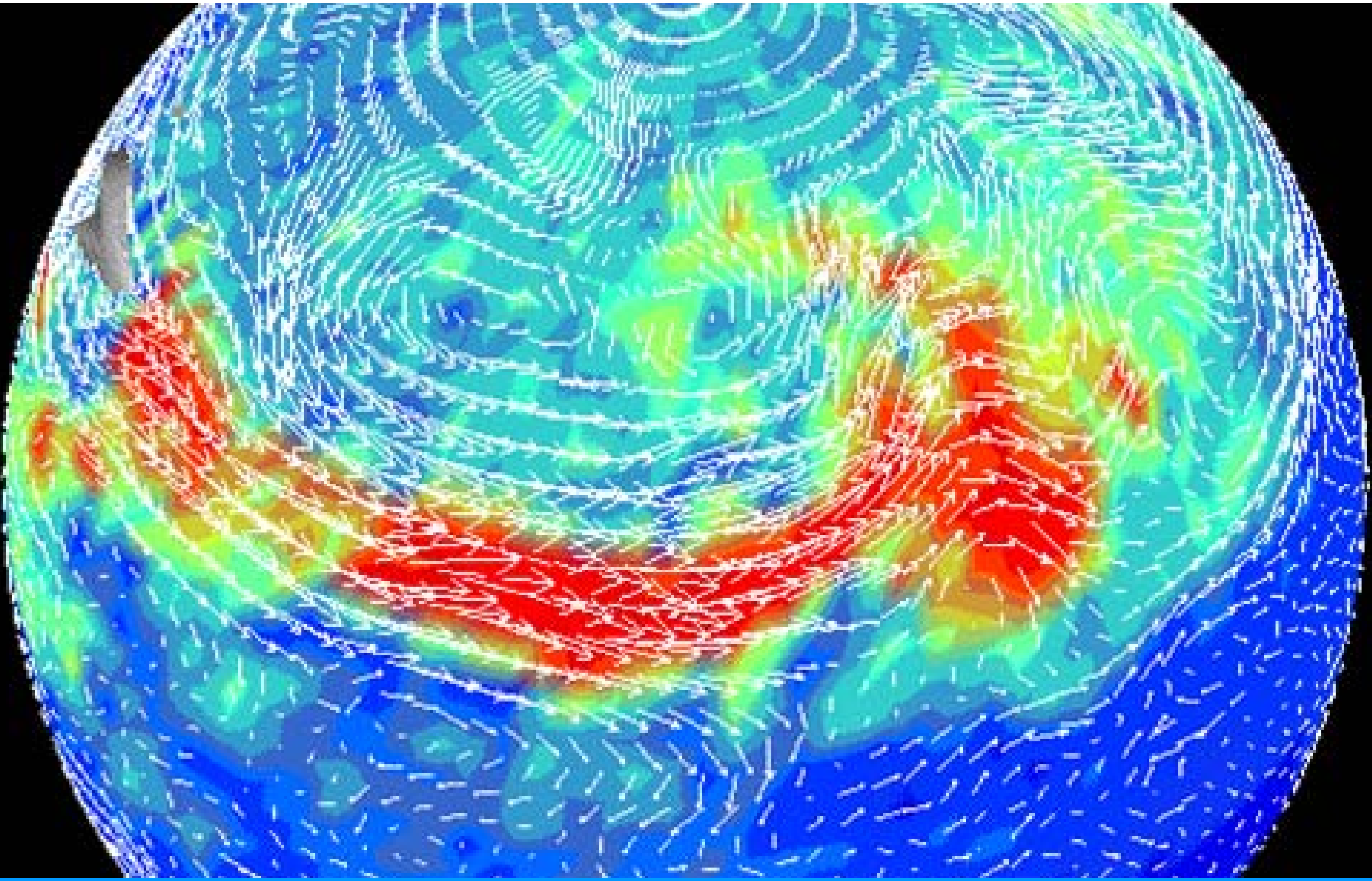
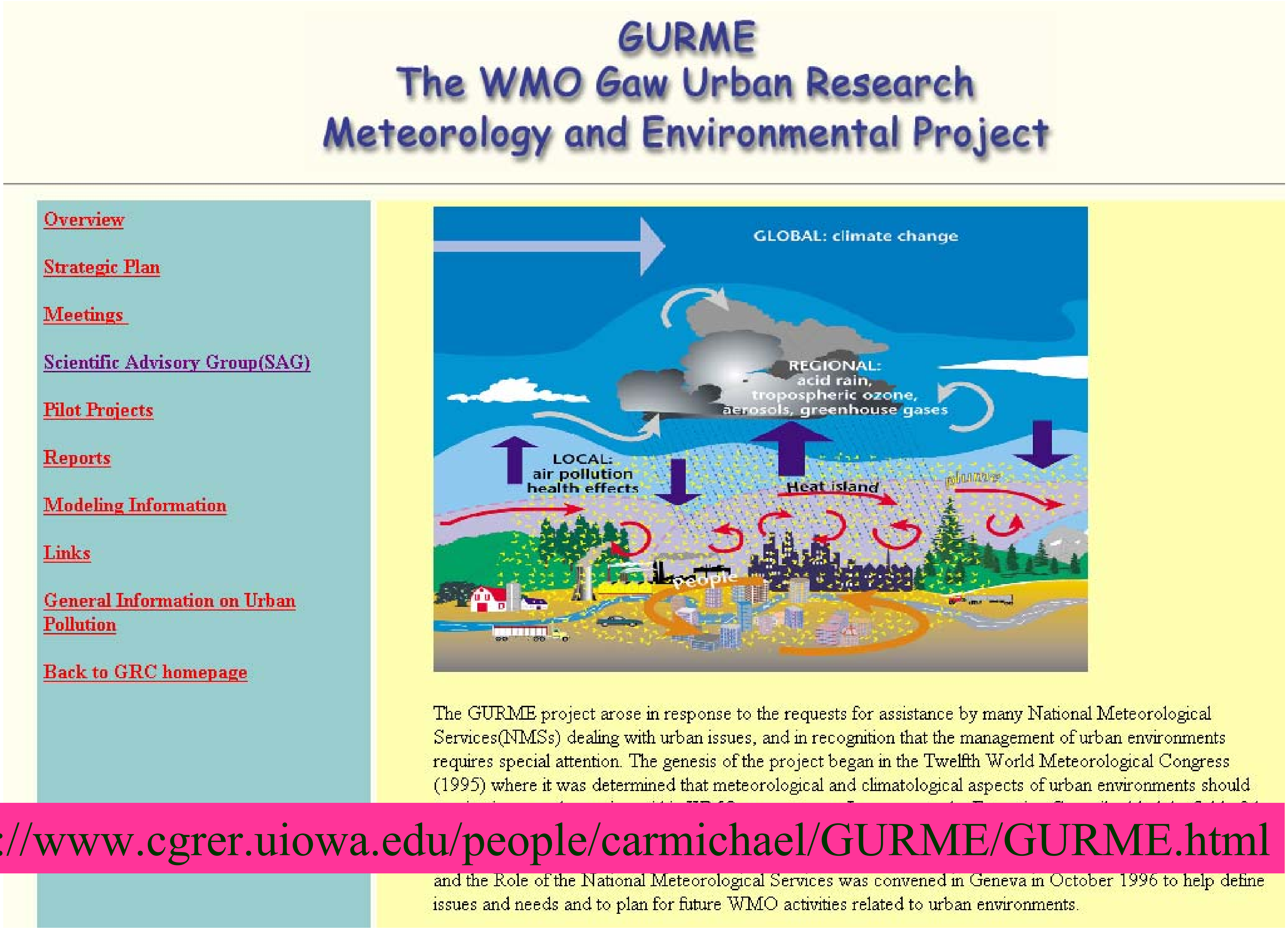
Chemical Weather Forecasting
Perspectives & Challenges



Gregory R. Carmichael
Department of Chemical & Biochemical Engineering
Center for Global & Regional Environmental Research and the
University of Iowa



GURME
The WMO Gaw Urban Research Meteorology and Environmental Project

- Overview
- Strategic Plan
- Meetings
- Scientific Advisory Group(SAG)
- Pilot Projects
- Reports
- Modeling Information
- Links
- General Information on Urban Pollution
- Back to GRC homepage

The GURME project arose in response to the requests for assistance by many National Meteorological Services(NMSs) dealing with urban issues, and in recognition that the management of urban environments requires special attention. The genesis of the project began in the Twelfth World Meteorological Congress (1995) where it was determined that meteorological and climatological aspects of urban environments should

and the Role of the National Meteorological Services was convened in Geneva in October 1996 to help define issues and needs and to plan for future WMO activities related to urban environments.

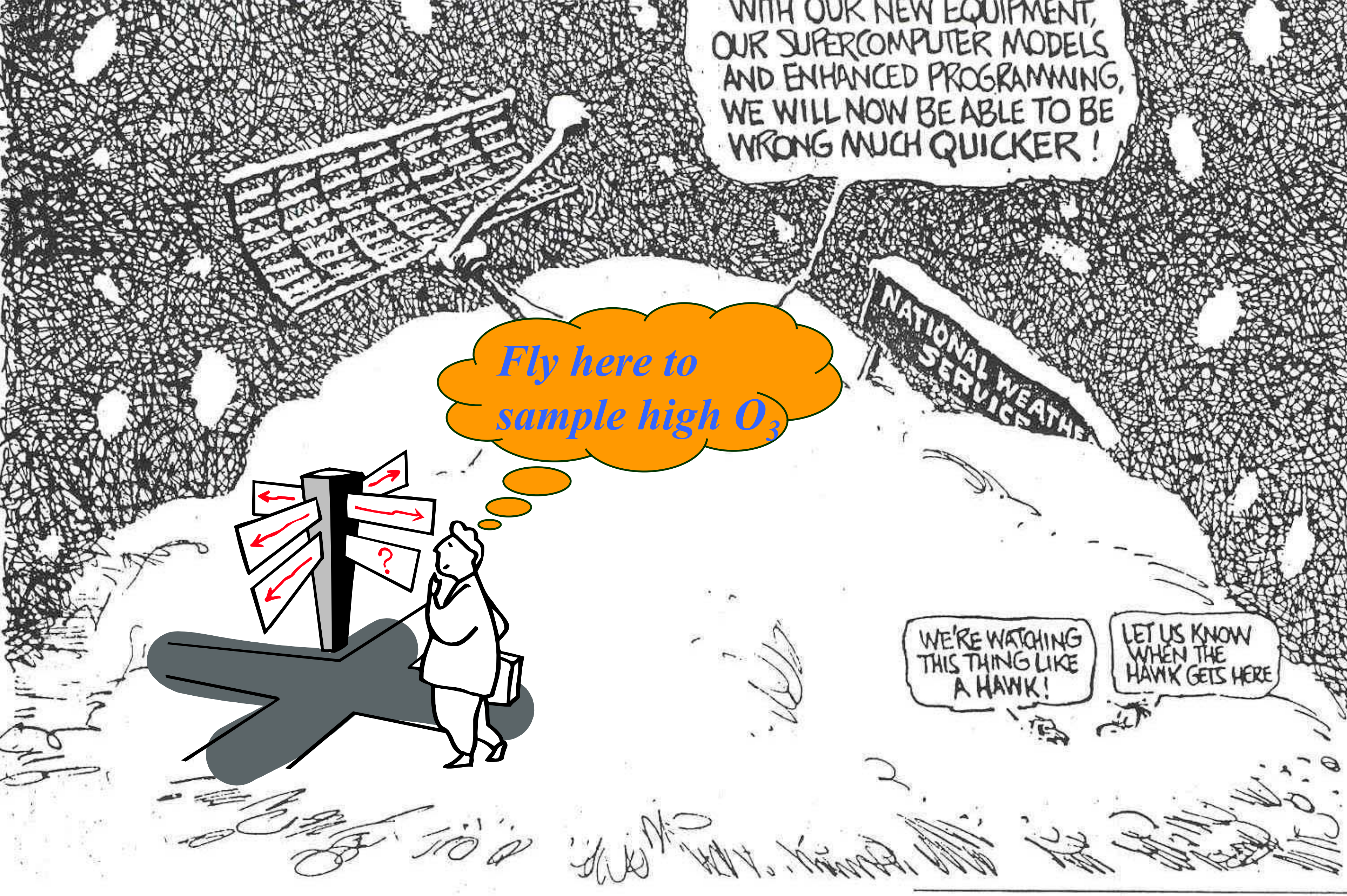
http://www.cgrer.uiowa.edu/people/carmichael/GURME/GURME.html

Why Forecast Air Quality?

