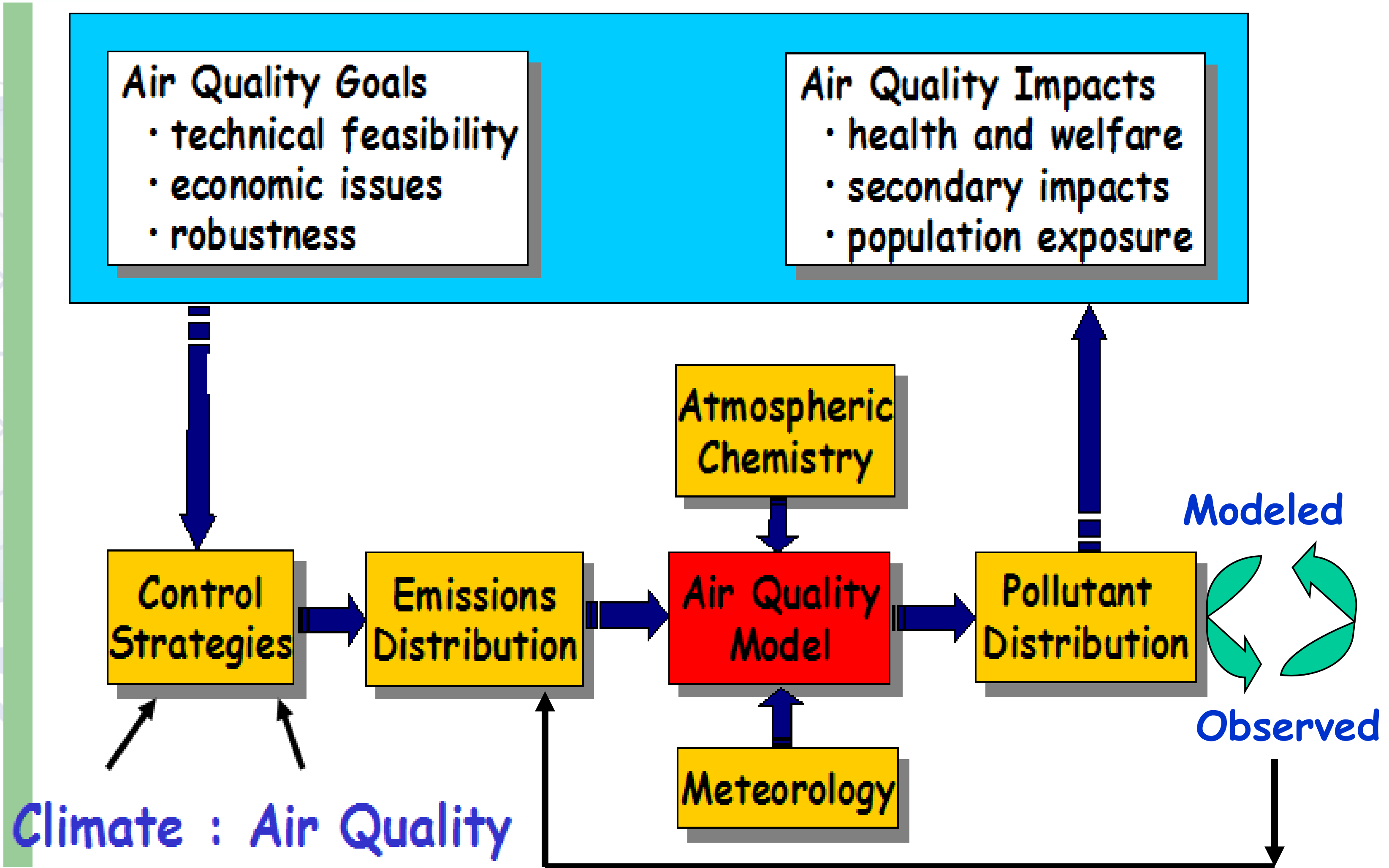
Introduction and Overview of Course

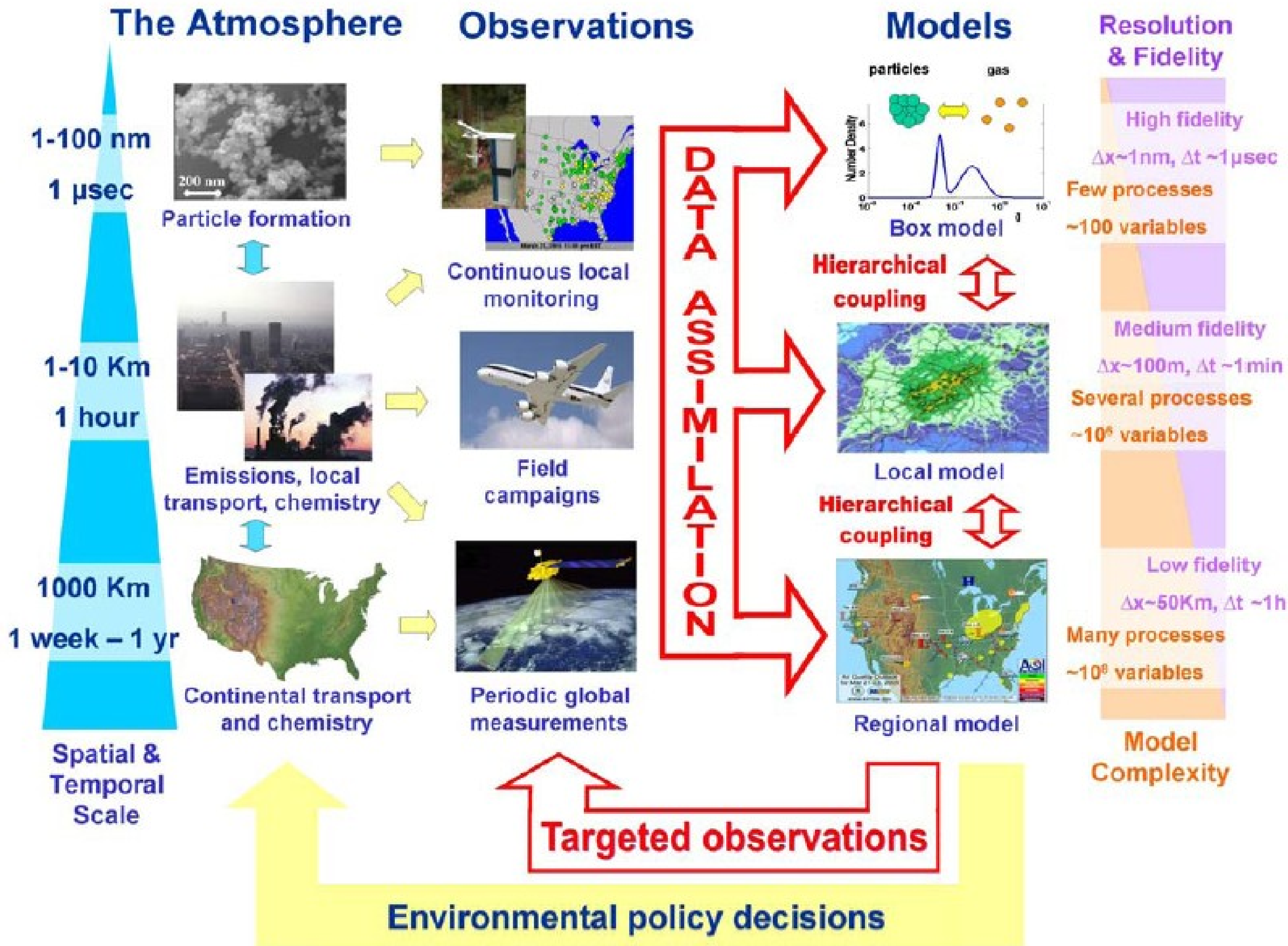
Air Quality Modeling Introduction

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



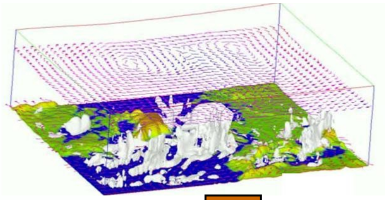
Models are an Integral Part of Air Quality Studies

- 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

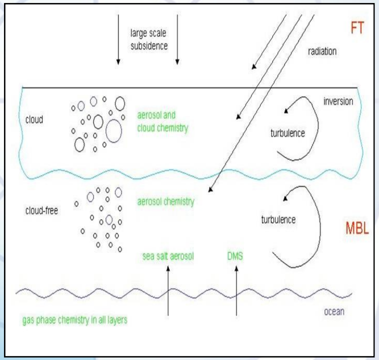

The Atmosphere
Observations
Models
Resolution & Fidelity
1-100 nm
1 μsec
200 nm
Particle formation
1-10 Km
1 hour
Emissions, local transport, chemistry
1000 Km
1 week – 1 yr
Continental transport and chemistry
Spatial & Temporal Scale
Continuous local monitoring
Field campaigns
Periodic global measurements
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
~10^6 variables
Low fidelity
Δx~50Km, Δt ~1h
Many processes
~10^8 variables
Model Complexity
Targeted observations
Environmental policy decisions

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

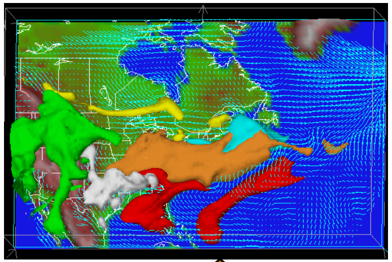
Met model



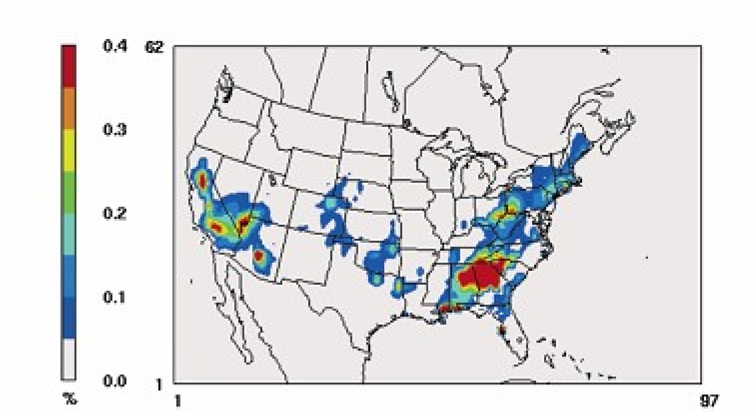
Chemical, Aerosol, Removal modules



CTM

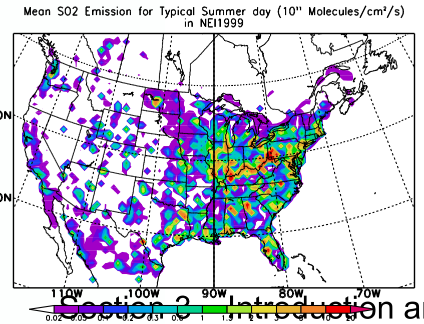


Predicted Quantity: e.g., *ozone AQ violation*

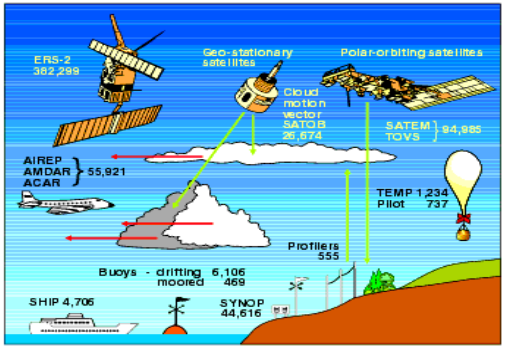


How confident are we in the models & predictions?

Emissions



Observations



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

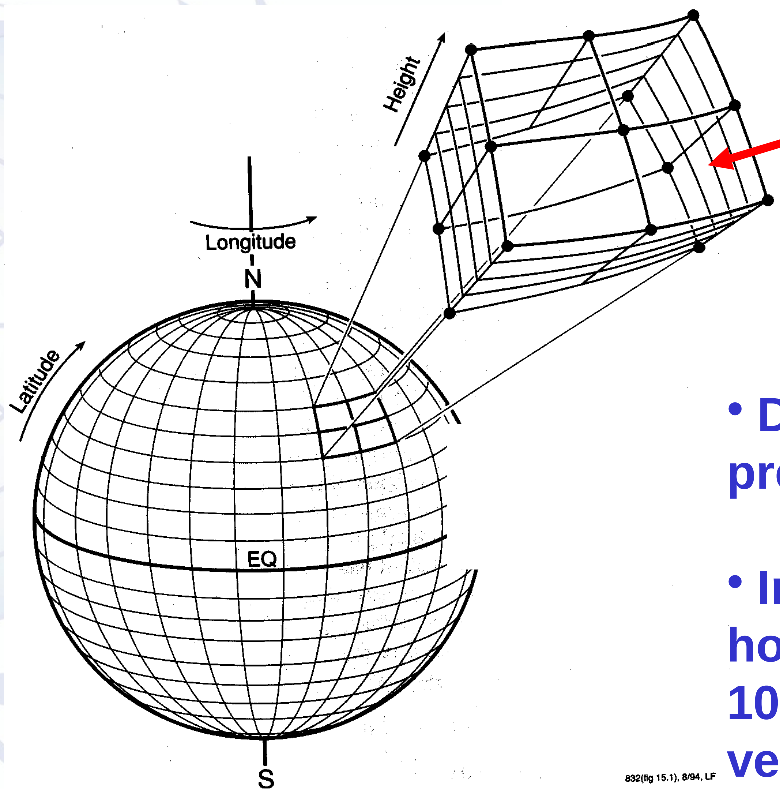
$$f_i(c) = P_i(c) - D_i(c) c_i$$

- Use operator splitting to solve CTM

$$M_{[t, t+\Delta t]} = T_X^{\Delta t/2} \, T_Y^{\Delta t/2} \, T_Z^{\Delta t/2} \, C^{\Delta t} \, T_Z^{\Delta t/2} \, T_Y^{\Delta t/2} \, T_X^{\Delta t/2}$$

EULERIAN MODELS PARTITION ATMOSPHERIC DOMAIN INTO GRIDBOXES

This discretizes the continuity equation in space



Solve continuity equation for individual gridboxes

- **Detailed chemical/aerosol models can presently afford -10^6 gridboxes**

- **In global models, this implies a horizontal resolution of ~ 0.5-1^o (~50 to 100 km) in horizontal and ~ 0.5-1 km in vertical**

