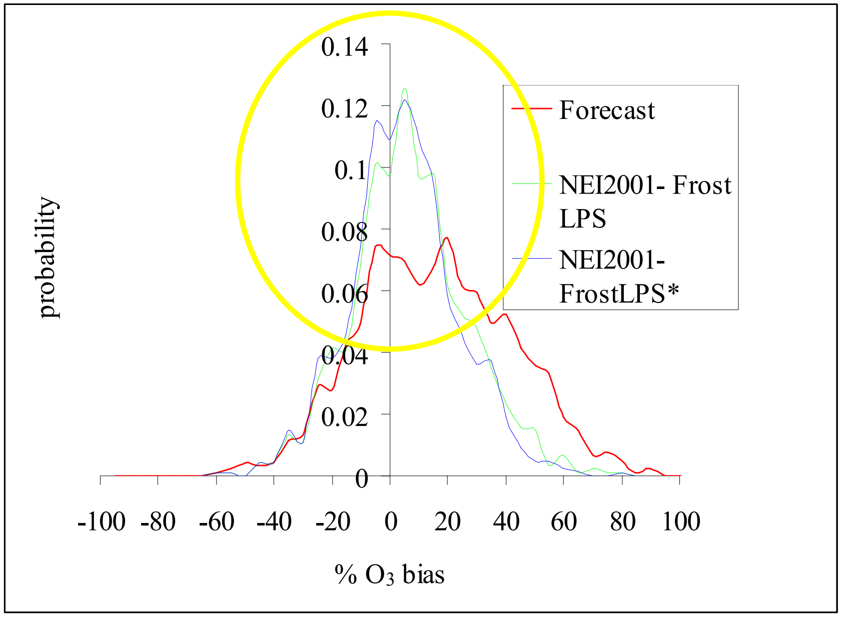


WMO
OMM

AREP
GAW

Documenting improvement (ICART)



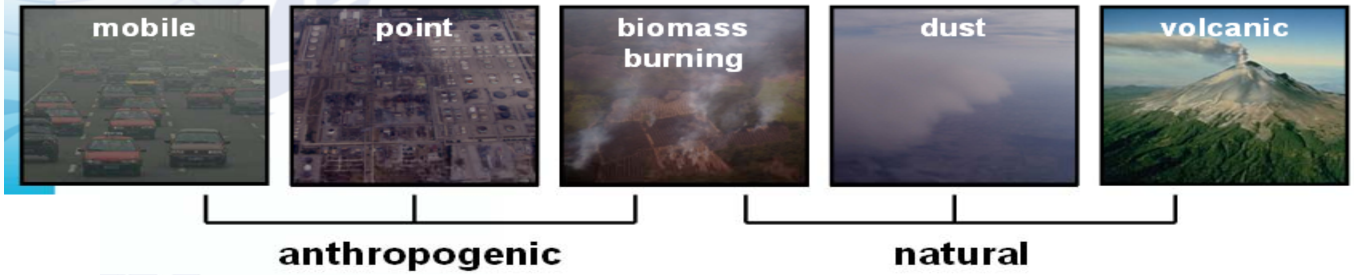


Left: Quantile-quantile plot of modeled ozone with observed ozone for DC-8 platform, data points collected at altitude less than 4000m, STEM-2K3, Forecast: NEI 1999, Post Analysis: NEI2001-Frost LPS*. MOZART-NCAR boundary conditions Right: Probability distribution of % ozone bias for Forecast (NEI 1999) and post analysis runs (NEI2001-FrostLPS and NEI2001-FrostLPS*) for DC-8 measurements under 4000m.