- Provide information to the public *operationally* to help them better manage their health and welfare (heat stress, comfort, pollen, flight operations, large scale pollution/fire events, safer more effective conditions to apply chemicals)

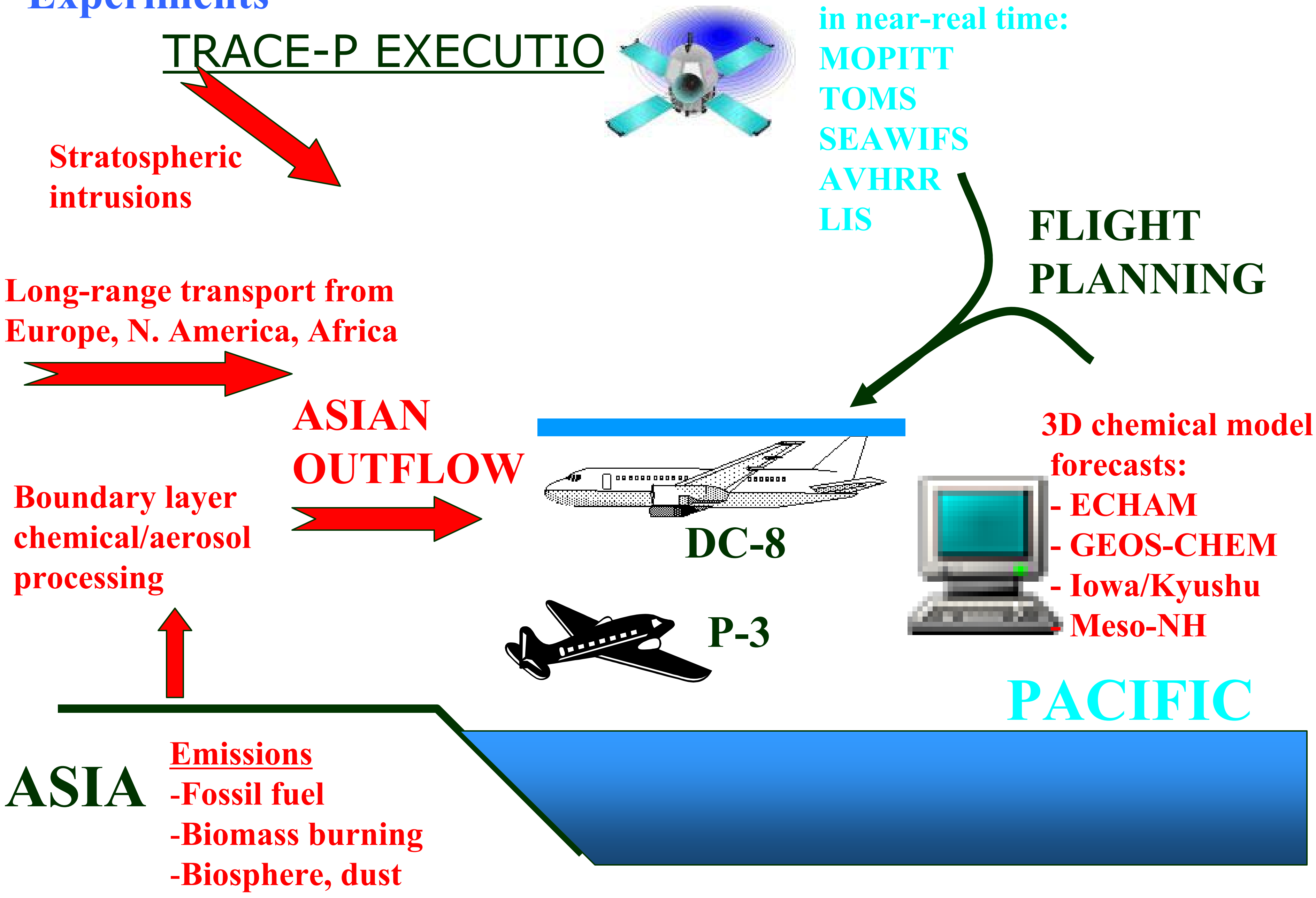
Why Forecast Air Quality?

- Strategic issues – if weather services don’t do it others certainly will !
- Weather infrastructure is invaluable – measurement, models, assimilation expertise.



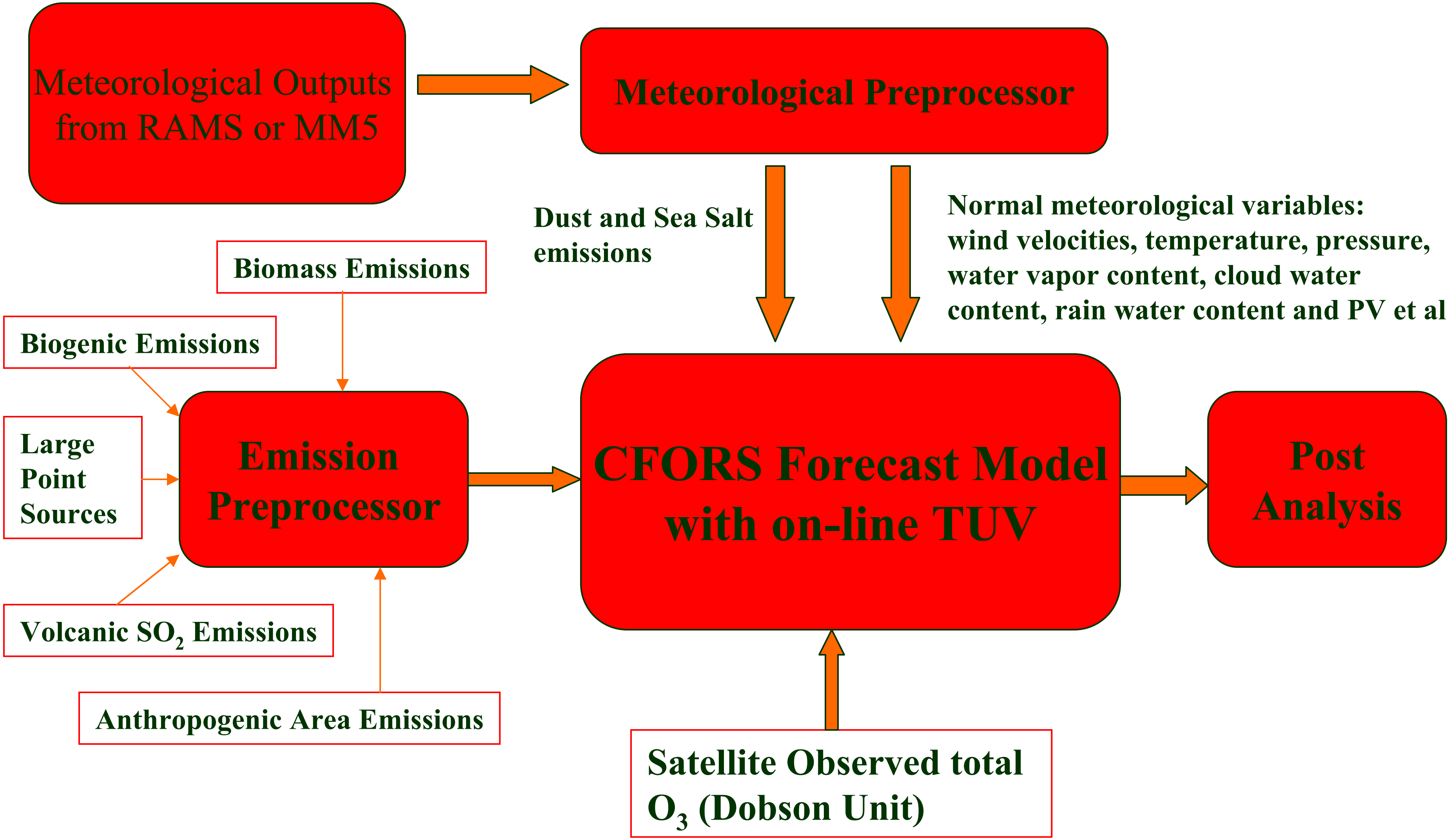
PAT OLPHANT/Universal Press Syndicat

Forecasting in Support of Field Experiments



Ace-Asia April/May 2001

CFORS/STEM Model Data Flow Chart



Meteorological Outputs from RAMS or MM5

Meteorological Preprocessor

Dust and Sea Salt emissions

Normal meteorological variables: wind velocities, temperature, pressure, water vapor content, cloud water content, rain water content and PV et al

