Global Forecasting System (GFS) Project: Improving National chemistry forecasting and assimilation capabilities

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Presented by Jay Al-Saadi (NASA-LaRC)

Applications Air Quality Modeling Focus at Langley Research Center

Objective: Benchmark prototype chemical data assimilation procedures to provide NASA constituent observations to environmental decision support systems of NOAA, EPA, Regional Planning Organizations, and State and Local air quality management agencies

CMAQ Project (FY ‘04 - ‘05)

Prototype/evaluate techniques for improving boundary conditions of *National* air quality assessment model

GFS Project (FY ‘06 - ‘07)

Improve operational *National* AQ forecasts through incorporation of NASA models and satellite data

TexAQS Rapid Prototype (FY ‘07)

Improve capability of *State/Local* agencies to assess extra-regional influences on local air quality

Enabling Synergies: EPA AMI projects, ROSES 2007 proposals

Tools, capabilities and *inter-organizational partnerships* developed under previous and ongoing projects applied to emerging opportunities/needs

Objective: Improve the use of space based ozone measurements in operational global chemical data assimilation and forecasting, and benchmark the impact of these improvements on National AQ forecasting decision support systems.

Background and Approach

•The Congressional Energy Policy Act of 2002 [H.R. 4, 2002] directed the Department of Commerce, through NOAA, to "establish a program to provide operational air quality forecasts and warnings for specific regions of the United States".

•Operational air quality guidance currently covers the Eastern U.S. and is based on chemical forecasts from the EPA Community Multi-scale Air Quality (CMAQ) model driven by regional meteorological forecasts from the NOAA Weather Research and Forecasting (WRF) Nonhydrostatic Mesoscale Model (NMM) system. WRF-NMM is in turn driven by global forecasts from the NOAA Global Forecasting System (GFS).

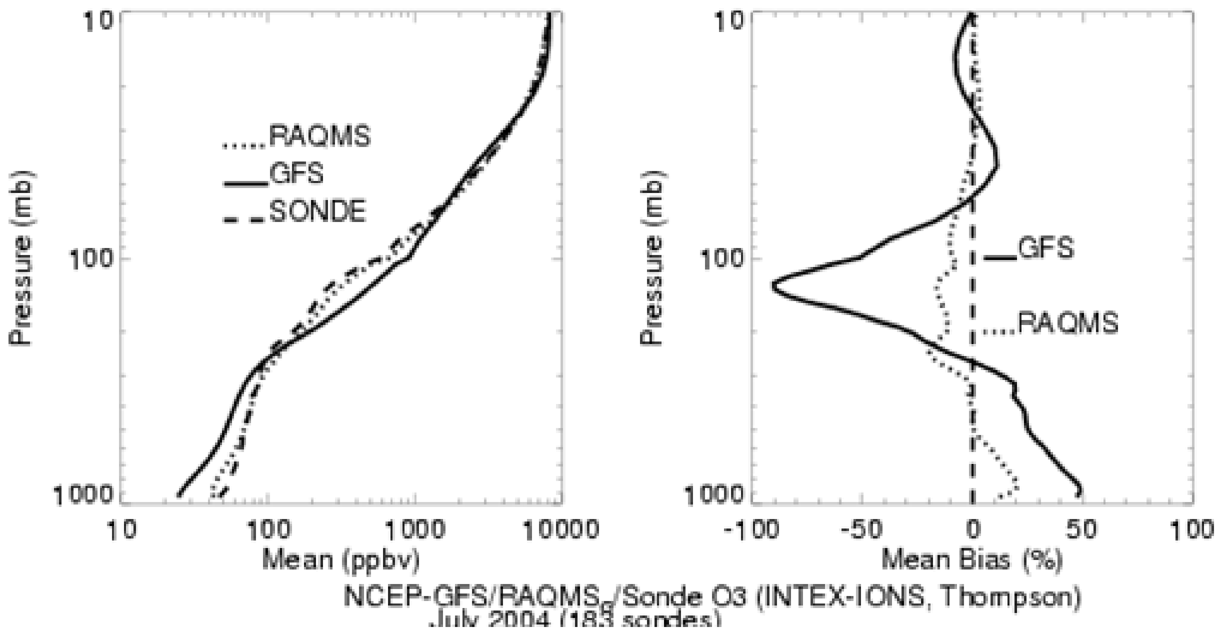
•Implement NASA chemical algorithms ("reduced chemistry") into NOAA GFS and validate improvements in GFS analyses due to operational assimilation of Aura and NPP constituent measurements

•Benchmark impact of improved operational global assimilation system on regional AQ forecasting using retrospective 2006 forecasts (follow-on to successful demonstration of impact of global chemical analyses on US-EPA CMAQ AQ assessment modeling during SOS 1999)