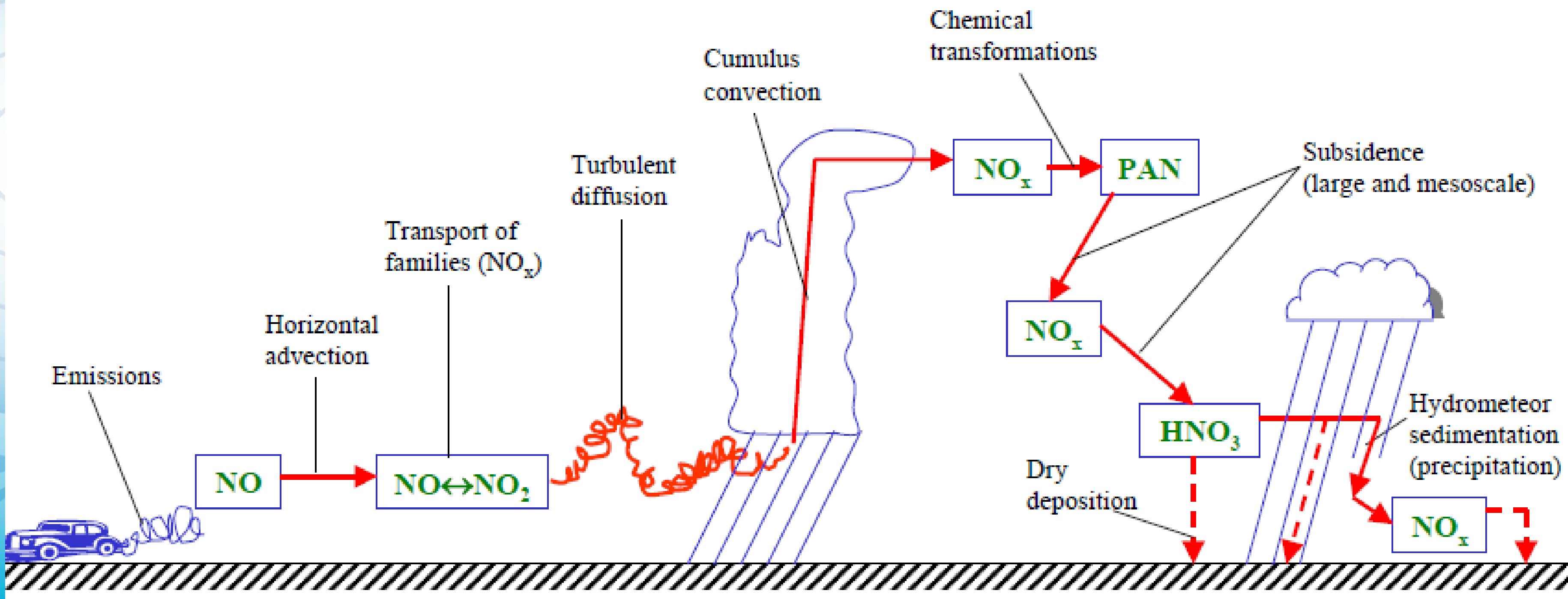
- **Chemical Transport Models (CTMs) use external meteorological data as input (or run on-line)**
- **General Circulation Models (GCMs) compute their own meteorological fields**

From D. Jacob

AREP
GAW

Factors Controlling Tracer Distributions

Example: Reactive Nitrogen

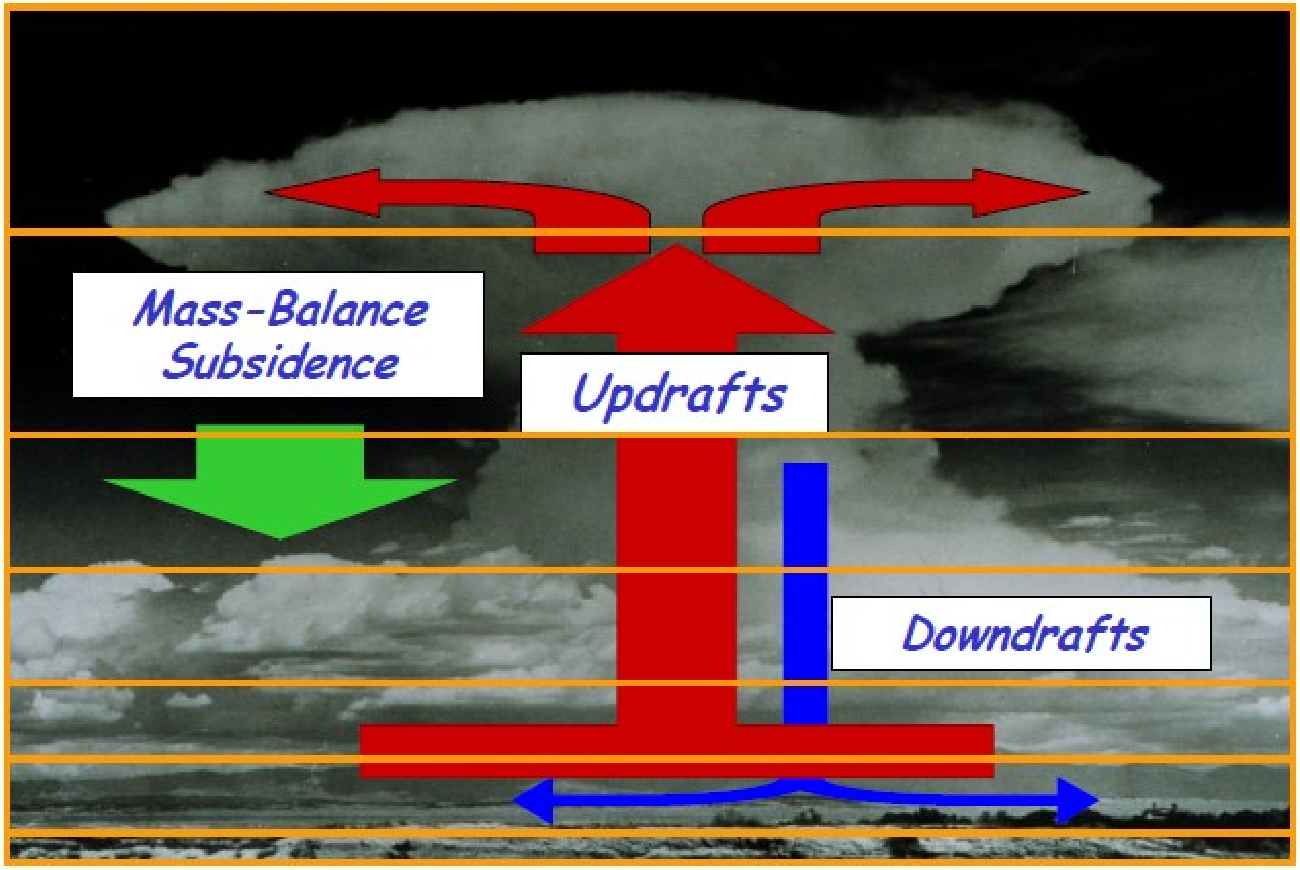


WMO
OMM

AREP
GAW

Cumulus Convection

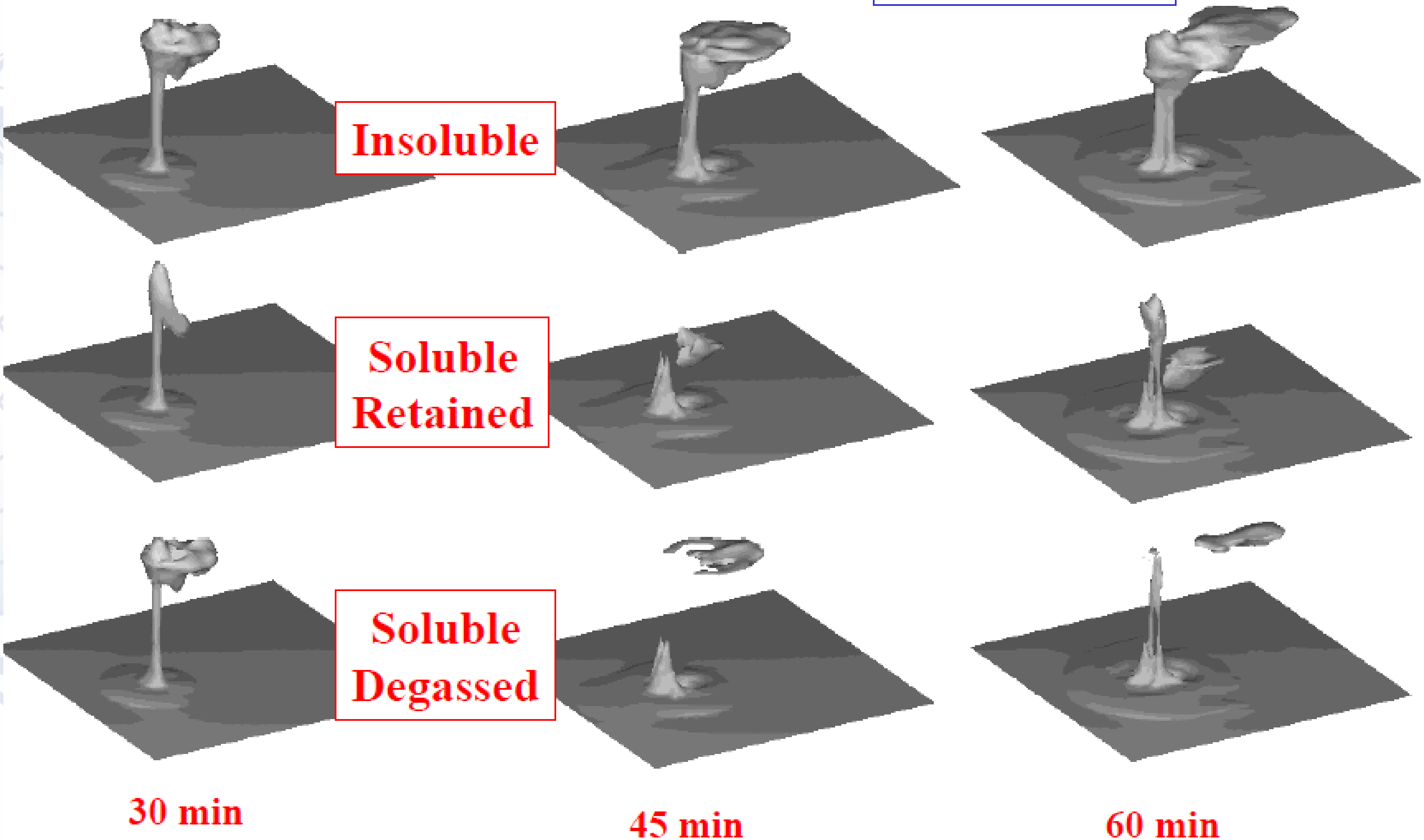
- *Issue:* How are θ, Q, and tracers affected by the full ensemble of different (deep) cumulus clouds within a model column?



WMO
OMM

Effects of Solubility and Retention in Ice

(Preliminary!)



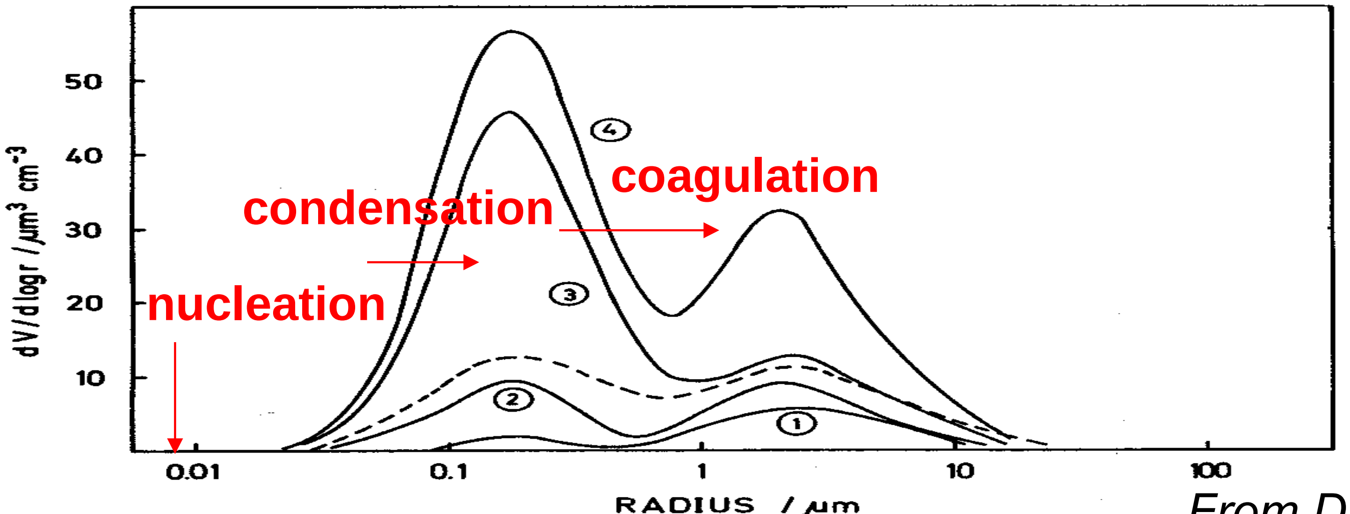
SPECIFIC ISSUES FOR AEROSOL CONCENTRATIONS

- A given aerosol particle is characterized by its size, shape, phases, and chemical composition – large number of variables!

- Measures of aerosol concentrations must be given in some integral form, by summing over all particles present in a given air volume that have a certain property

- If evolution of the size distribution is not resolved, continuity equation for aerosol species can be applied in same way as for gases

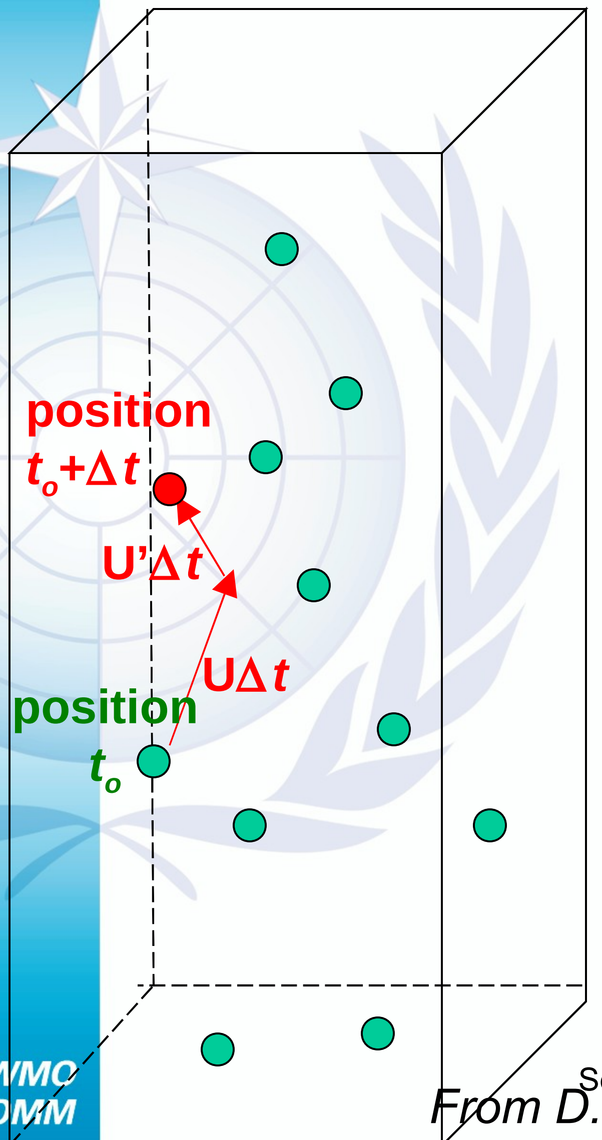
- Simulating the evolution of the aerosol size distribution requires inclusion of nucleation/growth/coagulation terms in P_i and L_i, and size characterization either through size bins or moments.