Biomass Emissions

Biogenic Emissions

Large Point Sources

Emission Preprocessor

CFORS Forecast Model with on-line TUV

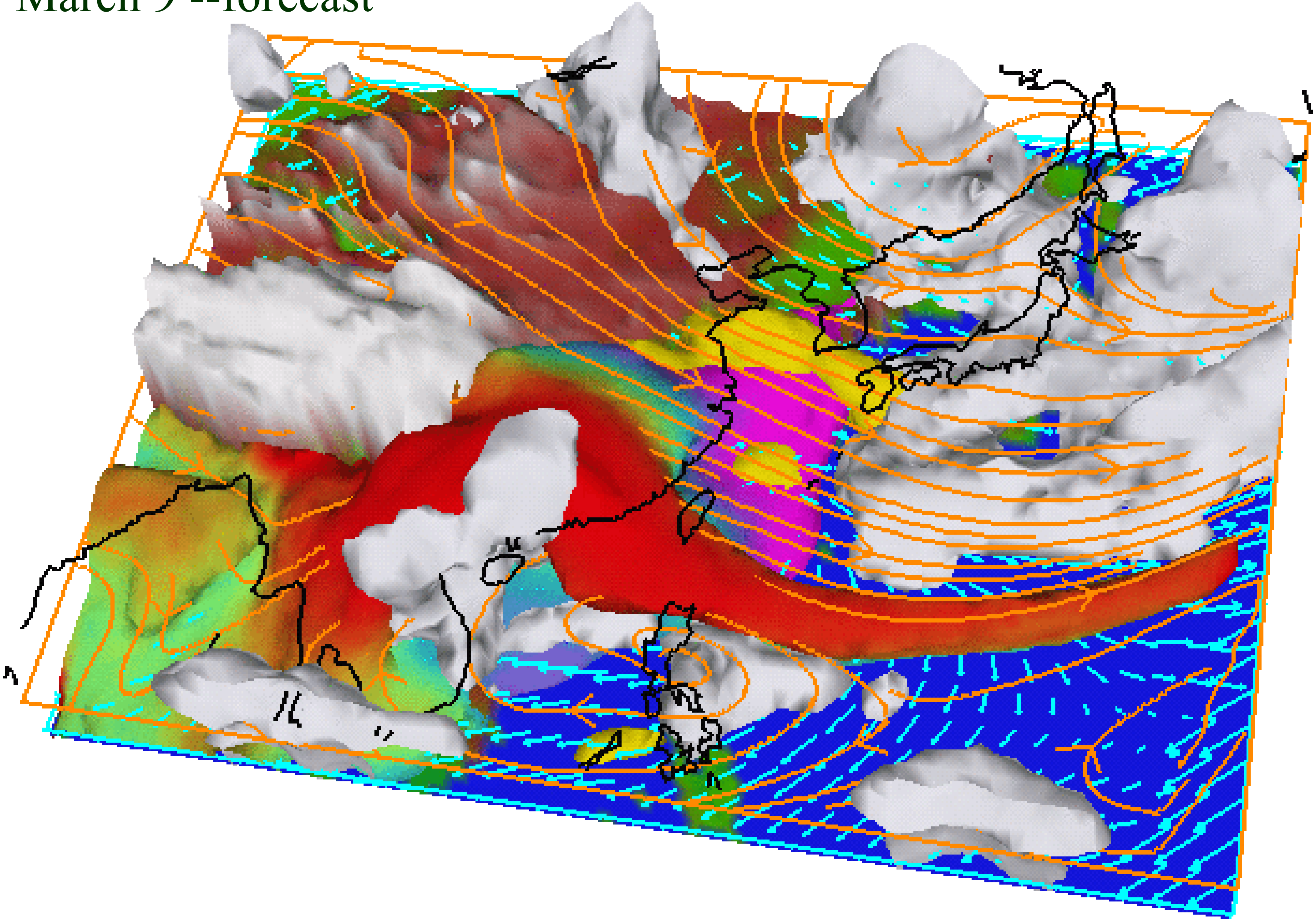
Post Analysis

Volcanic SO$_2$ Emissions

Anthropogenic Area Emissions

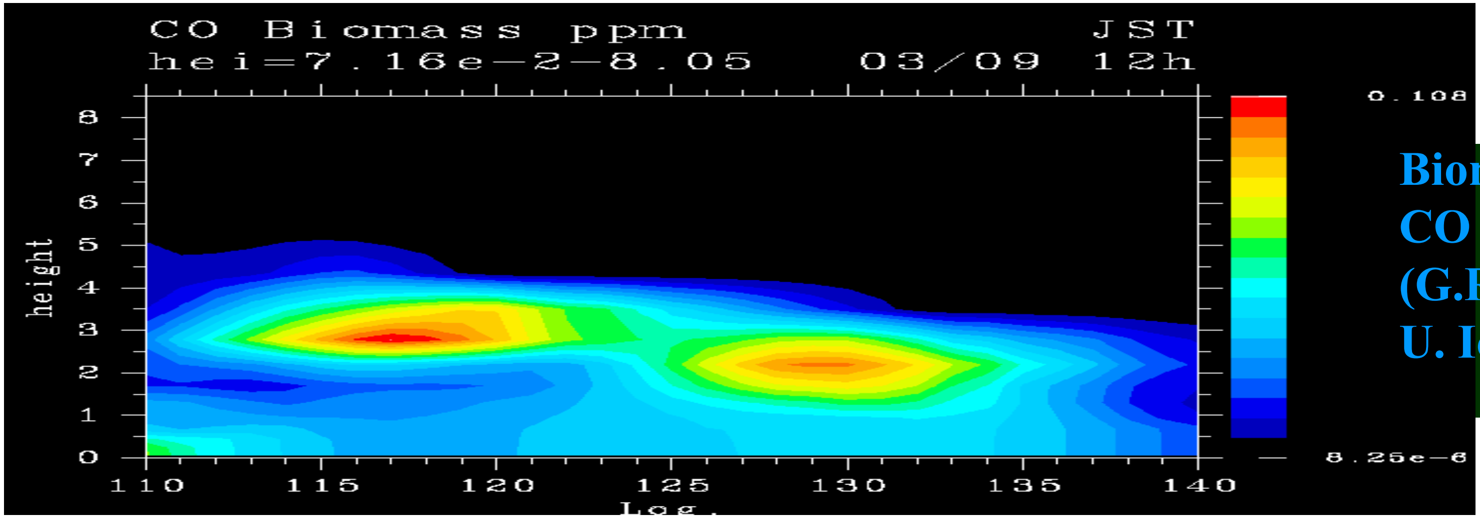
Satellite Observed total O$_3$ (Dobson Unit)

March 9 --forecast

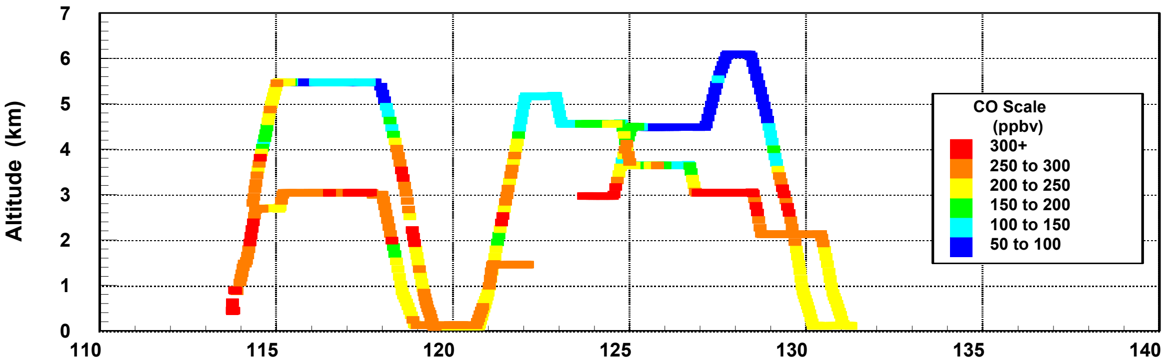


Vis5D

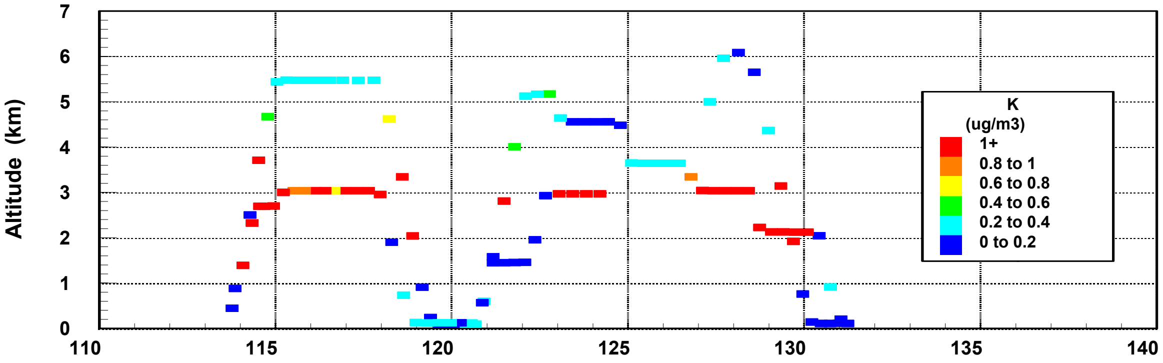
Frontal outflow of biomass burning plumes E of Hong Kong



Biomass burning CO forecast (G.R. Carmichael, U. Iowa)

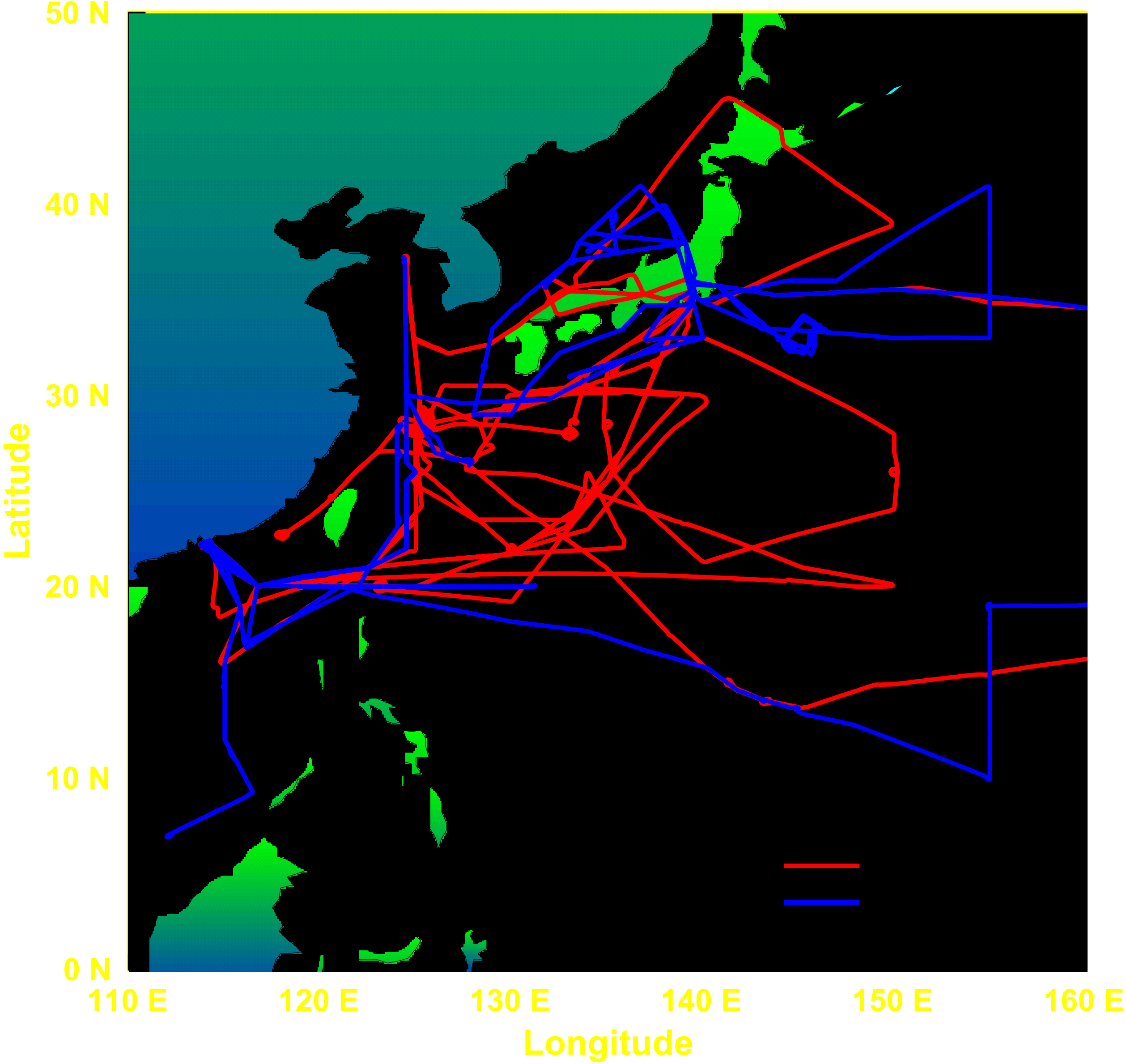


Observed CO (G.W. Sachse, NASA/LaRC)