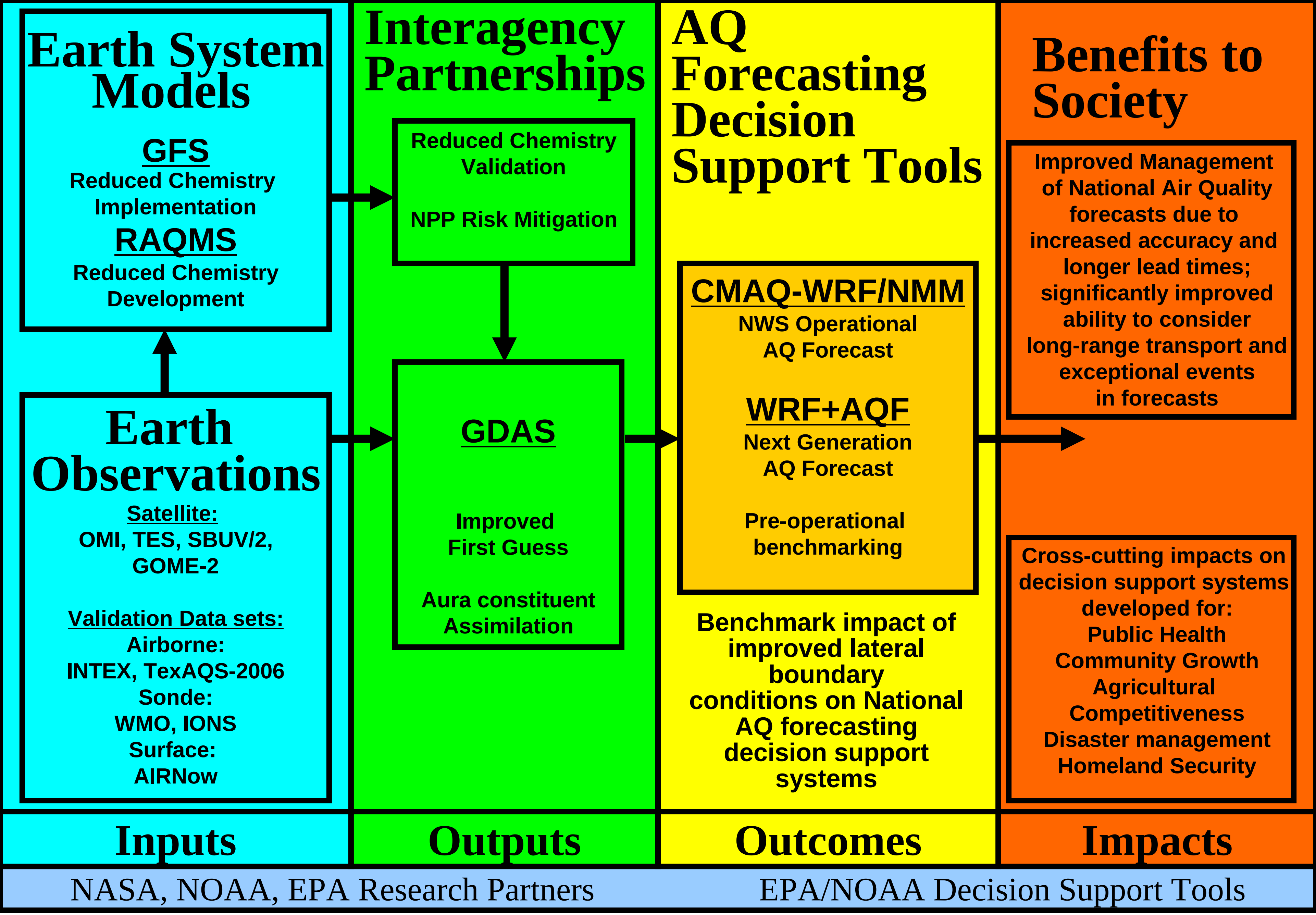
RAQMS and GFS vs CONUS Ozonesondes (IONS), July 2004

Mean O3 mixing ratio

Mean O3 bias



- GFS includes assimilation of SBUV2 Ozone but does not include chemistry
- RAQMS includes full chemistry with profile (solar occulatation) and column (TOMS) O3 assimilation



Integrated Systems Solutions Architecture for improving National global chemistry forecasting and assimilation capabilities and evaluation of impact on regional air quality prediction

History

•**January 20, 2005 -** Proposal submitted to NASA NASA CAN NN-H-04-Z-YO-010-C "Decision Support through Earth Science Results" entitled "Improving National global chemistry forecasting and assimilation capabilities and evaluation of the impacts on regional Air Quality Predictions" R. Pierce (NASA)/J. McQueen (NOAA) CO-PIs

•**May 26, 2005** – Proposal rejected, review panel summary states: "The research is high quality but the proposal is more a research proposal than an applications proposal."

•**August 30, 2005** – Negotiated first year funding of descoped proposal focusing on implementation of reduced chemistry into GFS.