Typical aerosol size distributions by volume

From D. Jacob

LAGRANGIAN APPROACH: TRACK TRANSPORT OF POINTS IN MODEL DOMAIN (NO GRID)



From D. Jacob

- Transport large number of points with trajectories from input meteorological data base (U) + random turbulent component (U') over time steps Δt
- Points have mass but no volume
- Determine local concentrations as the number of points within a given volume
- Nonlinear chemistry requires Eulerian mapping at every time step (semi-Lagrangian)

PROS over Eulerian models:

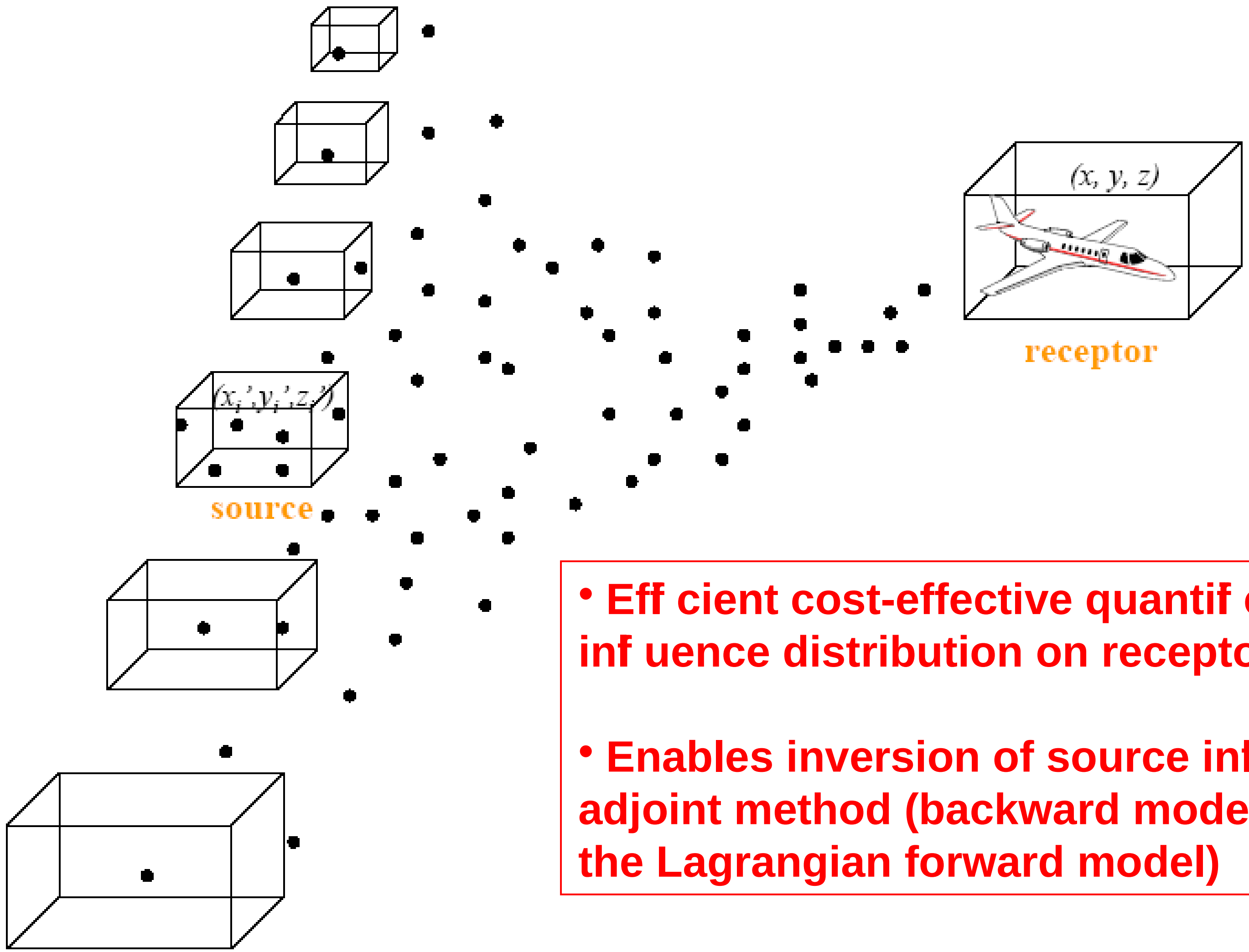
- no Courant number restrictions
- no numerical diffusion/dispersion
- easily track air parcel histories
- invertible with respect to time

CONS:

- need very large # points for statistics
- inhomogeneous representation of domain
- convection is poorly represented
- nonlinear chemistry is problematic

LAGRANGIAN RECEPTOR-ORIENTED MODELING

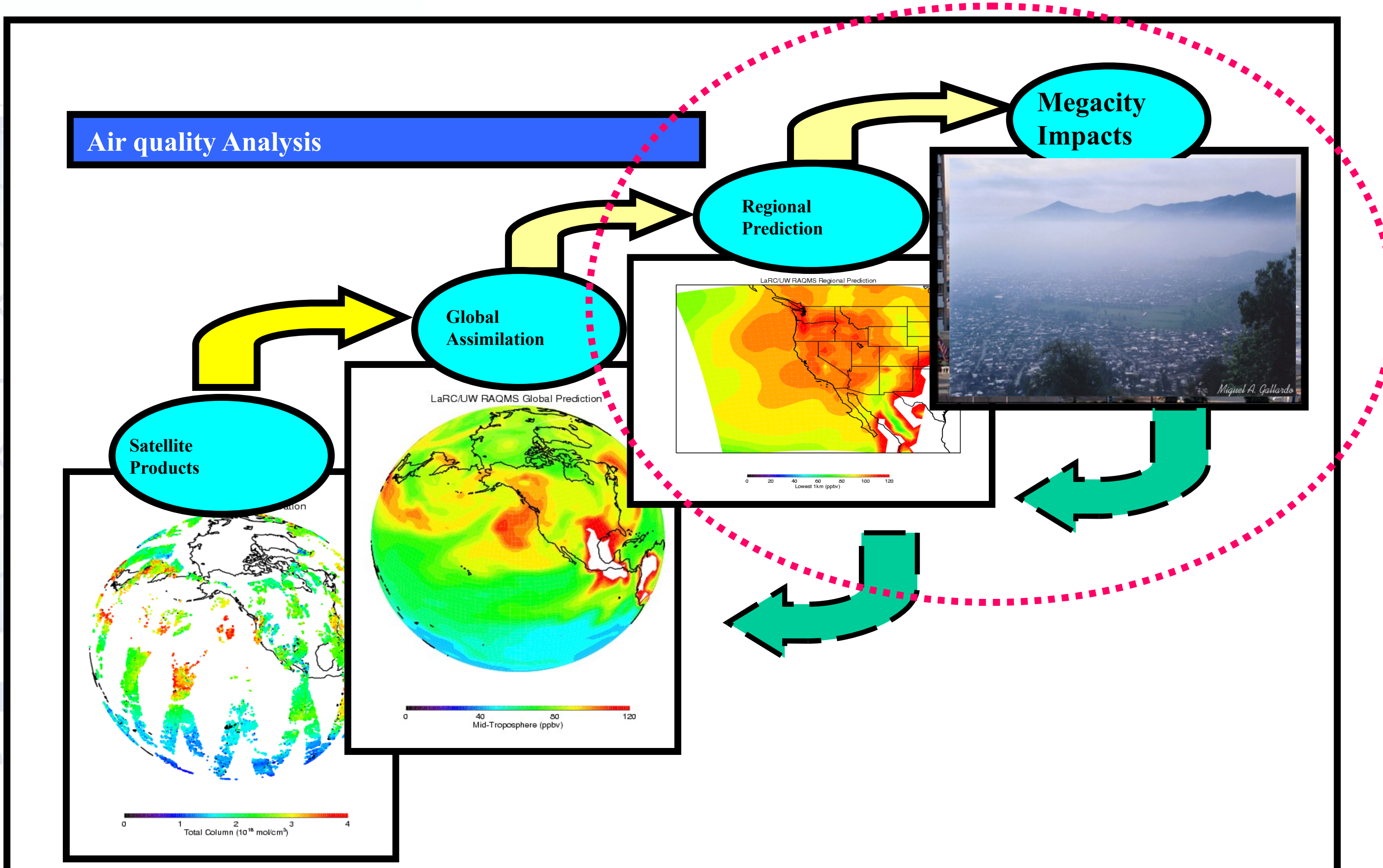
Run Lagrangian model backward from receptor location, with points released at receptor location only



- **Efficient cost-effective quantification of source influence distribution on receptor ("footprint")**
- **Enables inversion of source influences by the adjoint method (backward model is the adjoint of the Lagrangian forward model)**

From D. Jacob

Air Quality Prediction: A Challenge of Scales and Integration



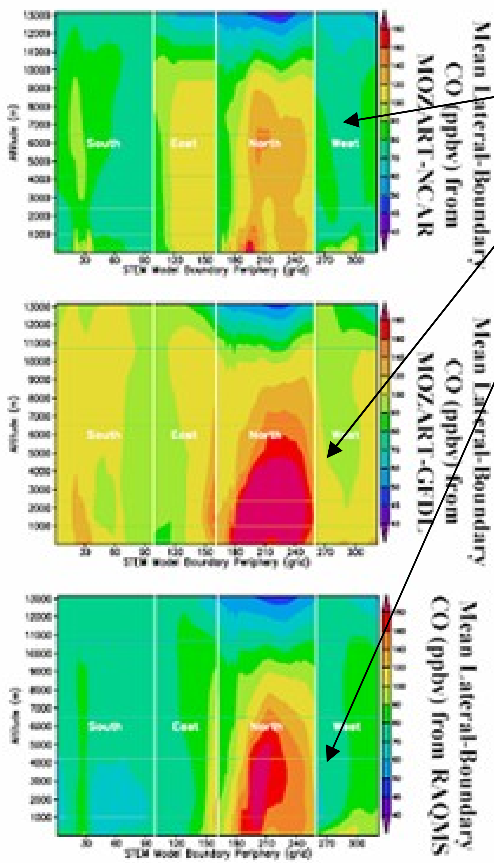
Modified after Pierce NASA/Langley

Integrated Science Studies:

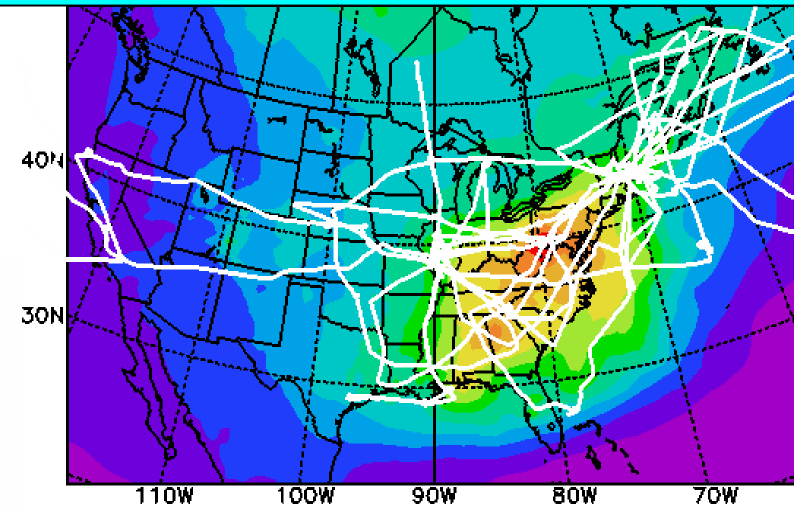
Impacts of Global Composition on Regional Air Quality