Observed aerosol potassium (R. Weber, Georgia Tech)

Flight Tracks Along the Asian Pacific Rim During the TRACE-P Mission



Results from Trace-P Intercomparison Study

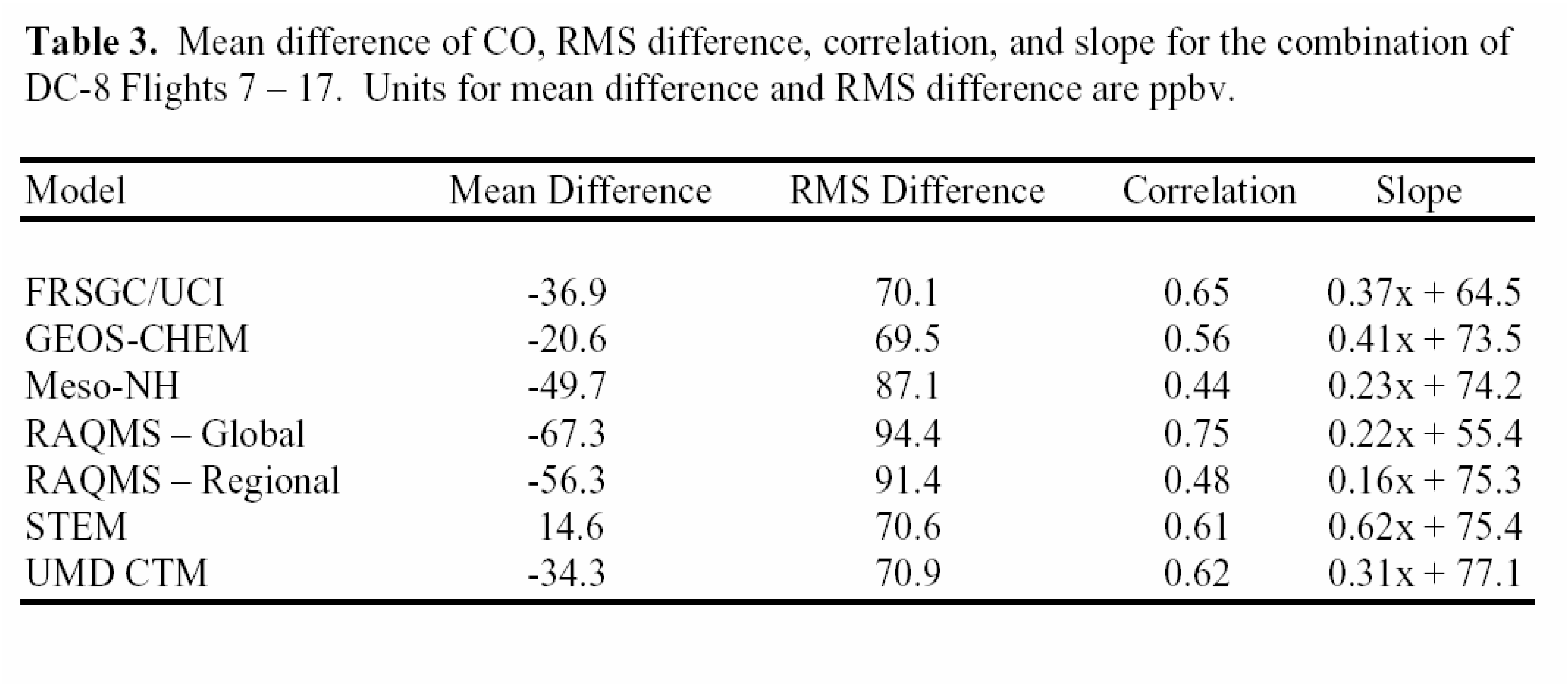
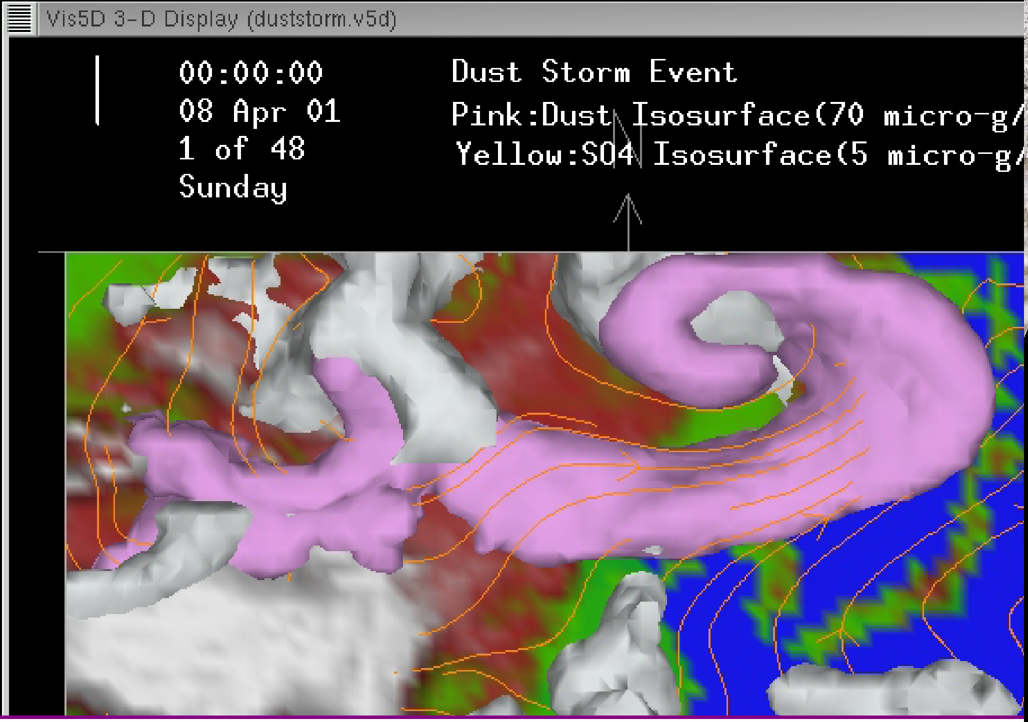


Table 3. Mean difference of CO, RMS difference, correlation, and slope for the combination of DC-8 Flights 7 – 17. Units for mean difference and RMS difference are ppbv.

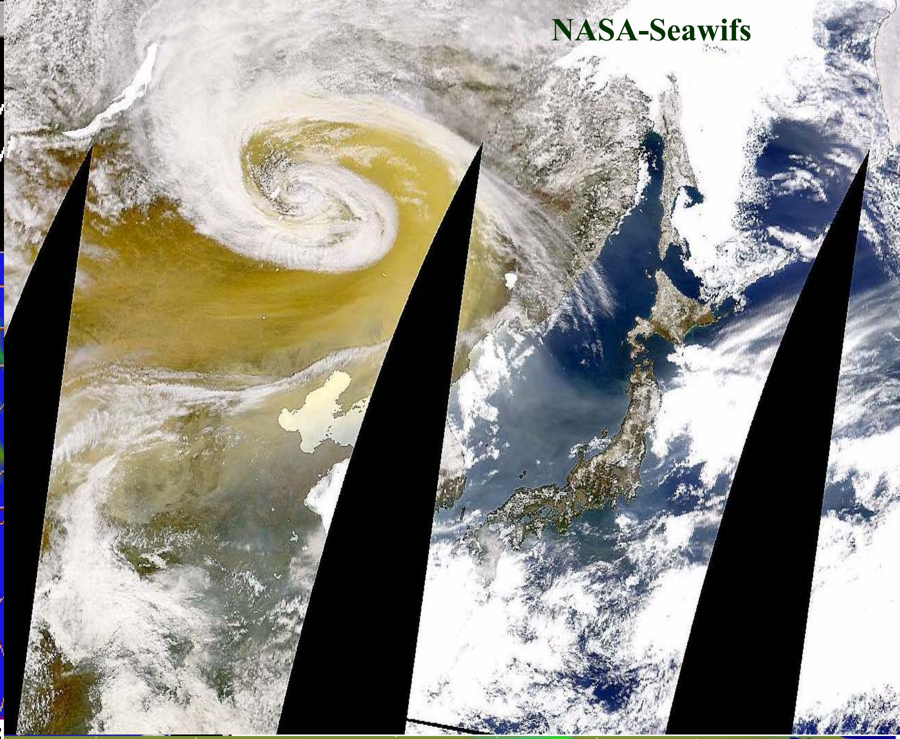
Model	Mean Difference	RMS Difference	Correlation	Slope
FRSGC/UCI	-36.9	70.1	0.65	0.37x + 64.5
GEOS-CHEM	-20.6	69.5	0.56	0.41x + 73.5
Meso-NH	-49.7	87.1	0.44	0.23x + 74.2
RAQMS – Global	-67.3	94.4	0.75	0.22x + 55.4
RAQMS – Regional	-56.3	91.4	0.48	0.16x + 75.3
STEM	14.6	70.6	0.61	0.62x + 75.4
UMD CTM	-34.3	70.9	0.62	0.31x + 77.1

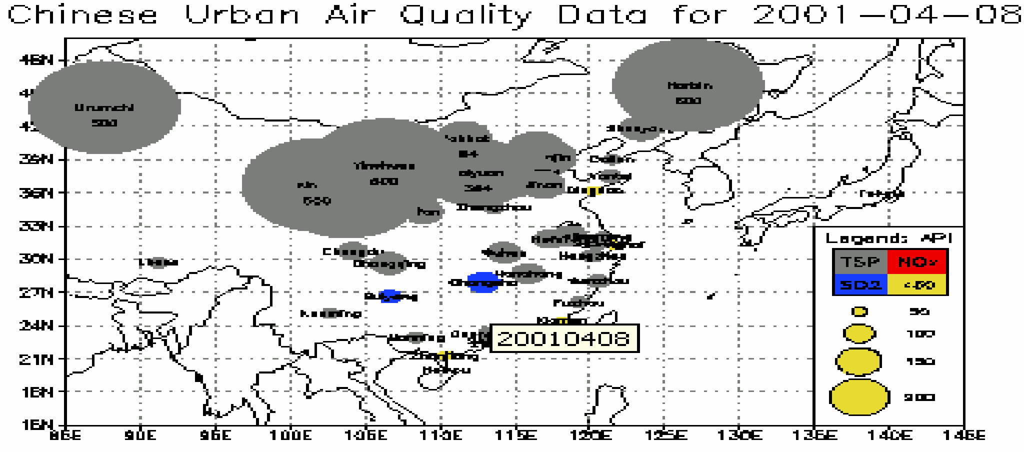


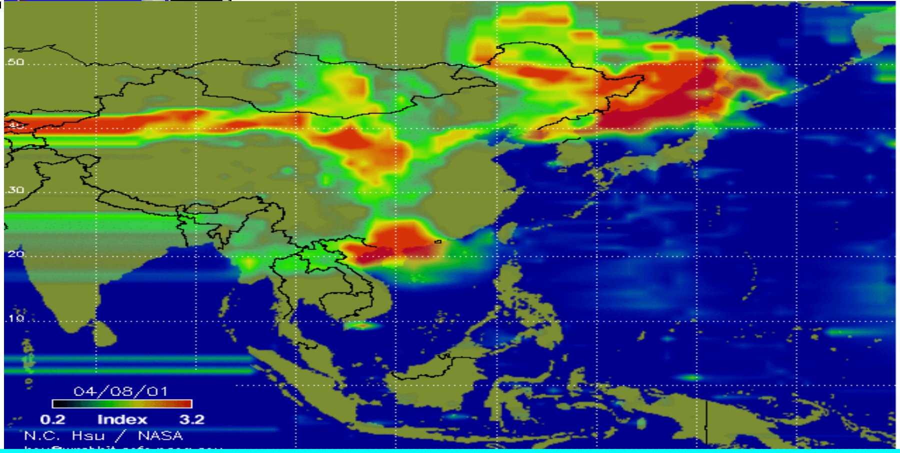
Vis5D 3-D Display (duststorm.v5d)