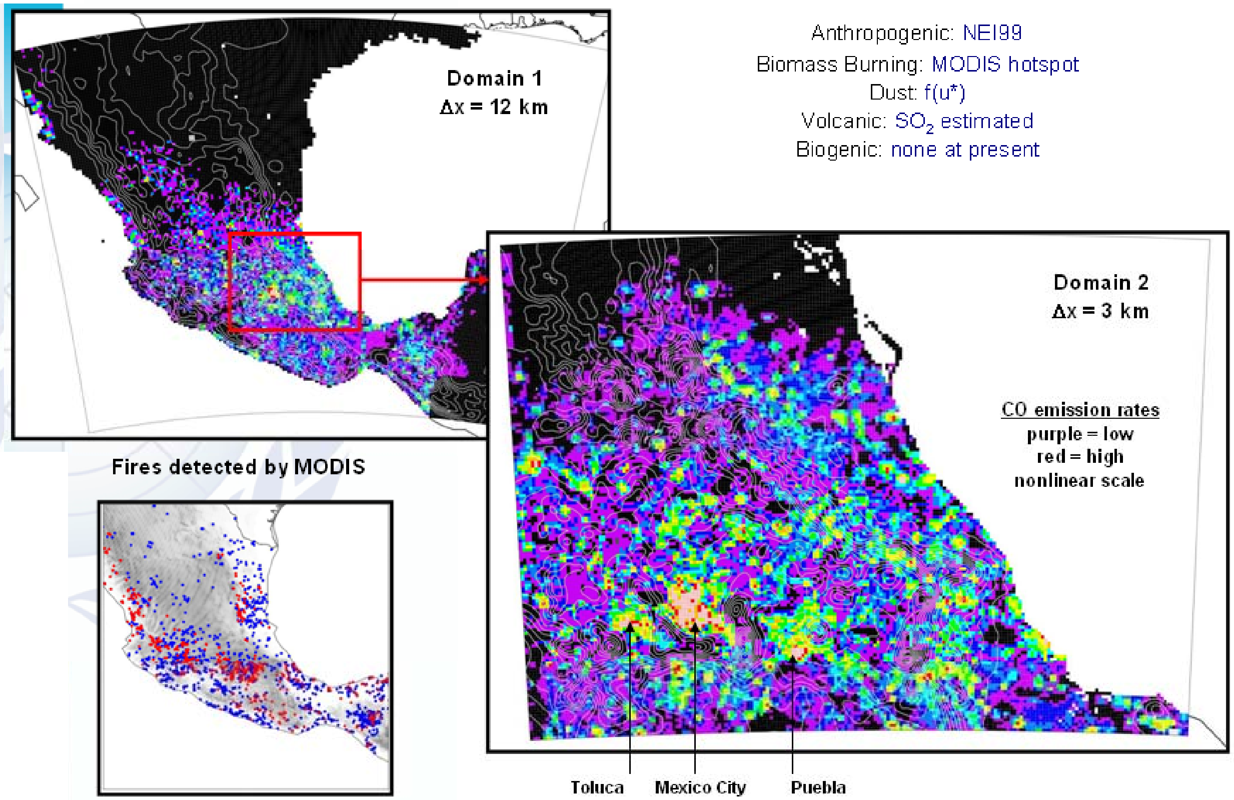
Mena et al., JGR, 2007

AREP
GAW

Need to Estimate Emissions at Appropriate Scales



Anthropogenic: NEI99
Biomass Burning: MODIS hotspot
Dust: f(u*)
Volcanic: SO_2 estimated
Biogenic: none at present



WMO
OMM

AREP GAW

Integrated Analysis Framework for Linking Meteorology, Air Quality and Human Exposure