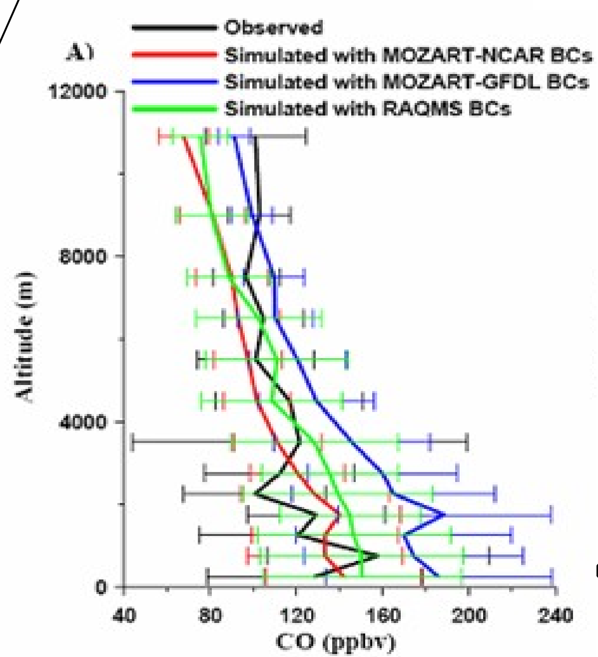
Global-Regional-Urban nesting of CTMs

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



Alaskan BB Impacts Northern Boundary



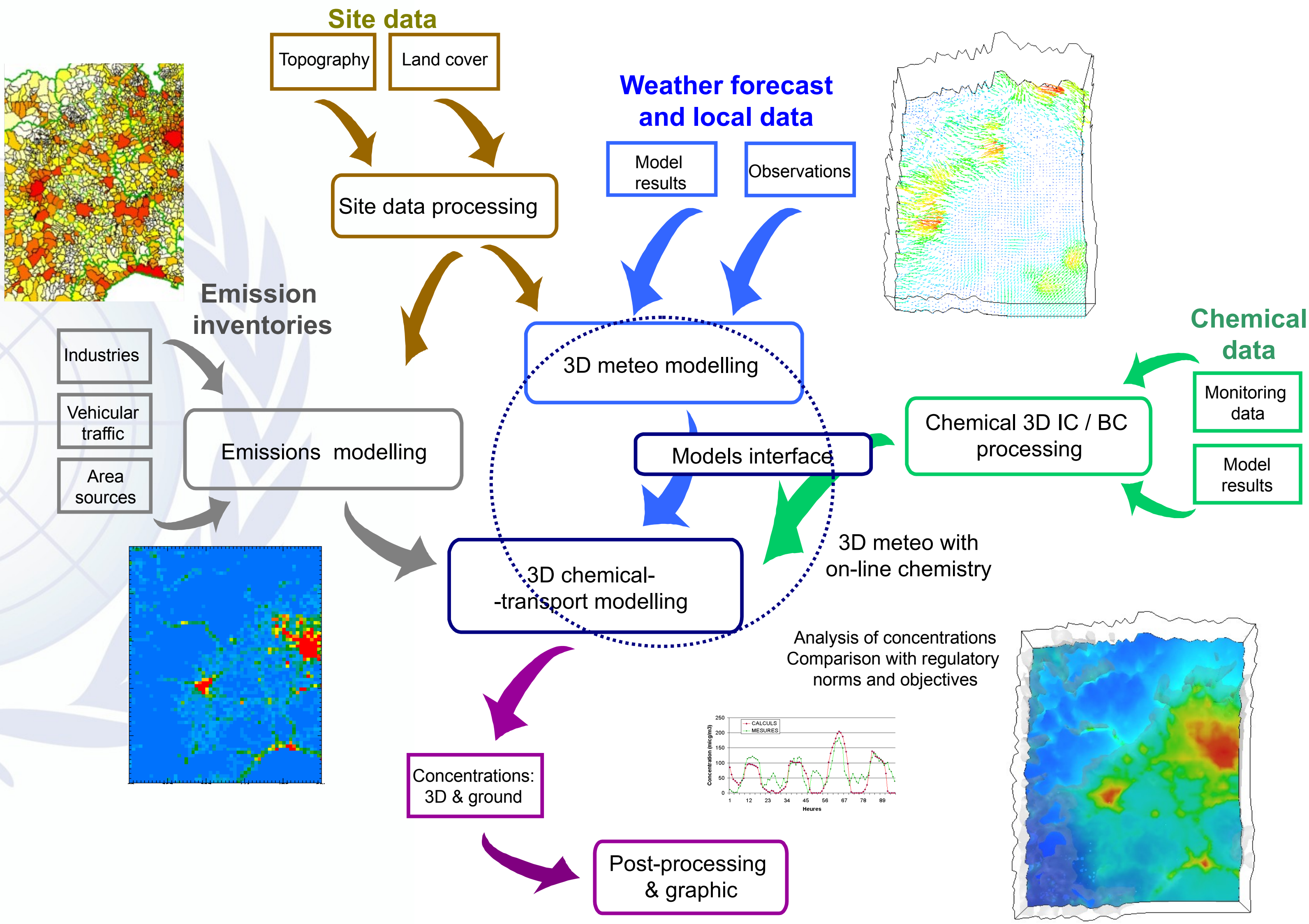


of

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

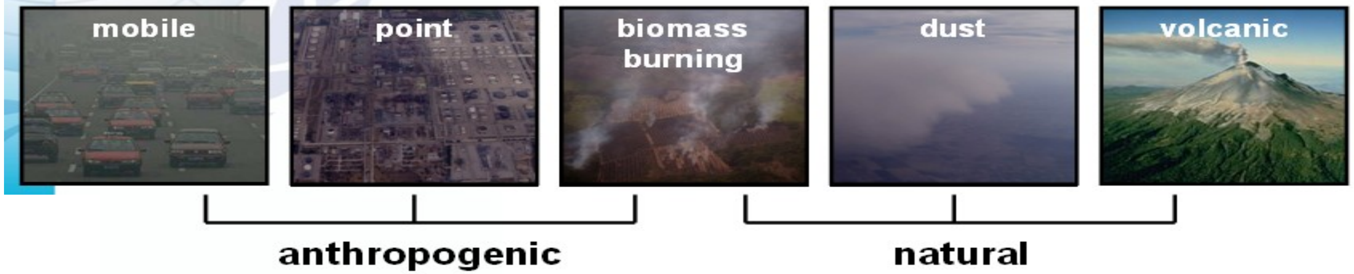
An Air Quality Modelling System

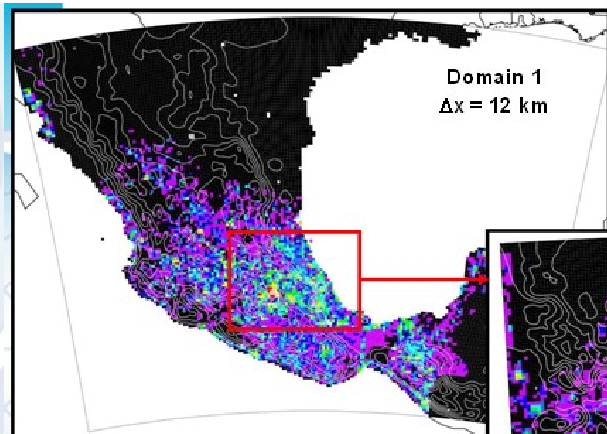


WMO
OMM

AREP GAW

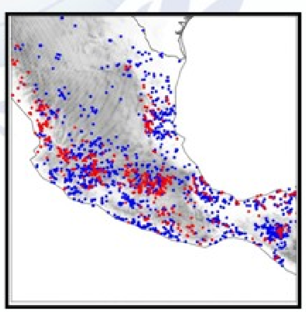
Need to Estimate Emissions at Appropriate Scales

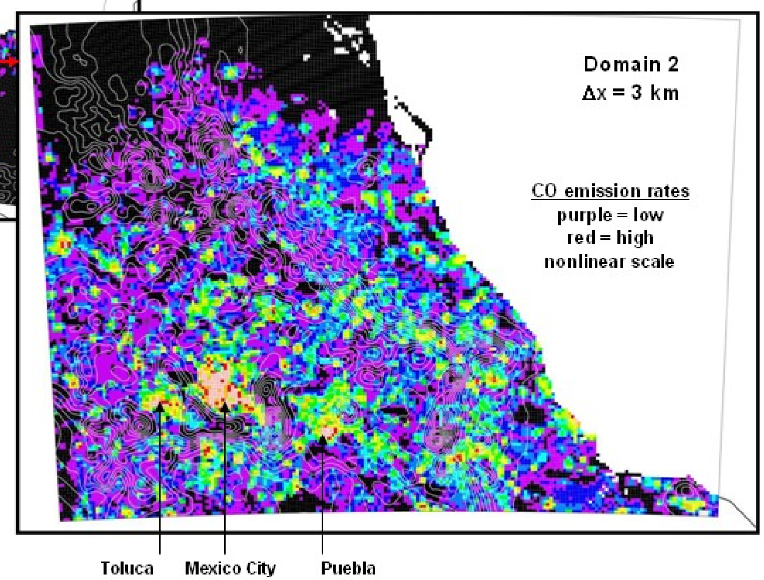




Anthropogenic: NEI99
Biomass Burning: MODIS hotspot
Dust: f(u*)
Volcanic: SO_2 estimated
Biogenic: none at present

Fires detected by MODIS

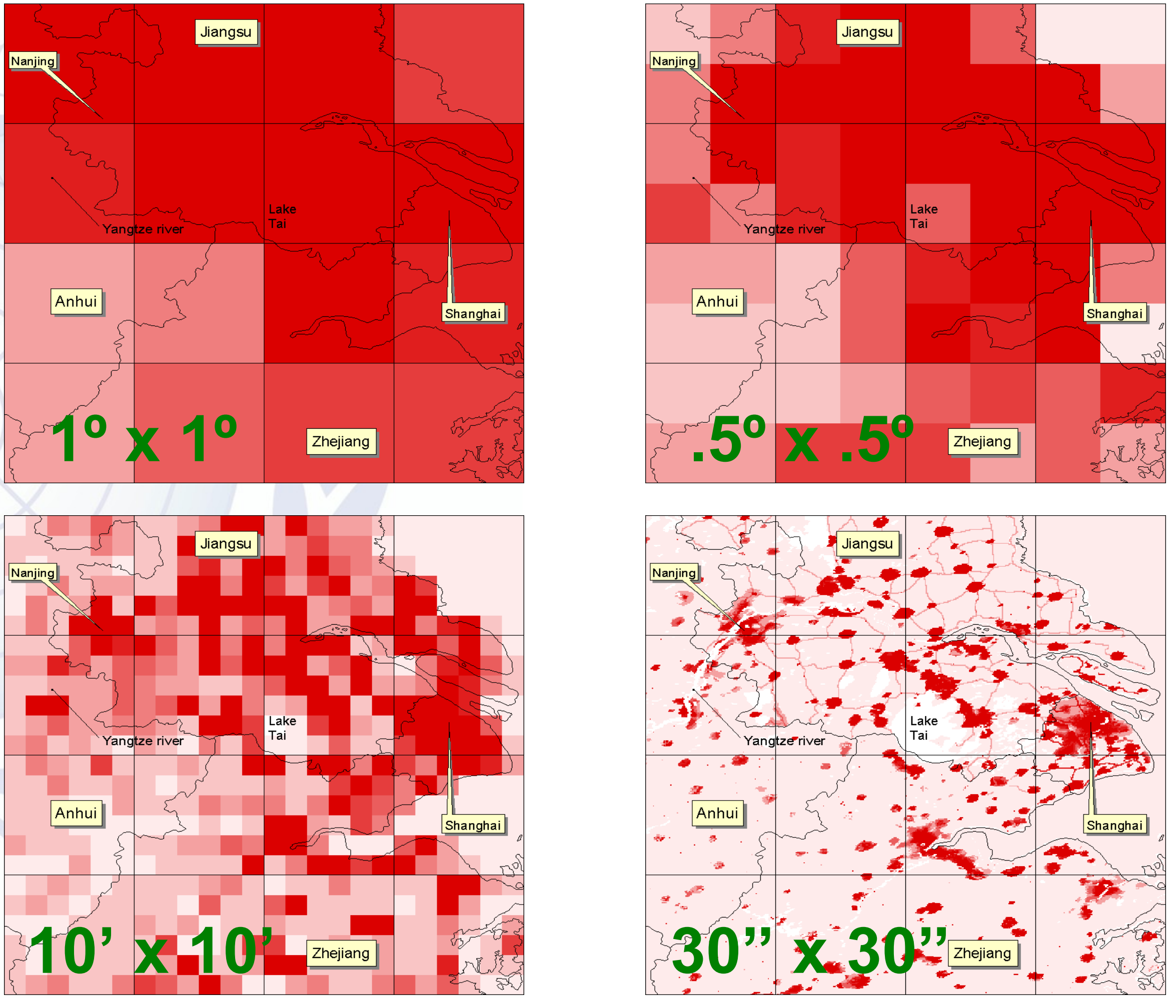




WMO OMM

AREP GAW

Detail: a matter of scale (3)



SO_2 emissions in the vicinity of Shanghai, China

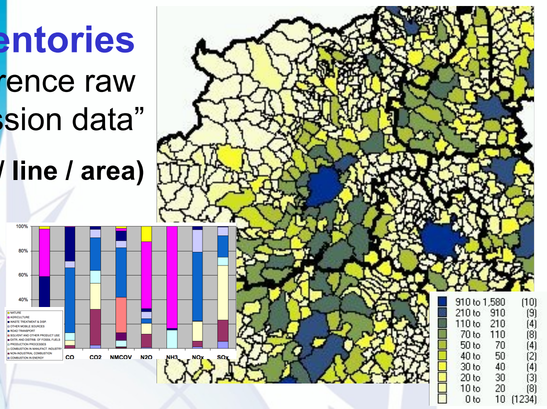
Section 3 – Introduction and Overview of Course

WMO OMM

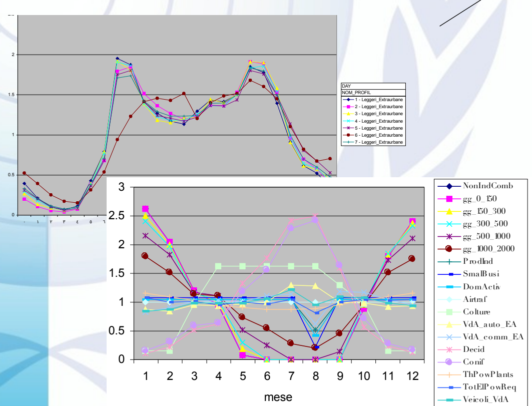
AREP
GAW

Emissions processing for AQM

Inventories
"reference raw emission data"
(point / line / area)



Modulation profiles
(hourly, daily, monthly)

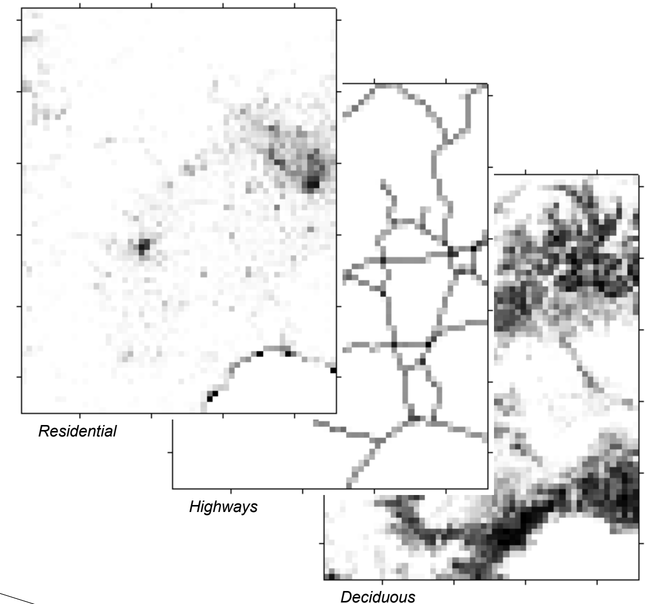


SPACE DISAGGREGATION

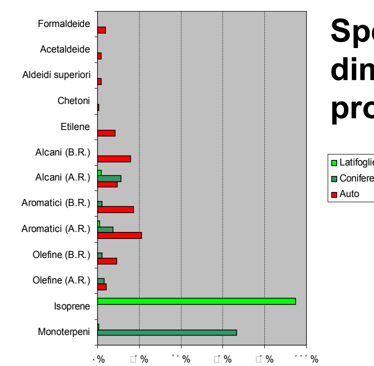
TIME MODULATION

NMVOC & PM SPECIATION & SIZE

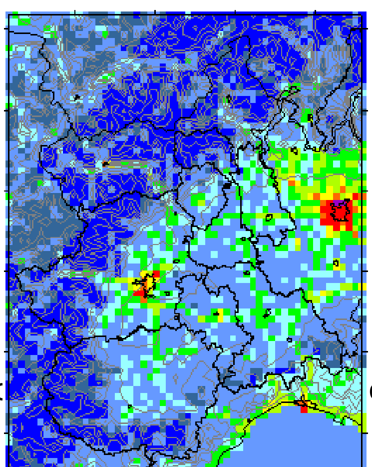
Thematic data



Speciation & dimensional profiles



Model-ready input
(hourly, gridded, speciated emissions)