00:00:00
08 Apr 01
1 of 48
Sunday

Dust Storm Event
Pink:Dust Isosurface(70 micro-g/
Yellow:SO4 Isosurface(5 micro-g/







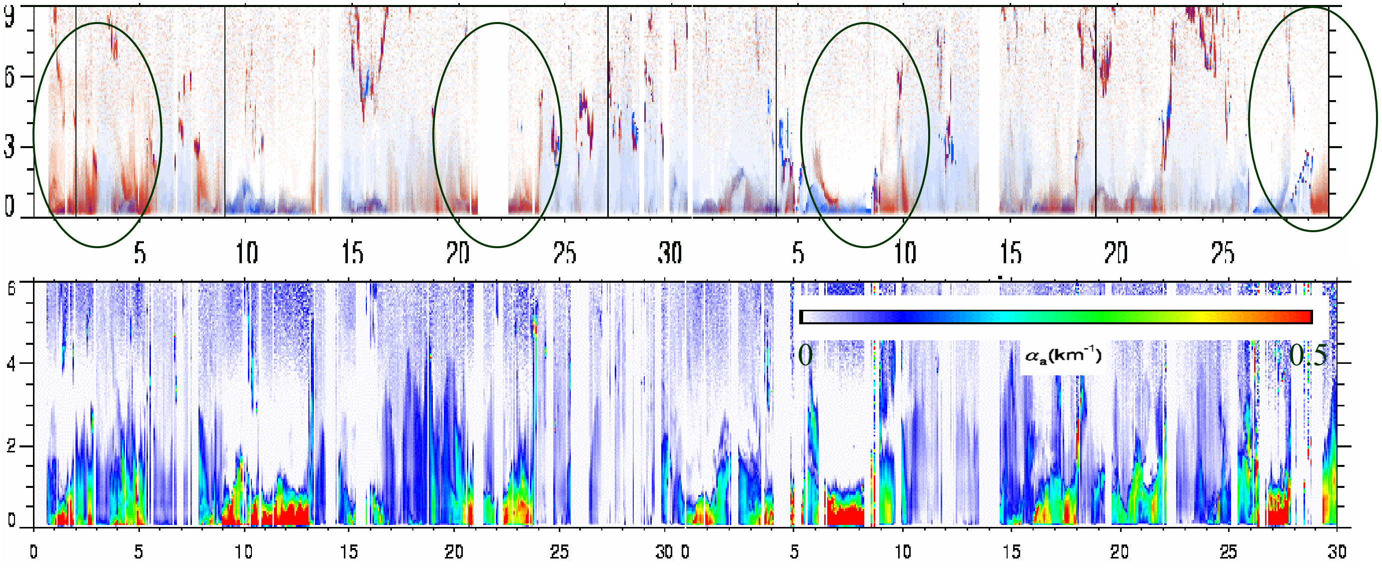
The CFORS forecast (upper left) of the two dust systems are shown above. The dust plume (pink) represents the region with dust concentrations greater than 200 μgrams/m³. White indicates clouds. The SeaWifs satellite image (upper right) also clearly shows the accumulation of dust spiraling into the Low Pressure center. Also note the strong outflow of dust in the warm sector "ahead" of the front over the Japan Sea. The two systems are clearly seen in the satellite derived TOMS-AI (aerosol index) (lower right). The dust event is clearly seen in the China SEPA air pollution monitoring network. Lower left hand panel shows extremely large ground level concentrations

These dust outbreaks caused severe problems in China

These photos are reduced-resolution versions of photos taken by Dr. Zev Levin while visiting Baicheng, Jilin Province, China (NE of Beijing) during the dust storm. The first two were taken on April 7th. The third was taken on April 8th. The two buildings seen in the foreground of the third image are also seen in the second

From P. Westphals web site:
http://www.nrlmry.navy.mil/aerosol/Case_studies/20010413_epac/

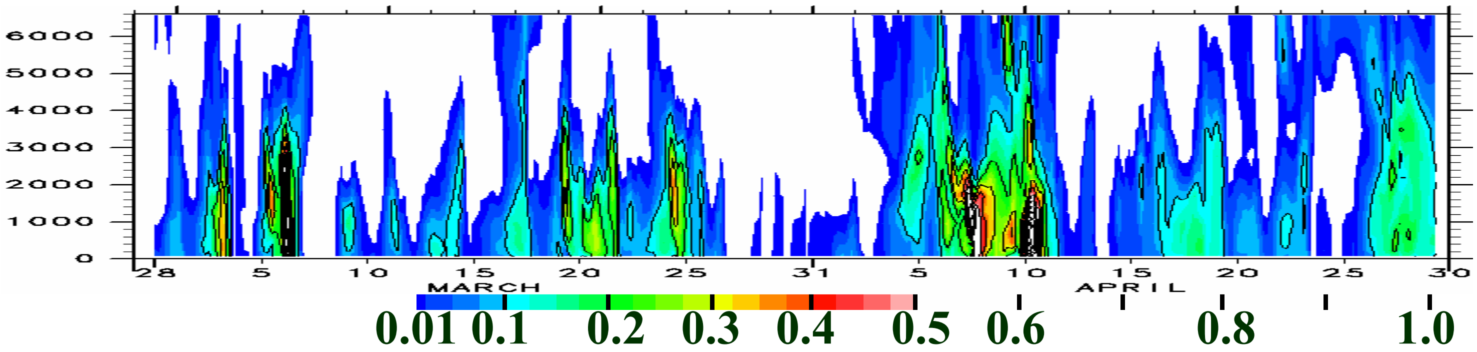
NIES Lidar Measurement at Beijing



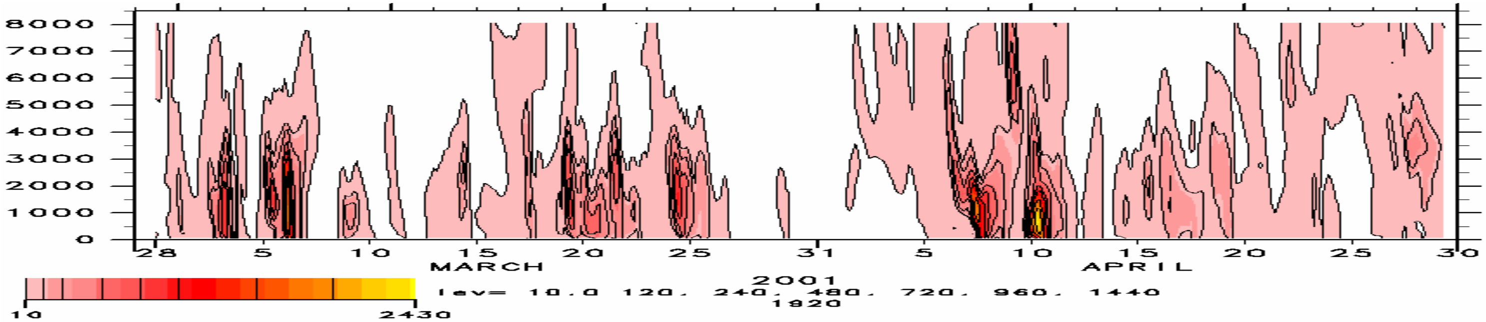
Ext. Coef.

(air pollution Part)

CFORS Model Simulation



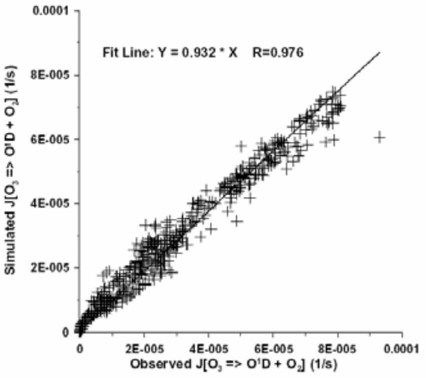
Ext. Coef. (1/Km)



Dust Conc.

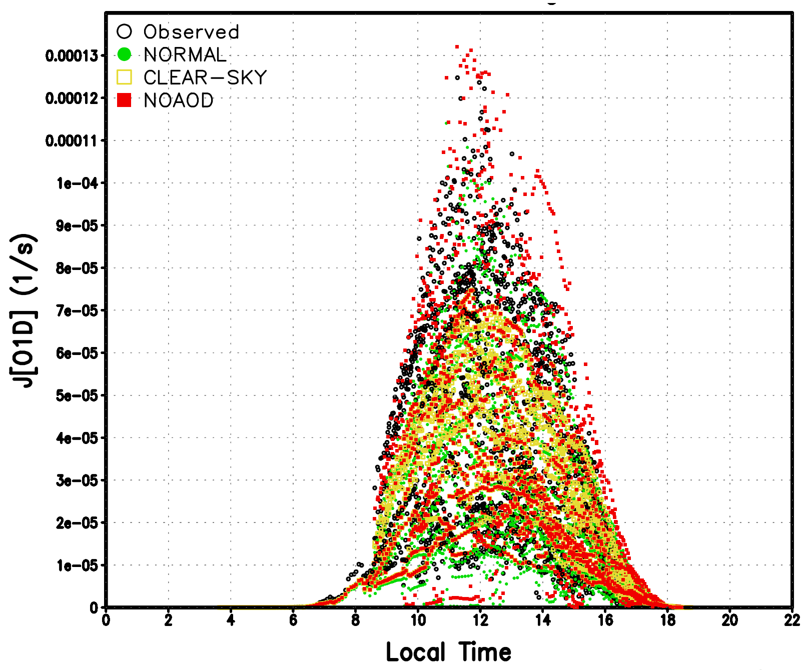
Accurate Calculation of Photolysis Rates is a Critical Element in Air Quality Forecasting

- **NORMAL:** standard STEM simulation. Aerosol and cloud optical properties are explicitly considered
- **NOAOD:** STEM simulation without aerosol optical properties, but with cloud impacts.
- **CLEARSKY:** STEM simulation without aerosol or cloud optical properties.