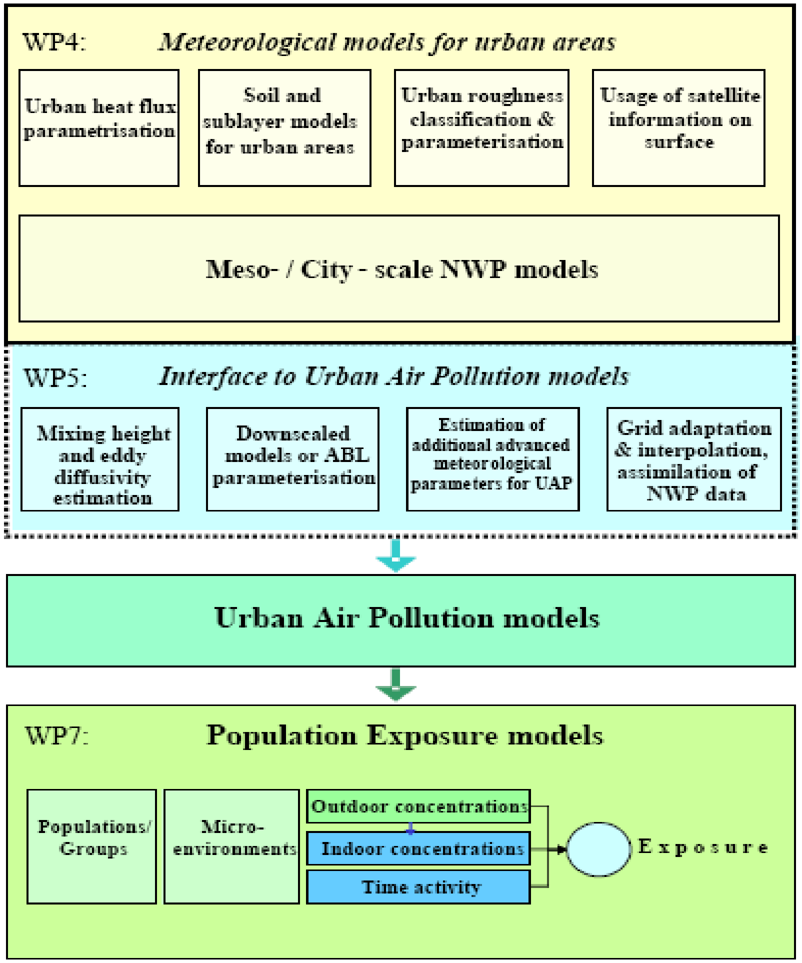


Fig. 1. Outline of the overall FUMAPEX methodology integrating models from urban meteorology to air quality and population exposure. The main improvements in meteorological forecasts (NWP) for urban areas, interfaces and integration with urban air pollution (UAP) and population exposure (PE) models for the Urban Air Quality Information Forecasting and Information Systems (UAQIFS) are mentioned in the scheme.