WMO
OMM

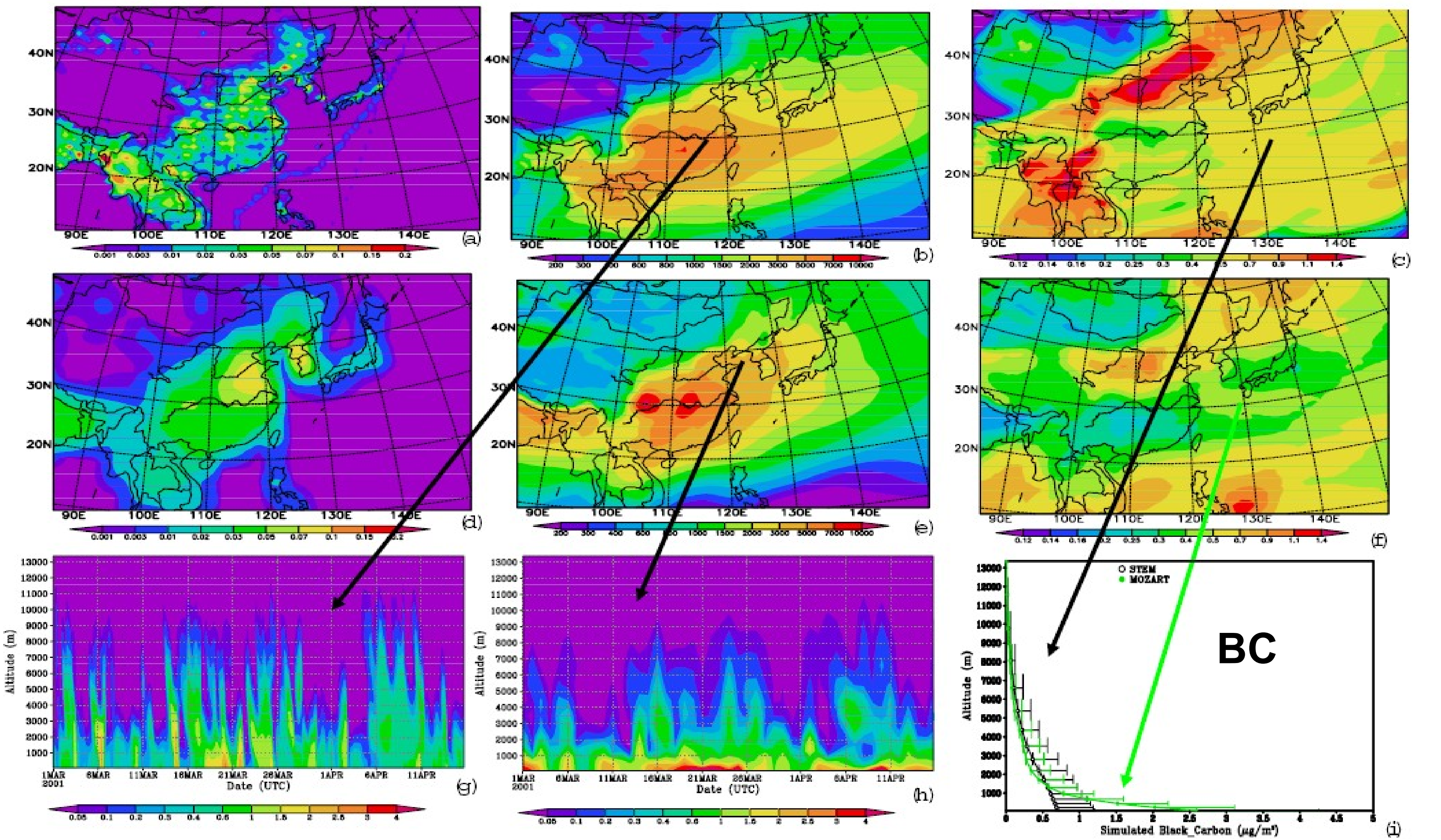
How do we build upon what is done and move beyond to improve air quality prediction?

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

AREP
GAW

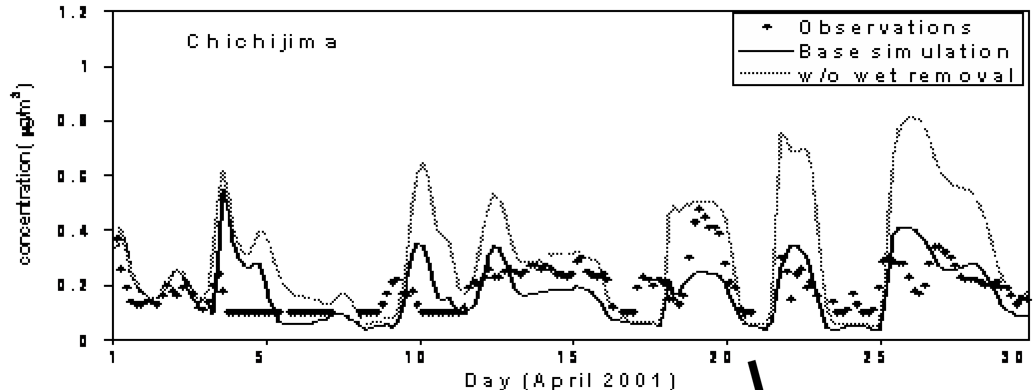
Model Resolution, Transport and Removal also Contribute to Differences

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



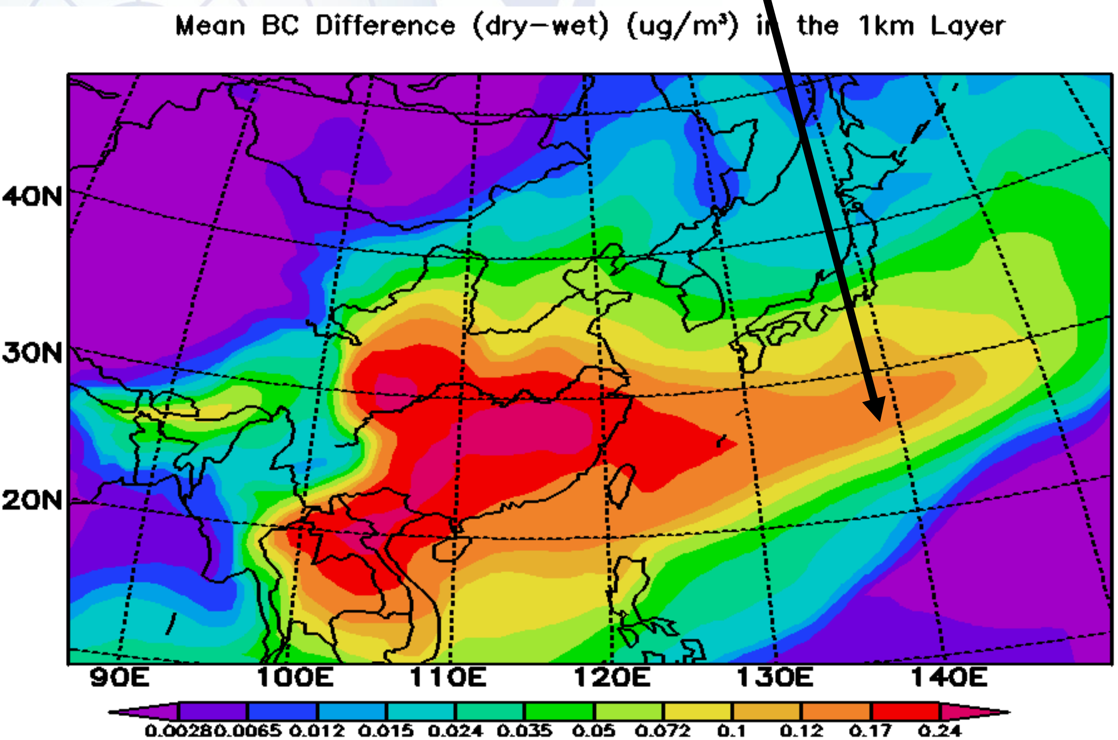
AREP
GAW

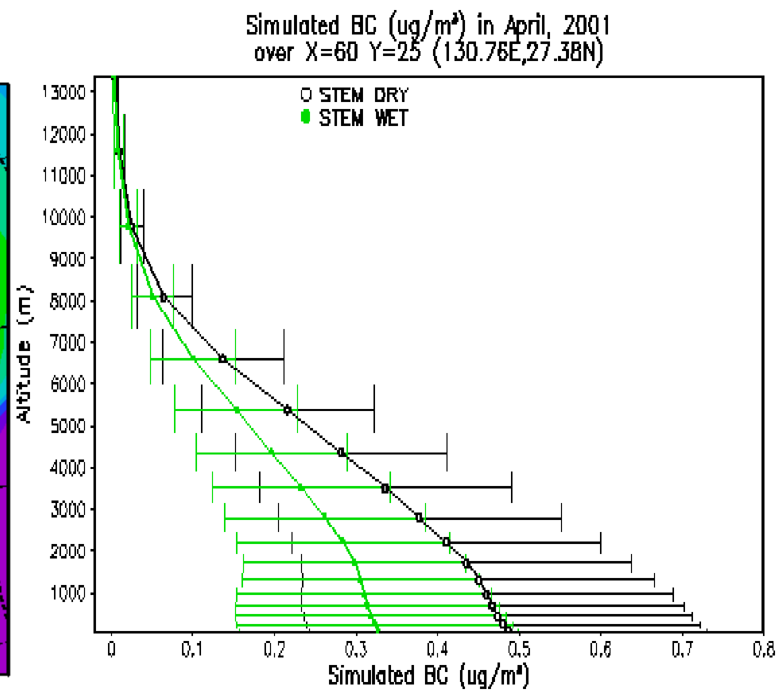
Removal Processes Remain Poorly Characterized in Models



Impact of Wet Removal on Predicted BC

Progress limited by lack of understanding and observations

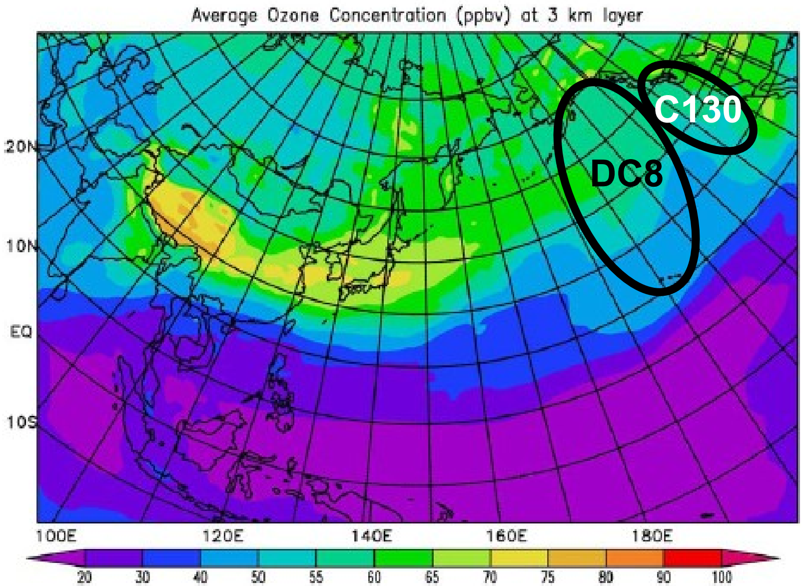


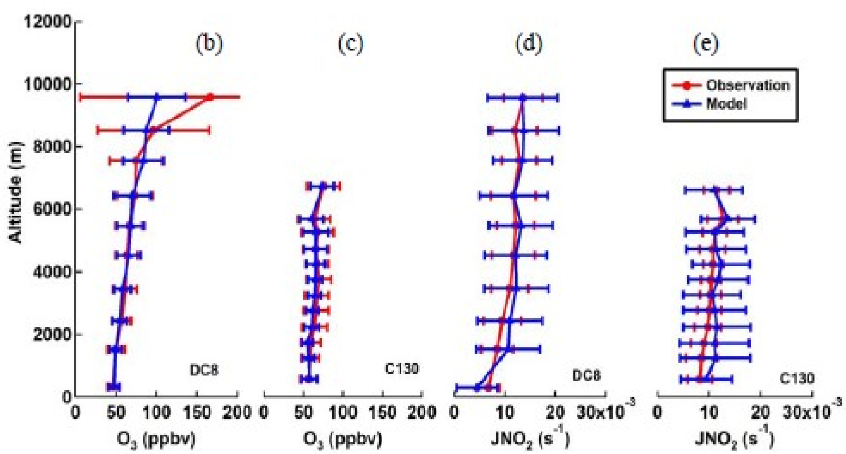


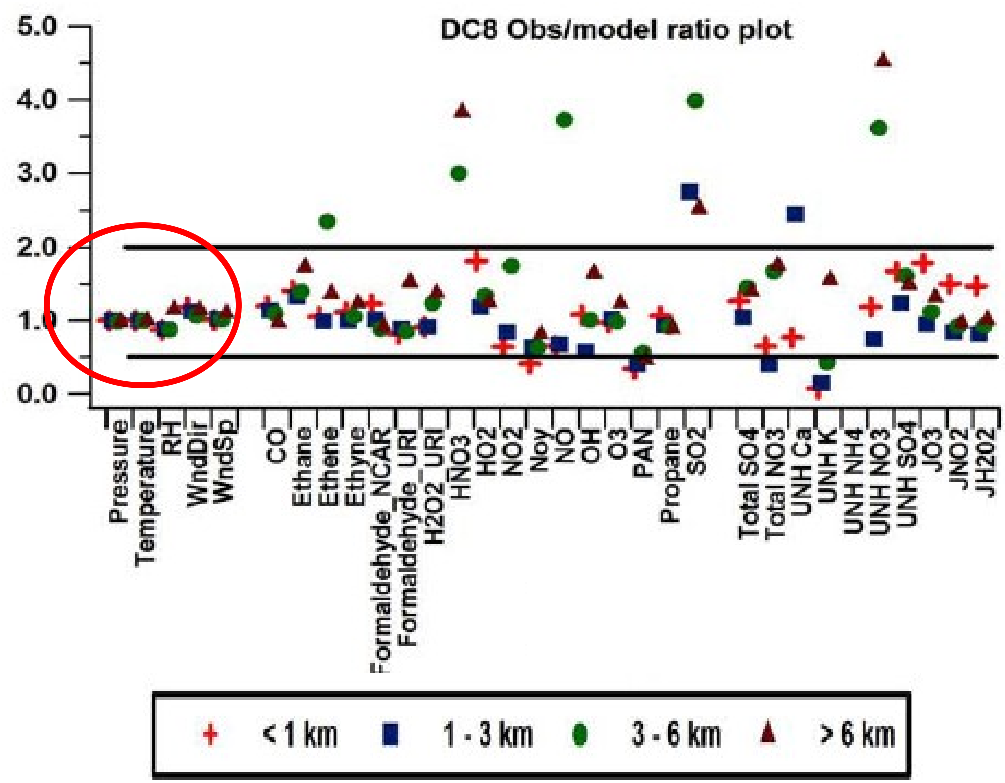
Intensive field experiments provide opportunities for comprehensive evaluations