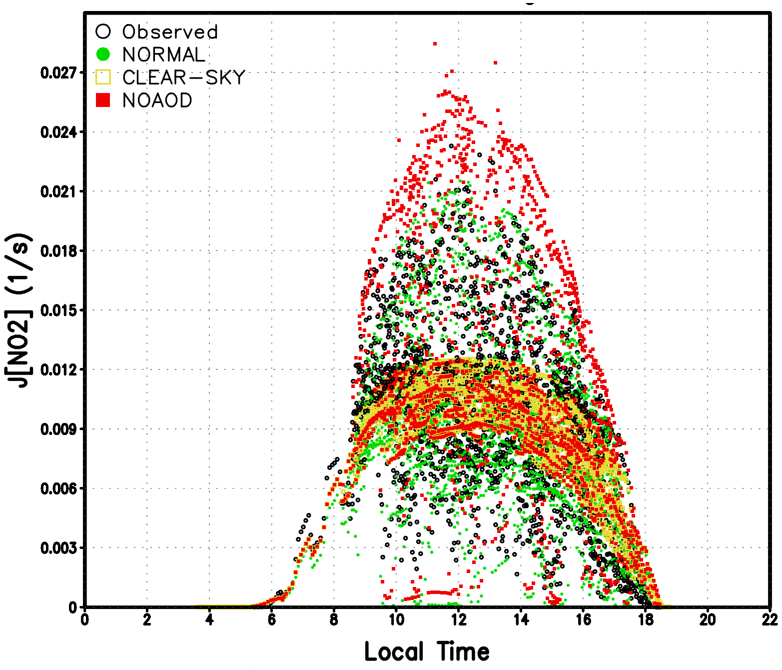


For TRACE-P all DC-8 and P-3 Flights:

$J[O_3 \rightarrow O^1D+O2]$



$J[NO_2 \rightarrow O^3P+NO]$



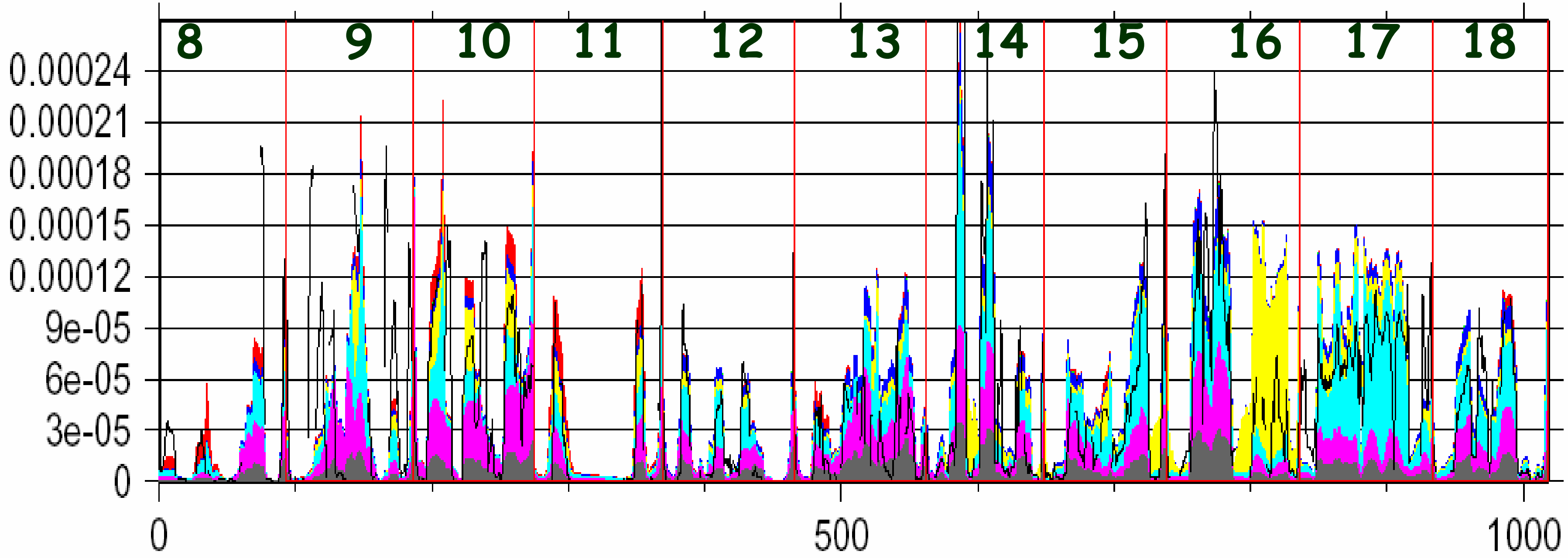
Data from Shetter et al.

TRACE-P Extinction

legend

🟥 Sea Salt 🟦 PM2.5 🟦 Sulfate 🟪 OC

🟩 PM10 🟨 DUST ⬛ BC



Data from Clarke et al.

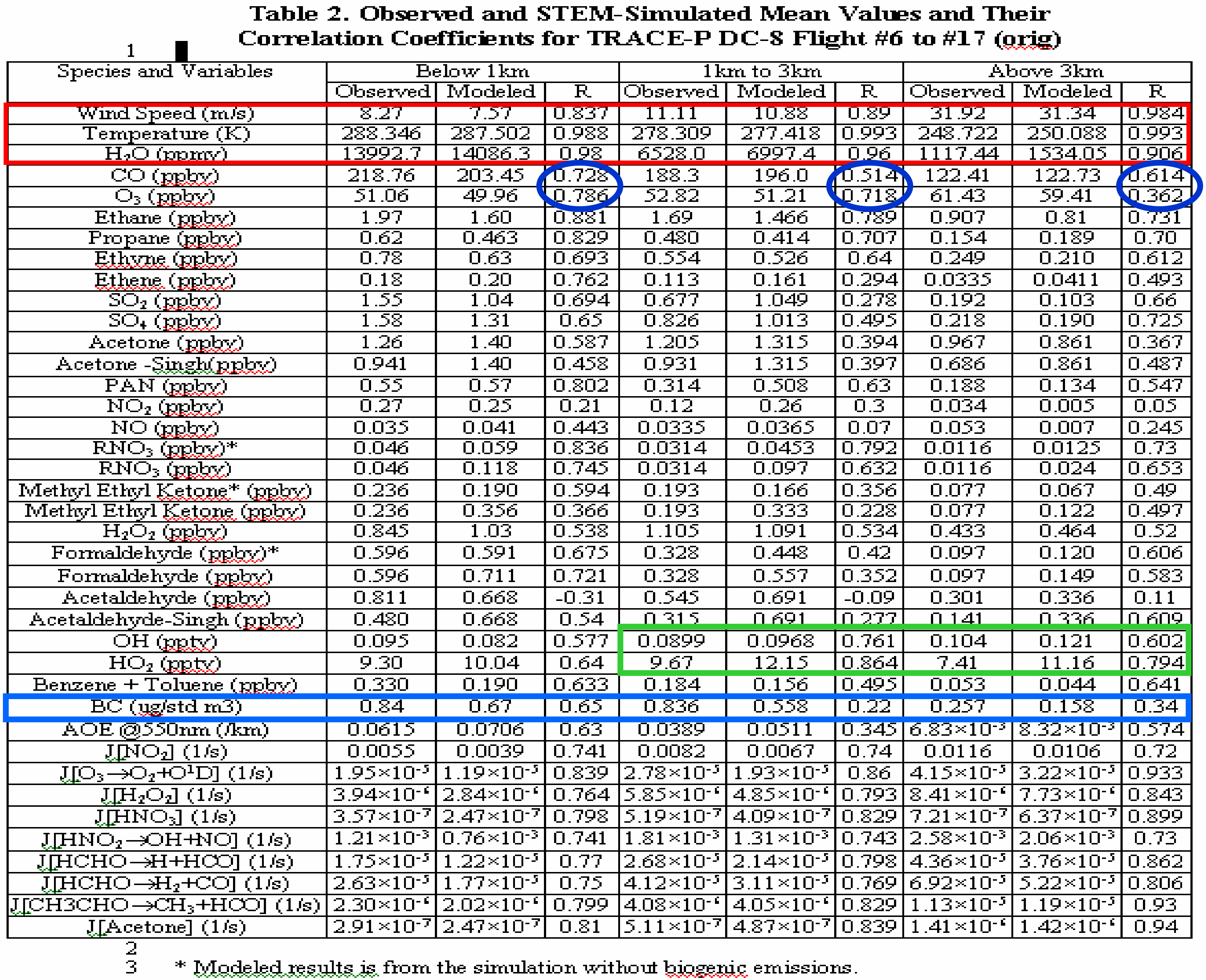


Table 2. Observed and STEM-Simulated Mean Values and Their Correlation Coefficients for TRACE-P DC-8 Flight #6 to #17 (orig)

Species and Variables	Below 1km			1km to 3km			Above 3km		
	Observed	Modeled	R	Observed	Modeled	R	Observed	Modeled	R
Wind Speed (m/s)	8.27	7.57	0.837	11.11	10.88	0.89	31.92	31.34	0.984
Temperature (K)	288.346	287.502	0.988	278.309	277.418	0.993	248.722	250.088	0.993
H_2O (ppmv)	13992.7	14086.3	0.98	6528.0	6997.4	0.96	1117.44	1534.05	0.906
CO (ppbv)	218.76	203.45	0.728	188.3	196.0	0.514	122.41	122.73	0.614
O_3 (ppbv)	51.06	49.96	0.786	52.82	51.21	0.718	61.43	59.41	0.362
Ethane (ppbv)	1.97	1.60	0.881	1.69	1.466	0.789	0.907	0.81	0.731
Propane (ppbv)	0.62	0.463	0.829	0.480	0.414	0.707	0.154	0.189	0.70
Ethyne (ppbv)	0.78	0.63	0.693	0.554	0.526	0.64	0.249	0.210	0.612
Ethene (ppbv)	0.18	0.20	0.762	0.113	0.161	0.294	0.0335	0.0411	0.493
SO_2 (ppbv)	1.55	1.04	0.694	0.677	1.049	0.278	0.192	0.103	0.66
SO_4 (ppbv)	1.58	1.31	0.65	0.826	1.013	0.495	0.218	0.190	0.725
Acetone (ppbv)	1.26	1.40	0.587	1.205	1.315	0.394	0.967	0.861	0.367
Acetone -Singh(ppbv)	0.941	1.40	0.458	0.931	1.315	0.397	0.686	0.861	0.487
PAN (ppbv)	0.55	0.57	0.802	0.314	0.508	0.63	0.188	0.134	0.547
NO_2 (ppbv)	0.27	0.25	0.21	0.12	0.26	0.3	0.034	0.005	0.05
NO (ppbv)	0.035	0.041	0.443	0.0335	0.0365	0.07	0.053	0.007	0.245
RNO_3 (ppbv)*	0.046	0.059	0.836	0.0314	0.0453	0.792	0.0116	0.0125	0.73
RNO_3 (ppbv)	0.046	0.118	0.745	0.0314	0.097	0.632	0.0116	0.024	0.653
Methyl Ethyl Ketone* (ppbv)	0.236	0.190	0.594	0.193	0.166	0.356	0.077	0.067	0.49
Methyl Ethyl Ketone (ppbv)	0.236	0.356	0.366	0.193	0.333	0.228	0.077	0.122	0.497
H_2O_2 (ppbv)	0.845	1.03	0.538	1.105	1.091	0.534	0.433	0.464	0.52
Formaldehyde (ppbv)*	0.596	0.591	0.675	0.328	0.448	0.42	0.097	0.120	0.606
Formaldehyde (ppbv)	0.596	0.711	0.721	0.328	0.557	0.352	0.097	0.149	0.583
Acetaldehyde (ppbv)	0.811	0.668	-0.31	0.545	0.691	-0.09	0.301	0.336	0.11
Acetaldehyde-Singh (ppbv)	0.480	0.668	0.54	0.315	0.691	0.277	0.141	0.336	0.609
OH (pptv)	0.095	0.082	0.577	0.0899	0.0968	0.761	0.104	0.121	0.602
HO_2 (pptv)	9.30	10.04	0.64	9.67	12.15	0.864	7.41	11.16	0.794
Benzene + Toluene (ppbv)	0.330	0.190	0.633	0.184	0.156	0.495	0.053	0.044	0.641
BC (ug/std m3)	0.84	0.67	0.65	0.836	0.558	0.22	0.257	0.158	0.34
AOE @550nm (/km)	0.0615	0.0706	0.63	0.0389	0.0511	0.345	6.83×10^{-3}	8.32×10^{-3}	0.574
$J[NO_2]$ (1/s)	0.0055	0.0039	0.741	0.0082	0.0067	0.74	0.0116	0.0106	0.72
$J[O_3 \rightarrow O_2+O^1D]$ (1/s)	1.95×10^{-5}	1.19×10^{-5}	0.839	2.78×10^{-5}	1.93×10^{-5}	0.86	4.15×10^{-5}	3.22×10^{-5}	0.933
$J[H_2O_2]$ (1/s)	3.94×10^{-6}	2.84×10^{-6}	0.764	5.85×10^{-6}	4.85×10^{-6}	0.793	8.41×10^{-6}	7.73×10^{-6}	0.843
$J[HNO_3]$ (1/s)	3.57×10^{-7}	2.47×10^{-7}	0.798	5.19×10^{-7}	4.09×10^{-7}	0.829	7.21×10^{-7}	6.37×10^{-7}	0.899
$J[HNO_2 \rightarrow OH+NO]$ (1/s)	1.21×10^{-3}	0.76×10^{-3}	0.741	1.81×10^{-3}	1.31×10^{-3}	0.743	2.58×10^{-3}	2.06×10^{-3}	0.73
$J[HCHO \rightarrow H+HCO]$ (1/s)	1.75×10^{-5}	1.22×10^{-5}	0.77	2.68×10^{-5}	2.14×10^{-5}	0.798	4.36×10^{-5}	3.76×10^{-5}	0.862
$J[HCHO \rightarrow H_2+CO]$ (1/s)	2.63×10^{-5}	1.77×10^{-5}	0.75	4.12×10^{-5}	3.11×10^{-5}	0.769	6.92×10^{-5}	5.22×10^{-5}	0.806
$J[CH3CHO \rightarrow CH_3+HCO]$ (1/s)	2.30×10^{-6}	2.02×10^{-6}	0.799	4.08×10^{-6}	4.05×10^{-6}	0.829	1.13×10^{-5}	1.19×10^{-5}	0.93
J[Acetone] (1/s)	2.91×10^{-7}	2.47×10^{-7}	0.81	5.11×10^{-7}	4.87×10^{-7}	0.839	1.41×10^{-6}	1.42×10^{-6}	0.94