uction ai

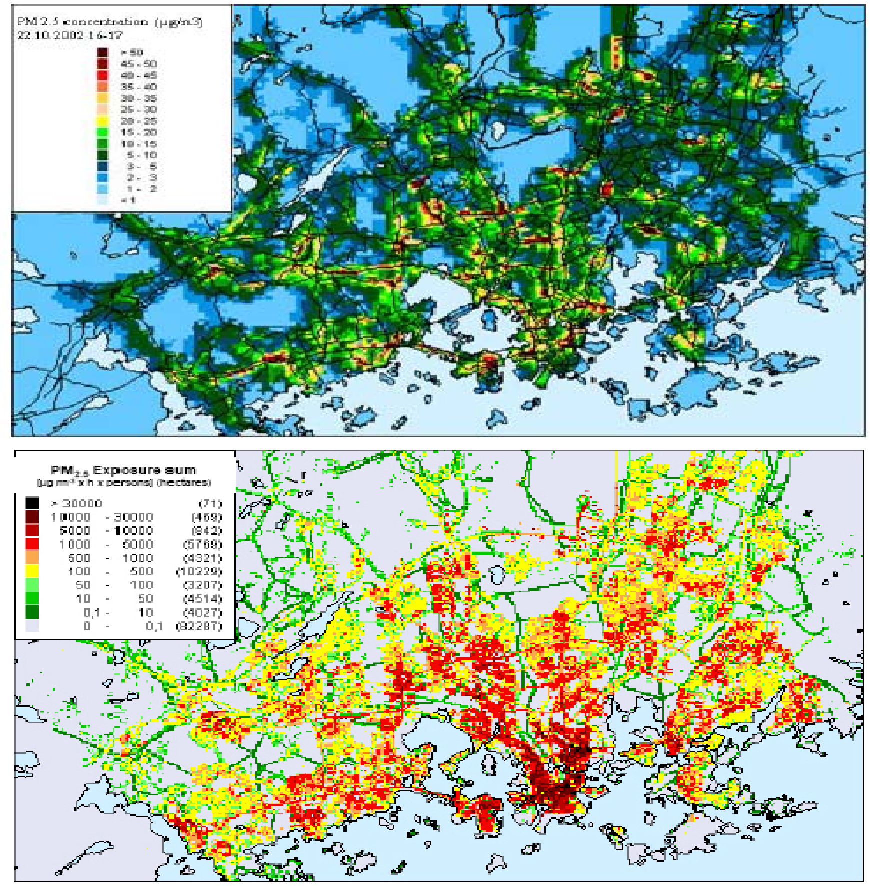
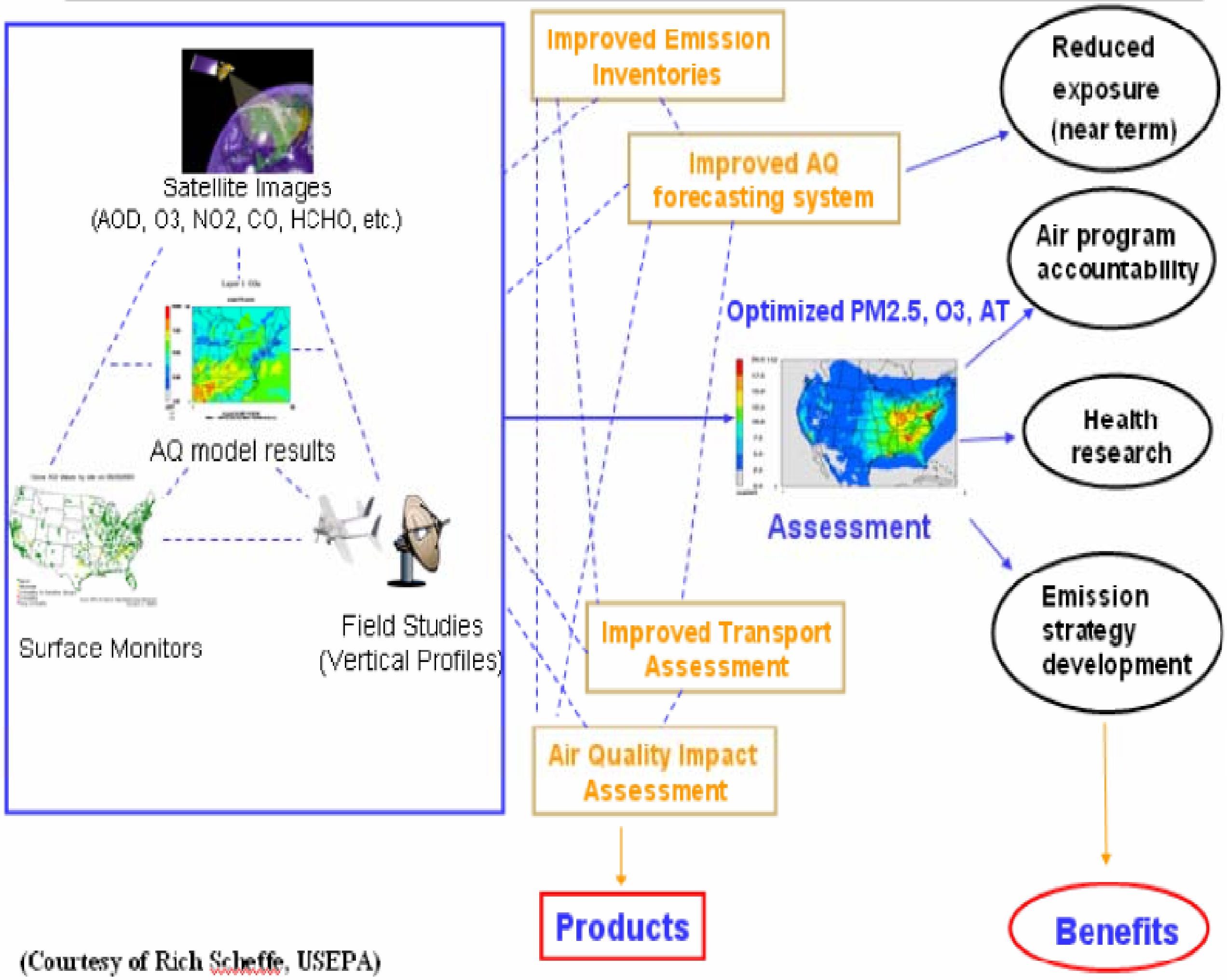


Fig. 2. Predicted spatial distribution of the concentrations of $PM_{2.5}$ in the Helsinki metropolitan area during an afternoon rush hour (from 04:00 to 05:00 p.m.; upper map), and the daily population exposure to $PM_{2.5}$, computed with the EXPAND model (lower map), both of these in the course of a peak pollution episode on 22 October 2002. The episode was mainly caused by stable atmospheric stratification combined with a strong ground-based temperature inversion.

Baklanov et al., ACP, 2007

AREP
GAW

Summary of Course – Introduction to Air Quality Modeling



(Courtesy of Rich Scheffe, USEPA)

WMO
OMM

AREP
GAW

WMO
OMM