Current CTMs Do Have Appreciable Skills In Predicting A Wide Variety Of Parameters

INTEX B – STEM Forecasts







WMO OMM

DC8 **C130**

AREP
GAW

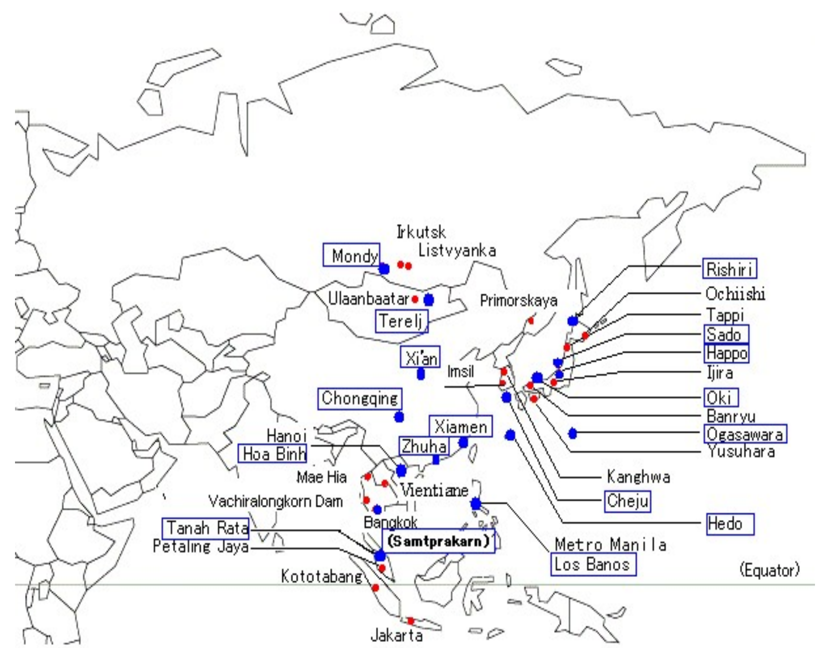
MICS-Asia < *M*odel *I*nter*C*omparison *S*tudy in *Asia* >

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

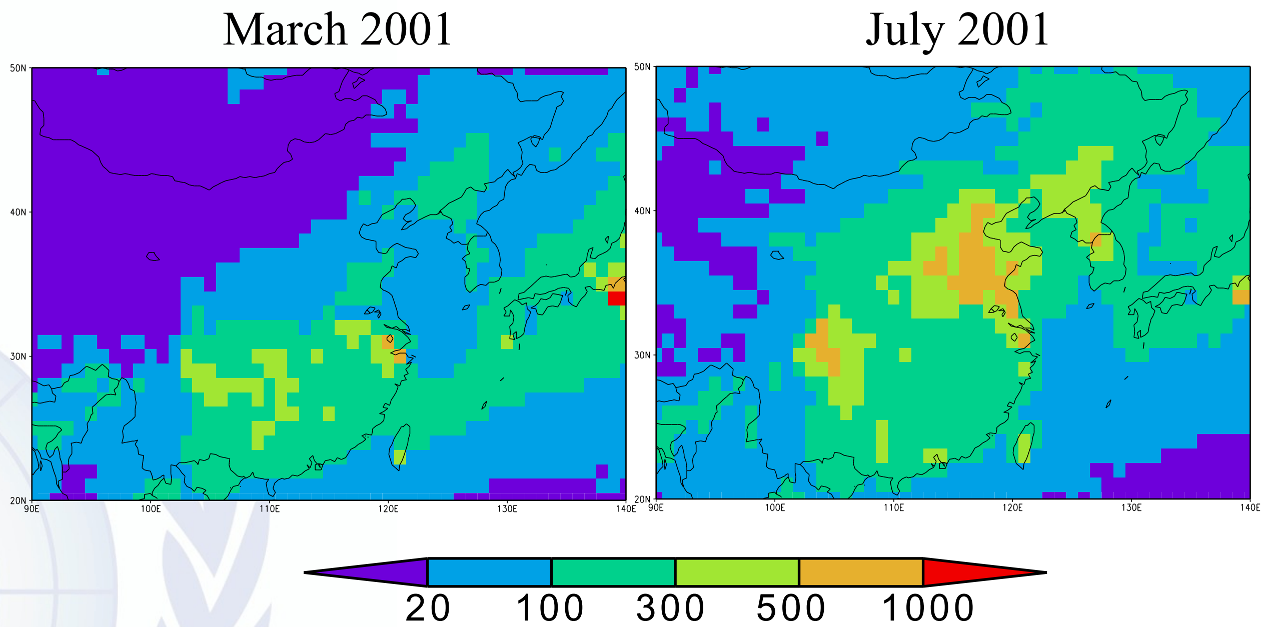
Observations:

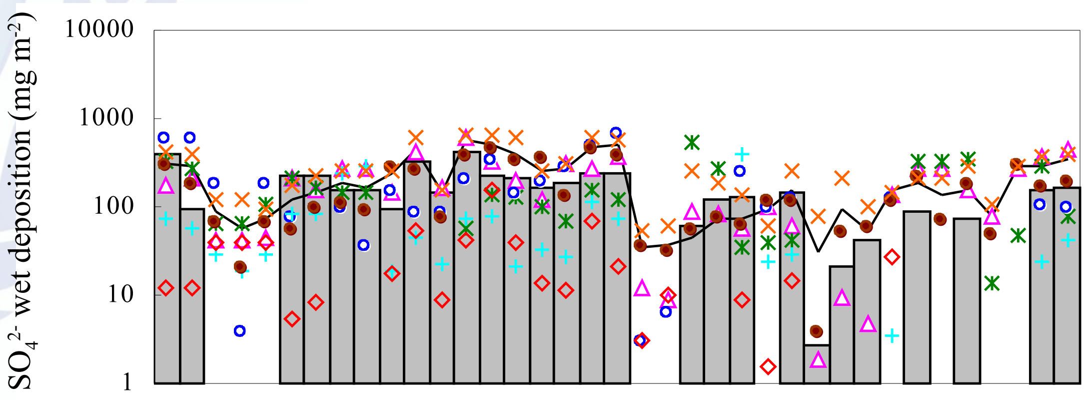
- EANET (47 sites) (gas, aerosol, deposition)
- Ozonesondes
- Trace-P Obs.
- Special obs. (aerosols)
- Met obs (sondes and surface)
- (daily & monthly analysis)
- Special Section of *Atmospheric Environment (8 papers)*



MICS-III Will look also at megacities

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



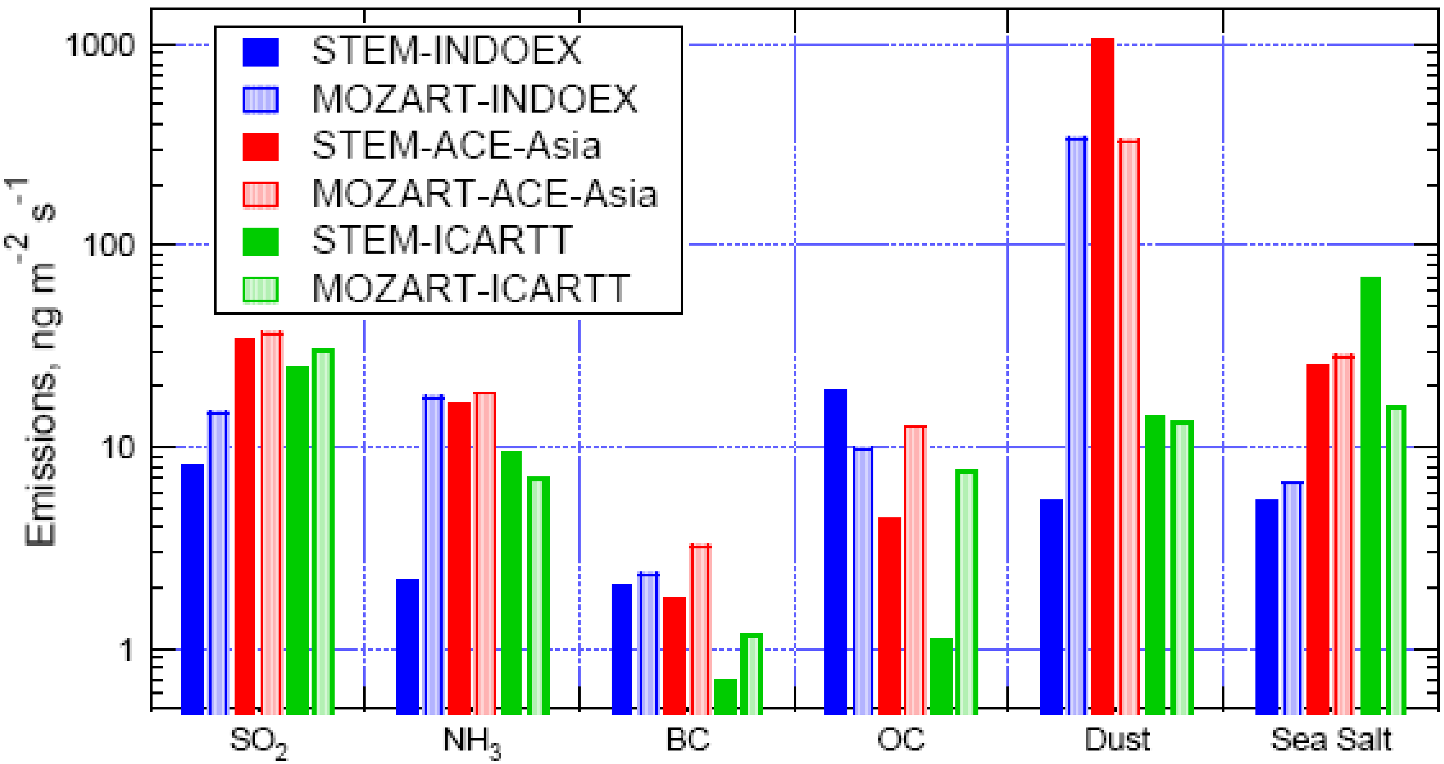


Nitrate quantities typically underestimated.

(mg m^{-2})