* Modeled results is from the simulation without biogenic emissions.

Added Considerations for Air Quality Forecasting

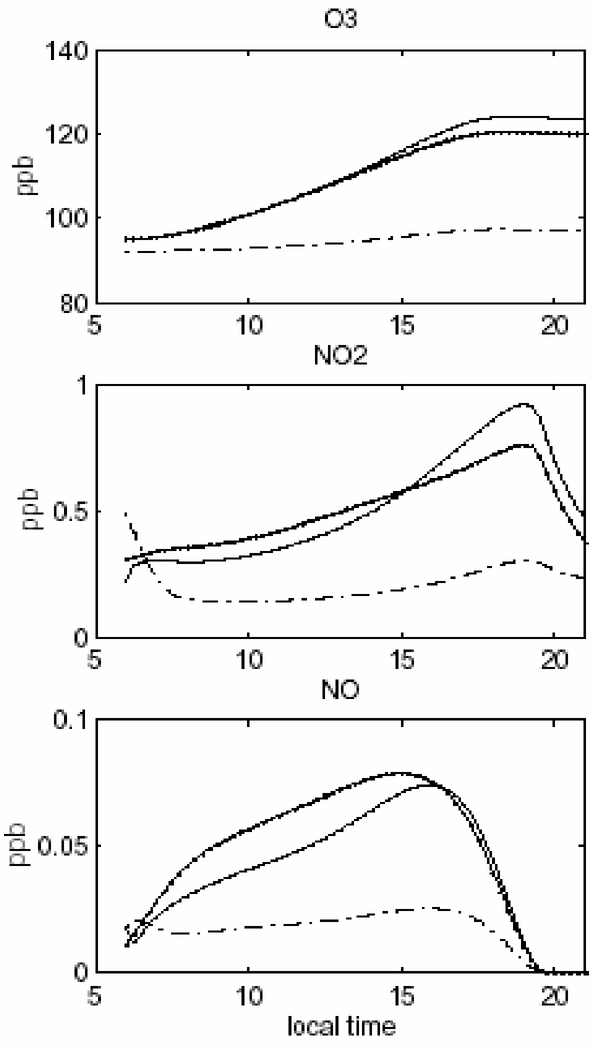
- System designed for synoptic scale meteorology.
- Air quality needs pbl info, cloud fluxes
- Deficiencies in met models – different requirements on transport, preservation of mass, etc.
- Sources needed at smaller scales, some sources intimately linked to meteorology
- Meteorological measurements for air quality (may) need to be designed differently (idea of urban:rural pairs)

The Future - Integrating Models and Measurements

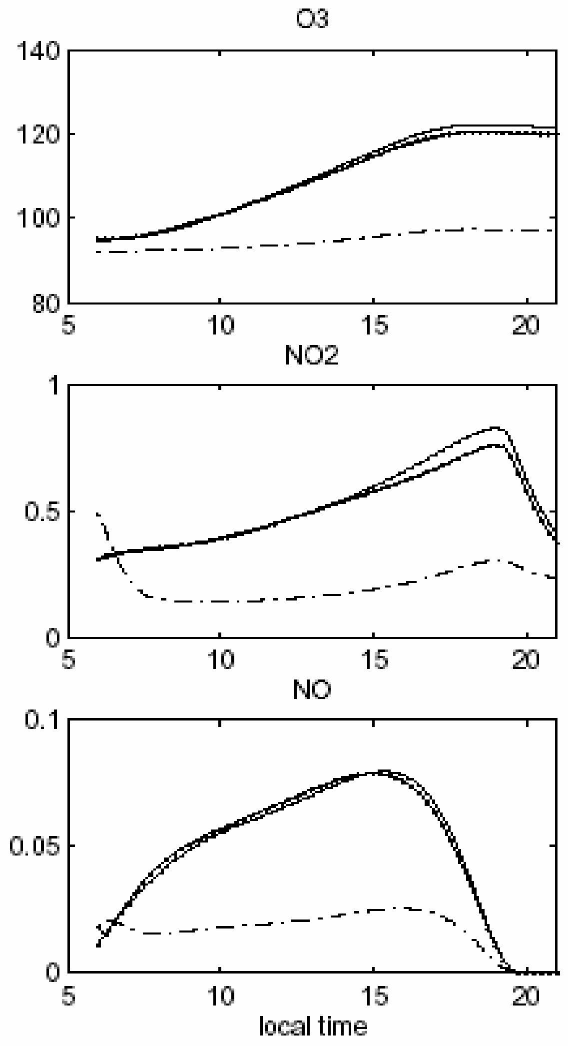
- Test forecasting skill – more emphasis on verification
- Test model resolution effects – for which problems is resolution critical?
- Data assimilation/sensitivity analysis in large models is “expanding” – great opportunity to think about how these experiments can help accelerate the science
- Data assimilation – satellite, surface obs….
- Characterize errors….., and co-variances, and species/species correlations and other ways of filling in data for use in assimilation
- How to best link measurements in space & time

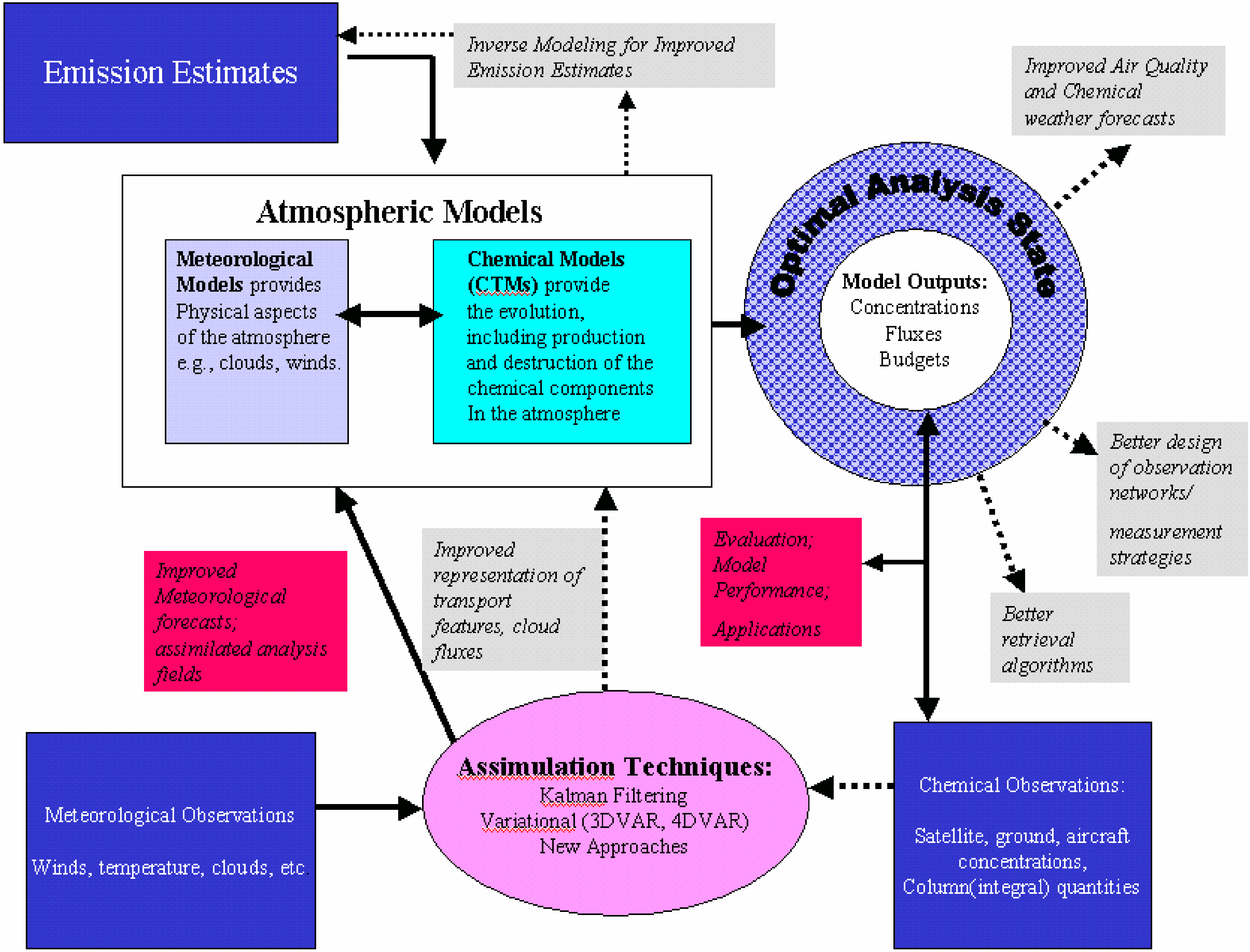
4D-var Data Assimilation

O_3



$O_3 + NO_2$





Emission Estimates

Inverse Modeling for Improved Emission Estimates

Improved Air Quality and Chemical weather forecasts

Atmospheric Models

Meteorological Models provides Physical aspects of the atmosphere e.g., clouds, winds.

Chemical Models (CTMs) provide the evolution, including production and destruction of the chemical components In the atmosphere

Optimal Analysis State

Model Outputs:
Concentrations
Fluxes
Budgets

Better design of observation networks/

measurement strategies

Improved Meteorological forecasts; assimilated analysis fields

Improved representation of transport features, cloud fluxes

Evaluation; Model Performance;

Applications

Better retrieval algorithms

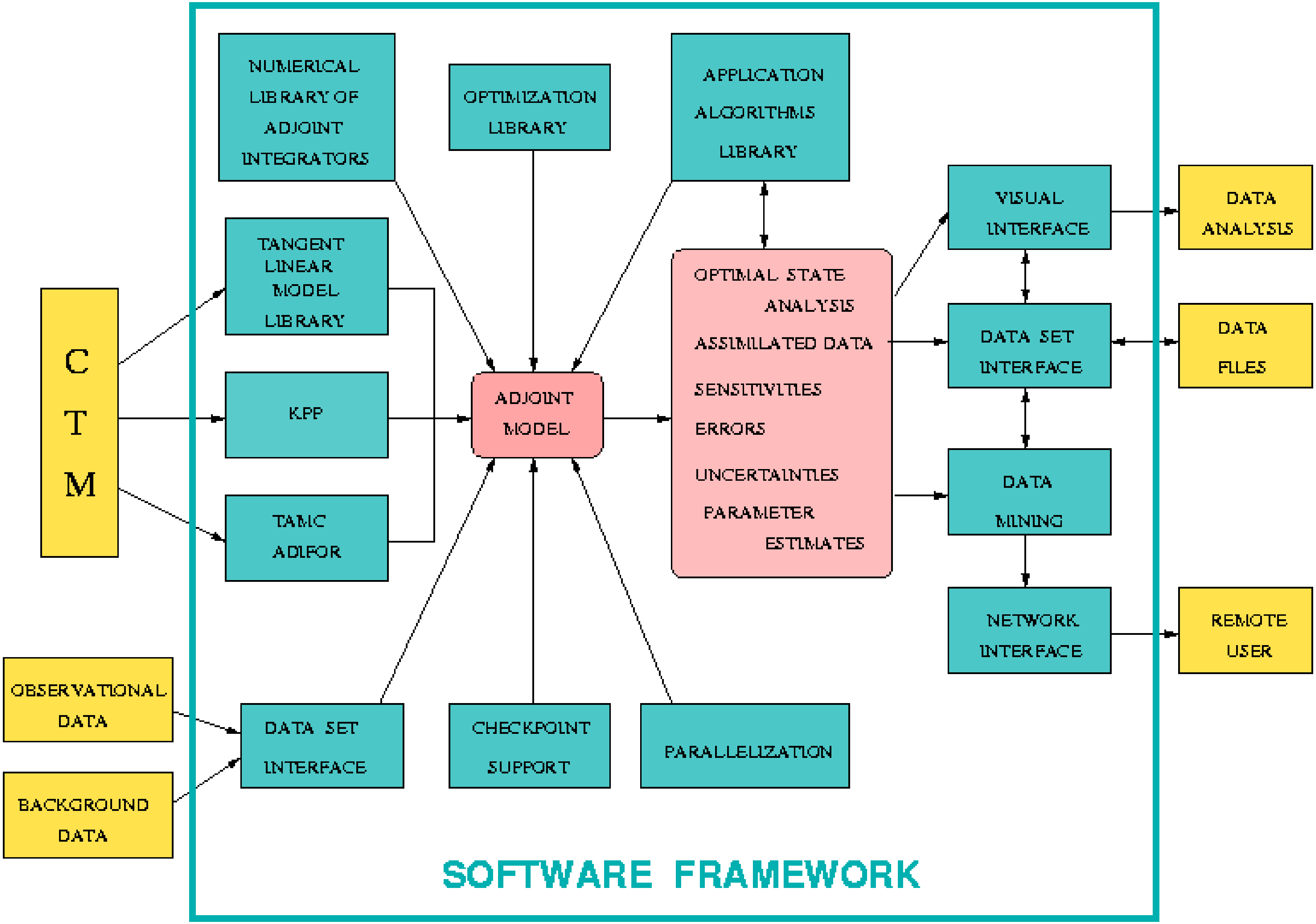
Meteorological Observations

Winds, temperature, clouds, etc.

Assimilation Techniques:
Kalman Filtering
Variational (3DVAR, 4DVAR)
New Approaches

Chemical Observations:

Satellite, ground, aircraft concentrations,
Column(integral) quantities



CTM

NUMERICAL LIBRARY OF ADJOINT INTEGRATORS

OPTIMIZATION LIBRARY

APPLICATION ALGORITHMS LIBRARY

TANGENT LINEAR MODEL LIBRARY

KPP

TAMC ADIFOR

ADJOINT MODEL

OPTIMAL STATE ANALYSIS

ASSIMILATED DATA

SENSITIVITIES

ERRORS

UNCERTAINTIES

PARAMETER ESTIMATES

VISUAL INTERFACE

DATA SET INTERFACE

DATA MINING

NETWORK INTERFACE

DATA ANALYSIS

DATA FILES

REMOTE USER

OBSERVATIONAL DATA

BACKGROUND DATA

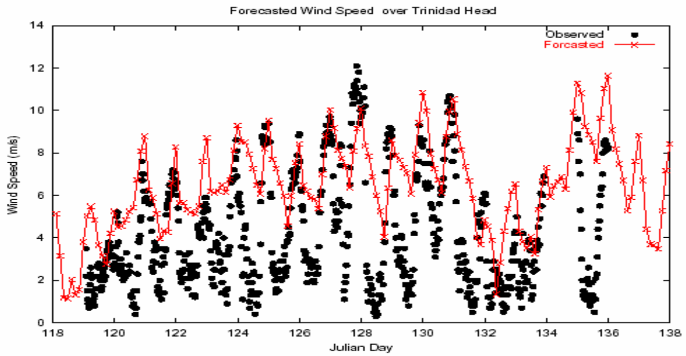
DATA SET INTERFACE

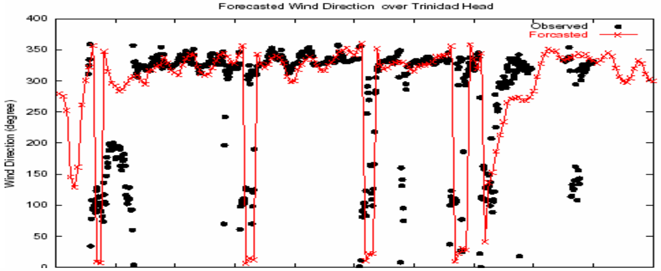
CHECKPOINT SUPPORT

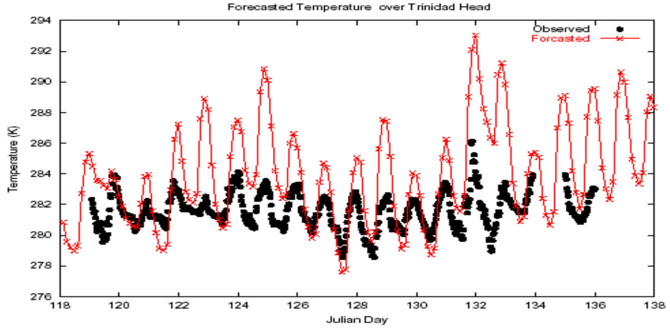
PARALLELIZATION

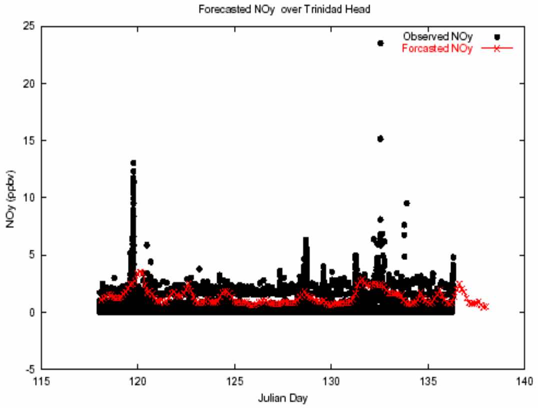
SOFTWARE FRAMEWORK

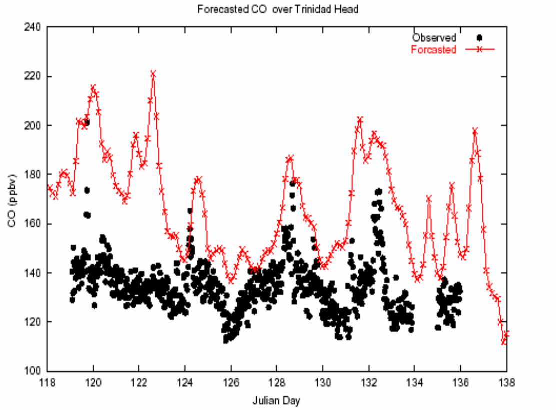
Trinidad Head Surface Measurements during ITCT Y2K- Model Forecasts were Provided Daily

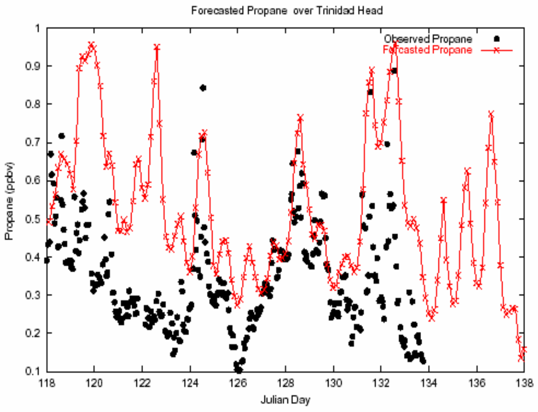

Forecasted Wind Speed over Trinidad Head

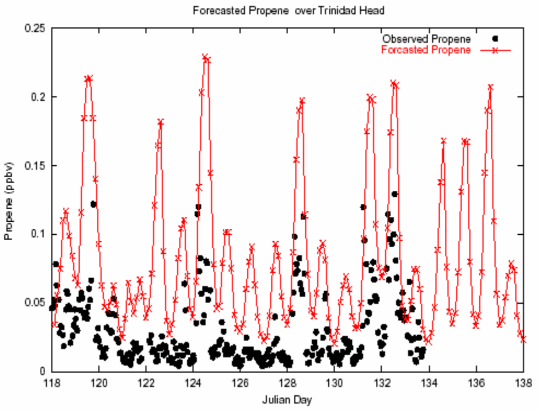

Forecasted Wind Direction over Trinidad Head


Forecasted Temperature over Trinidad Head


Forecasted NOy over Trinidad Head


Forecasted CO over Trinidad Head


Forecasted Propane over Trinidad Head


Forecasted Propene over Trinidad Head

Thoughts on Forecasting and Modeling

- Roles of models are expanding
- Challenge: How to make the best use of having a suite of forecasting products AND modelers in the field
- Challenge: How best to use the models to meet the mission objectives
- Challenge: How to optimally integrate measurements and model data

Final Thoughts on Priorities/Objectives

- Achieve improvements in met forecasts by considering air pollution elements.
- Add operational information to help protect public health and welfare, and to support more detailed air quality studies.
- Focus on the tools to facilitate the integration of measurements and models that are needed to support operational air quality forecasting systems.