AREP
GAW

Emissions are the Largest Single Source of Uncertainty

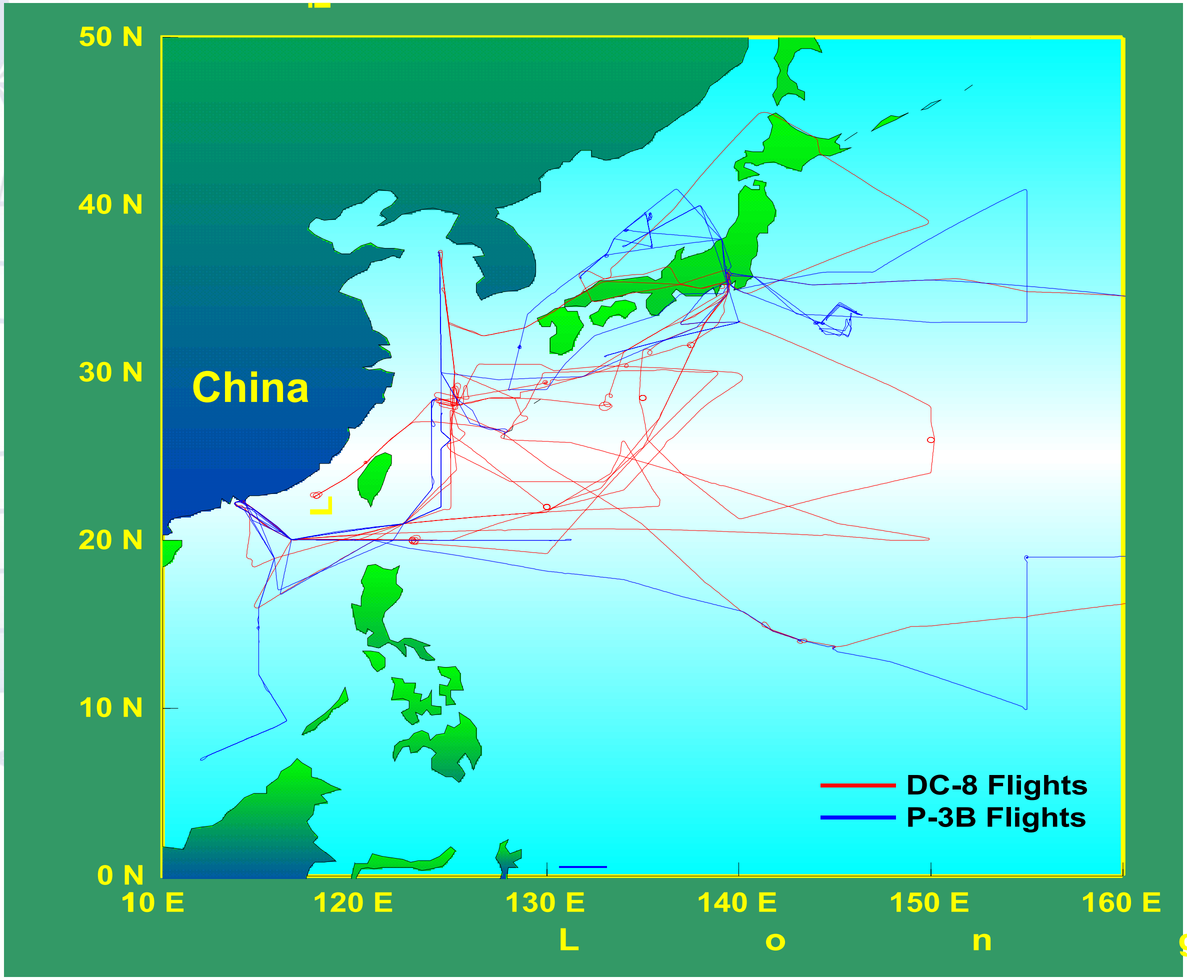


Uncertainties: SO2 <BC & OC < Dust & Sea Salt

WMO
OMM

AREP GAW

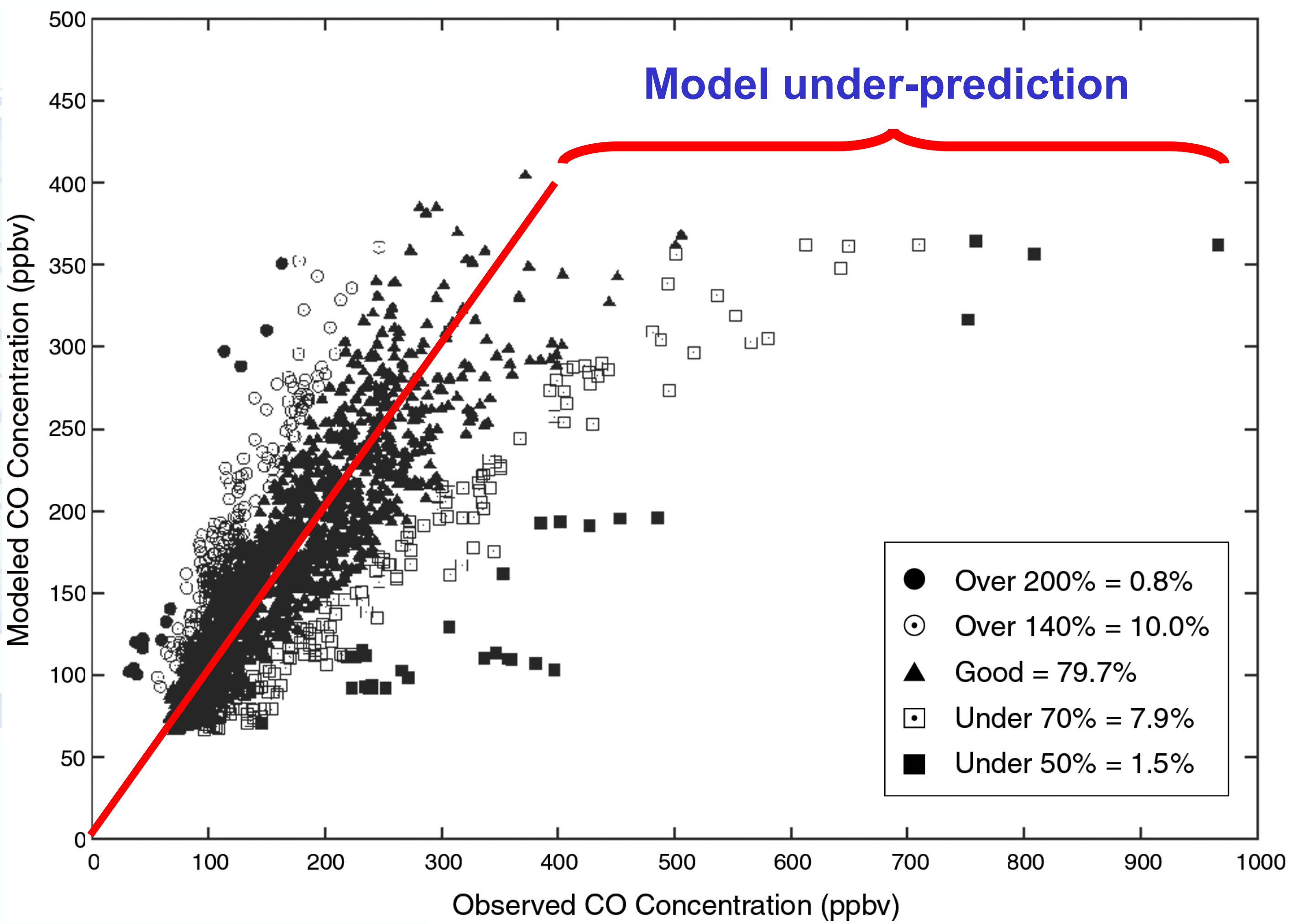
Experiments such as TRACE-P and ACE-Asia employ mobile "Super-Sites" and study pollution outflow from source regions



Spring 2001

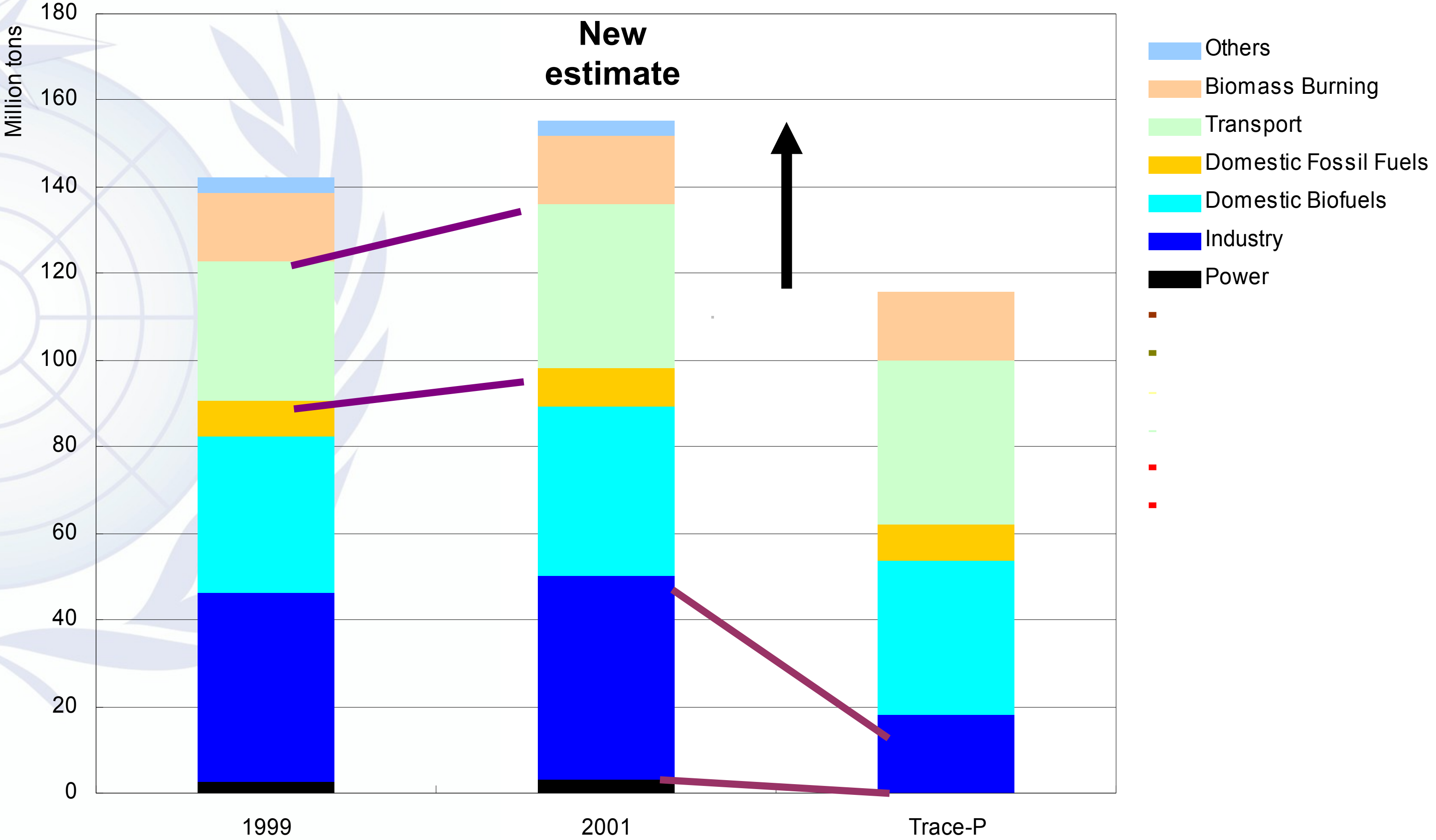
WMO OMM

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

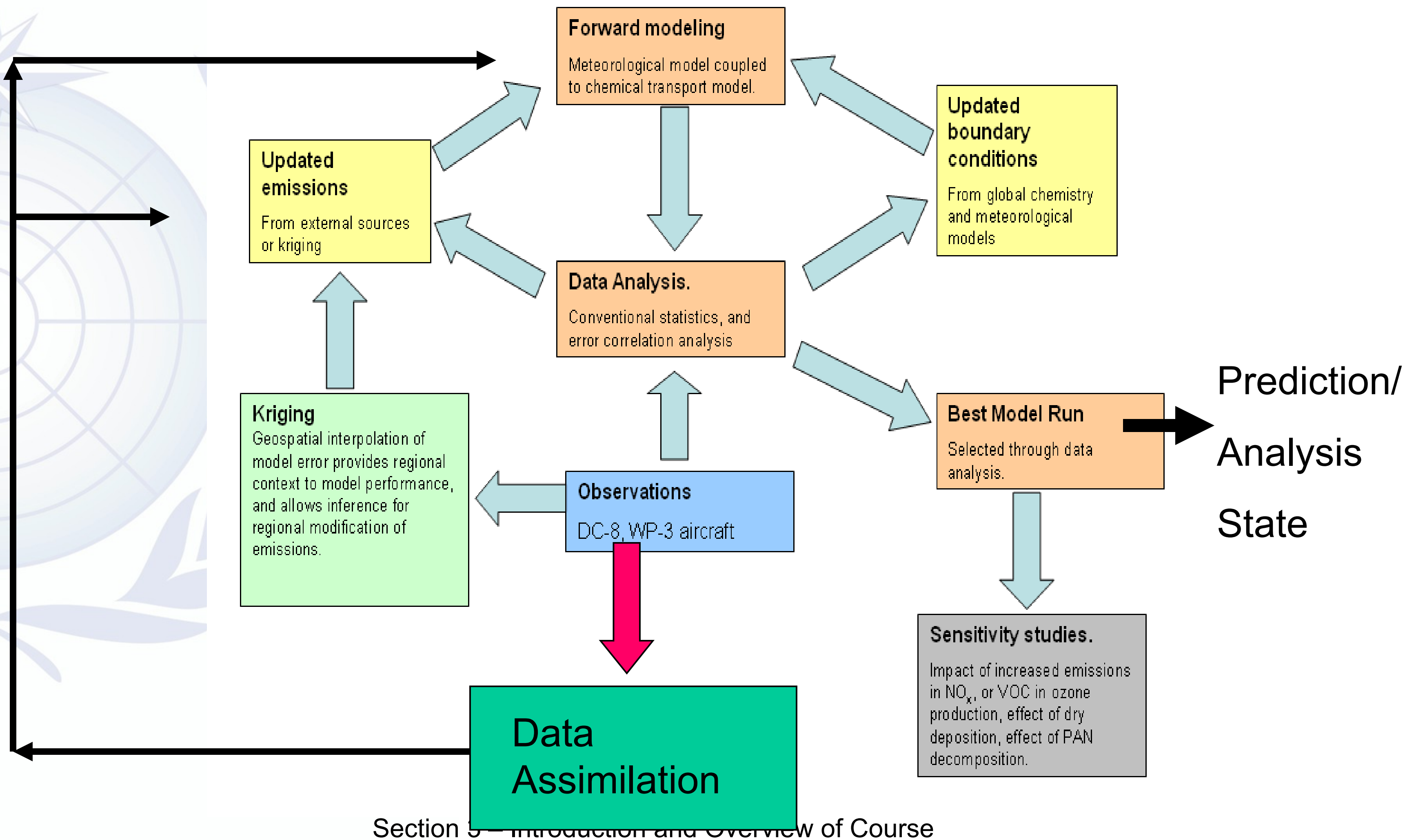


(Carmichael et al., JGR, 2003)

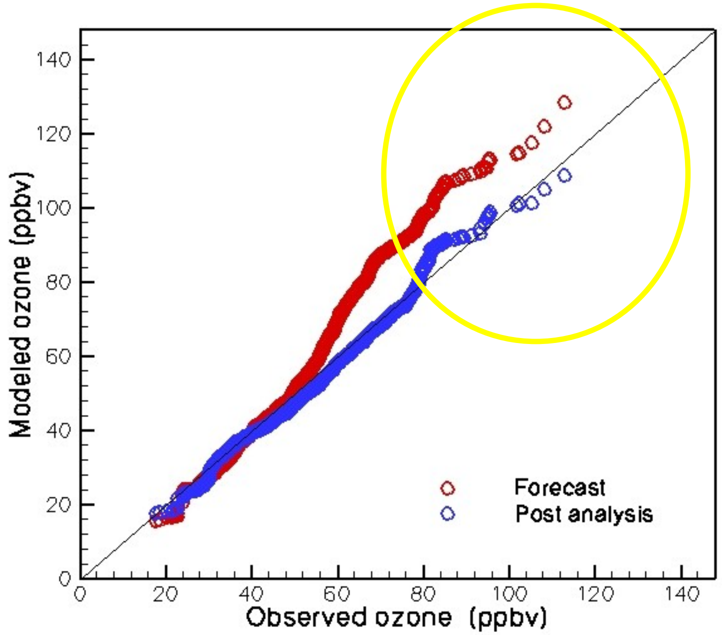
Comparison of New CO Inventory with Trace-P

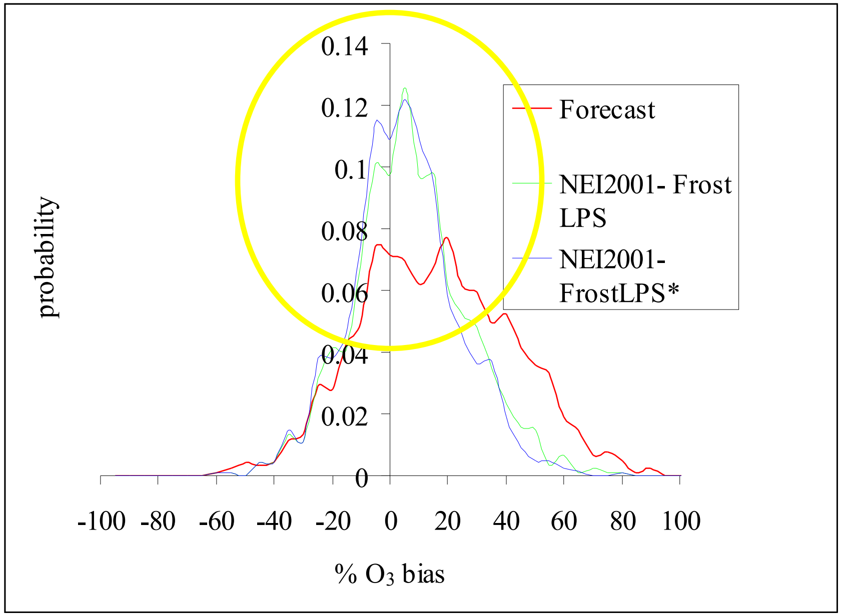


Our Analysis Approach



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

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

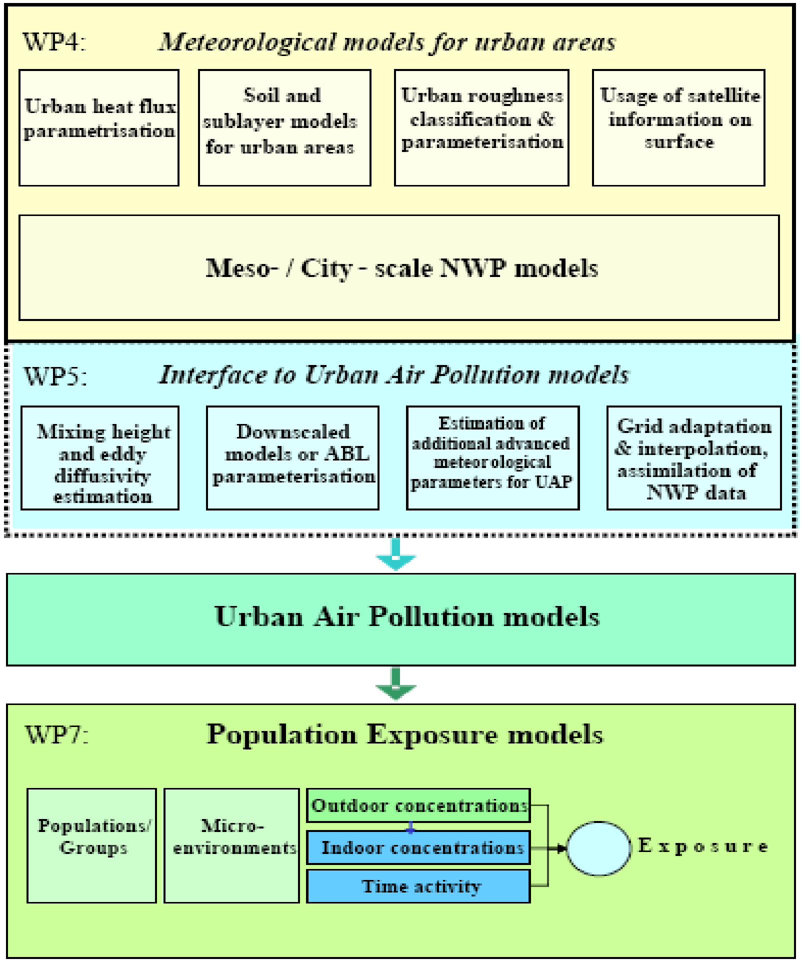


Fig. 1. Outline of the overall FUMAPEX methodology integrating models from urban meteorology to air quality and population exposure. The main improvements in meteorological forecasts (NWP) for urban areas, interfaces and integration with urban air pollution (UAP) and population exposure (PE) models for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

uction a

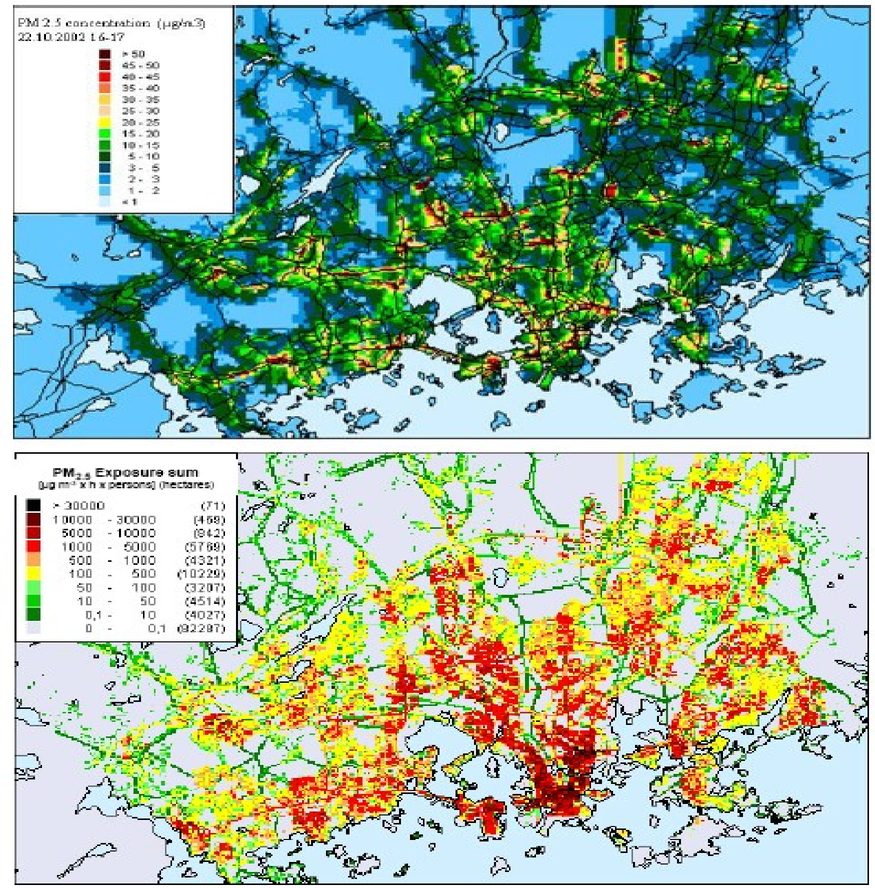
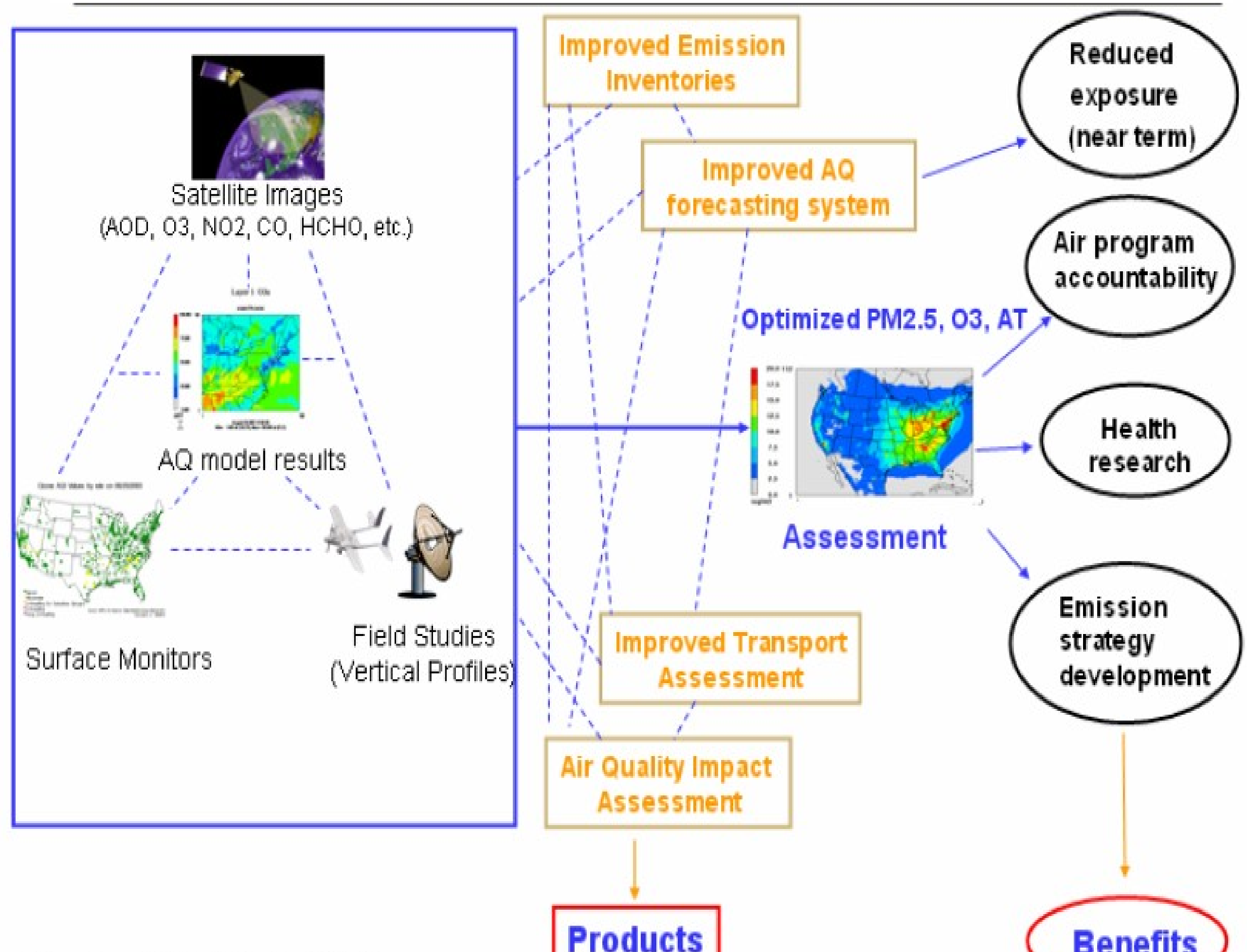


Fig. 2. Predicted spatial distribution of the concentrations of $PM_{2.5}$ in the Helsinki metropolitan area during an afternoon rush hour (from 04:00 to 05:00 p.m.; upper map), and the daily population exposure to $PM_{2.5}$, computed with the EXPAND model (lower map), both of these in the course of 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

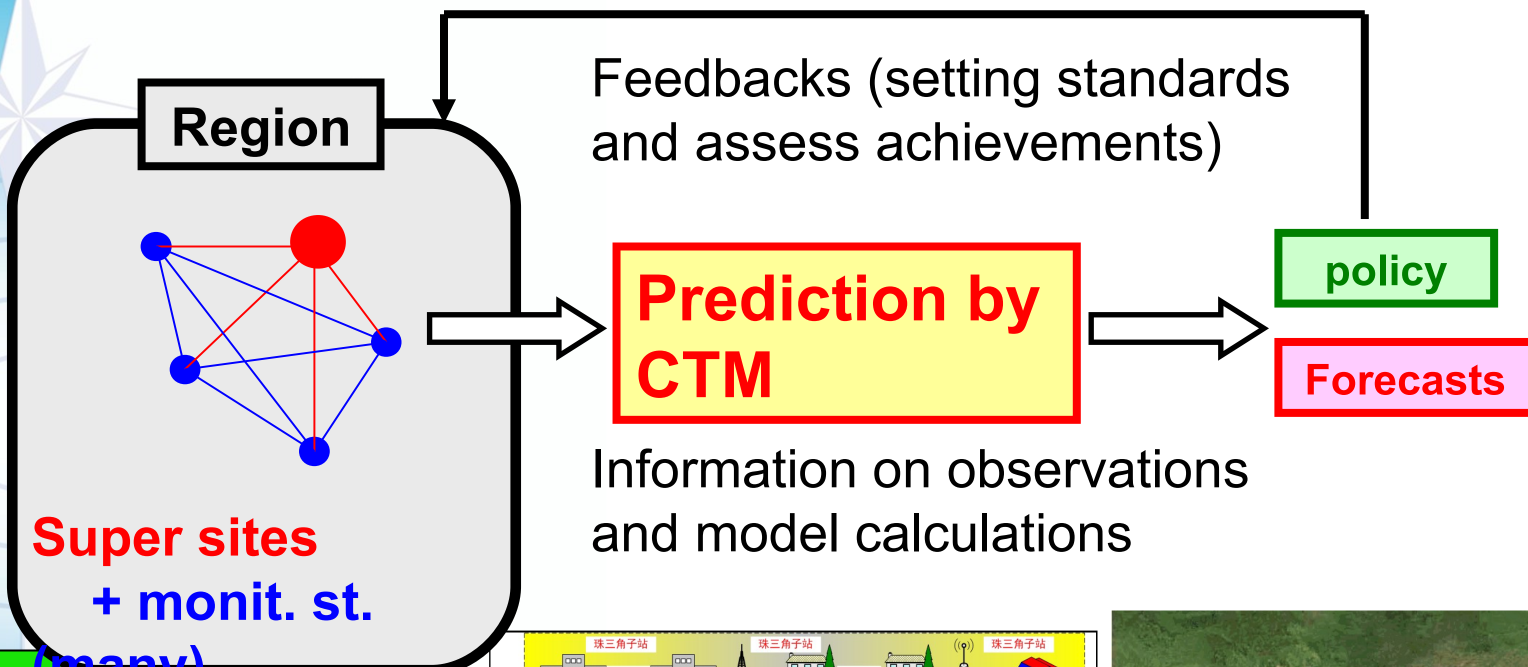
Summary of Course – Introduction to Air Quality Modeling

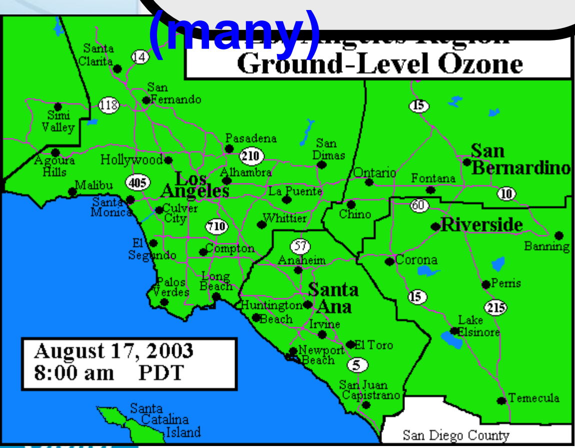


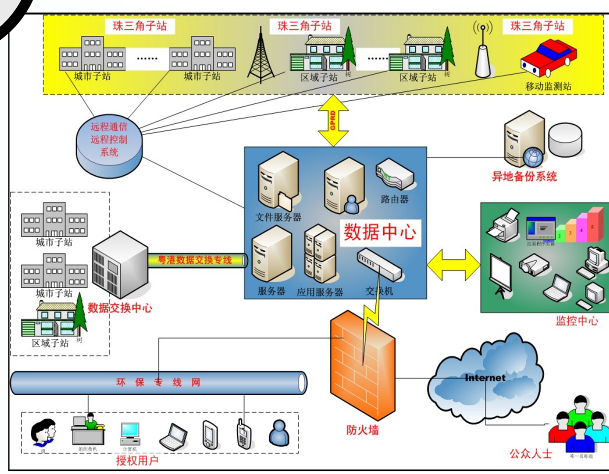
(Courtesy of Rich Scheffe, USEPA)

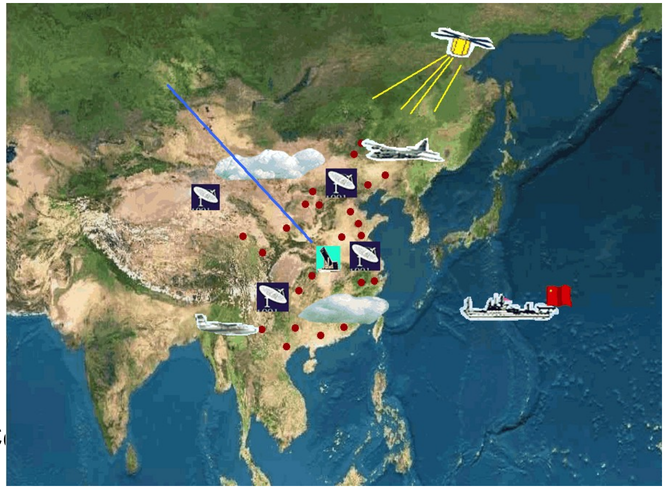
WMO
OMM

Air quality monitoring and ensemble forecasting framework.









Modified from Y. Zhang , Guangzhou Meeting 2007

Many Meteorological Services Already Supply Operational Chemical Weather Products (e.g., FMI)