•**June 2006 -** First year funding sent to LaRC, work on reduced chemistry initiated. Amendment to the Memorandum of Agreement between NASA LaRC and NOAA ESRL/GSD was added to include "Improvements in Air Quality Forecasting with the WRF-Chem Model".

Task Description

Task 1: Development of “reduced chemistry” version of RAQMS chemical mechanism for incorporation into GFS.

Task 2: Preliminary evaluation of the impact of RAQMS reduced and full chemistry BC on regional Air Quality Prediction.

Task 3: Incorporate reduced chemistry into the NOAA GFS.

Task 4: Prototype NOAA assimilation of Aura constituent measurements and provide guidance for operational use of NPP limb scattering measurements

Task 5: Evaluate the impact of improved GFS BC on regional Air Quality Prediction

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Task 5: Evaluate the impact of improved GFS BC on regional Air Quality Prediction

Notes:

1. Descoped proposal focuses on Task 1 and 3
2. Progress on Task 2 associated with INTEX-B and TexAQS field mission work (NASA Atmospheric Composition, Rapid Prototyping)

Task 1. RAQMS unified (strat/trop) chemistry

(55 species/families explicitly transported, 86 calculated, PCE assumptions for "fast" species)

1) Ox
2) Noy
3) Cly
4) Bry
5) HNO3
6) N2O5
7) H2O2
8) HCl
9) ClONO2
10) OClO
11) N2O
12) CFCl3 (F11)
13) CF2Cl2 (F12)
14) CCl4
15) CH3Cl
16) CH3CCl3 (MTCFM)
17) CH3Br
18) CF3Br (H1301)
19) CF2ClBr (H1211)
20) HF
21) CFClO
22) CF2O
23) CH4
24) HNO4
25) HOCl
26) H2O
27) NO3
28) NO2
29) CH2O
30) CH3OOH
31) CO
32) HBr
33) BrONO2
34) HOBr
35) BrCl
36) Cl2

Stratosphere+CH4&CO oxidation

37) C2H6 (ethane, 2C)
38) ALD2 (acetaldehyde+higher group, 2C)
39) ETHOOH (ethyl hydrogen peroxide, 2C)
40) PAN (2C)
41) PAR (paraffin carbon bond group, 1C)
42) ONIT (organic nitrate group, 1C)
43) AONE (acetone, 3C)
44) ROOH (C3+hydrogen peroxides group, 1C)
45) MGLY (methylglyoxal, 3C)
46) ETH (ethene, 2C)
47) XOLET (terminal olefin carbon group, 2C)
48) XOLEI (internal olefin carbon group, 2C)
49) XISOP (isoprene, 5C)
50) XISOPRD (isoprene oxidation product-long lived, 5C)
51) PROP_PAR (propane paraffin, 1C)
52) CH3OH (methanol)
53) XMVK (methyl vinyl ketone, 4C)
54) XMACR (methacrolein, 4C)
55) XMPAN (peroxymethacryloyl nitrate, 4C)

NMHC Chemistry

Chemical families

Ox=O(1D)+O(3P)+O3+NO2+HNO3+2(NO3)+3(N2O5)+HNO4+PAN+MPAN
NOy=N+NO+NO2+NO3+2(N2O5)+HNO3+HNO4+BrNO3+ClNO3+PAN+ONIT+MPAN
Cly=HCl+ClONO2+ClO+2(Cl2O2)+OClO+ClO2+2(Cl2)+BrCl+HOCl+Cl
Bry=HBr+BrONO2+BrO+BrCl+HOBr+Br

Task 1. RAQMS reduced (strat/trop) chemistry

(12 species/families explicitly transported, 3 species and ClOx/BrOx loss from climatologies)

1) Ox
2) NOy
3)
4)
5) HNO3
6) N2O5
7) H2O2
8)
9) ClONO2
10)
11) N2O
12)
13)
14)
15)
16)
17)
18)

19)
20)
21)
22)
23) CH4
24) HNO4
25)
26) H2O
27) NO3
28) NO2
29) CH2O
30) CH3OOH
31) CO
32)
33)
34)
35)
36)

37) C2H6 (ethane, 2C)
38) ALD2 (acetaldehyde+higher group, 2C)
39) ETHOOH (ethyl hydrogen peroxide, 2C)
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52) CH3OH (methanol)
53) XMVK (methyl vinyl ketone, 4C)
54) XMACR (methacrolein, 4C)
55) XMPAN (peroxymethacryloyl nitrate, 4C)

Enhance CO emissions with ISOPRENE Source

Ox-HOx-NOx+CH4+CO oxidation

NMHC Chemistry

Chemical families

Ox=O(1D)+O(3P)+O3+NO2+HNO3+2(NO3)+3(N2O5)+HNO4

NOy=N+NO+NO2+NO3+2(N2O5)+HNO3+HNO4+ClNO3

Climatological Species:
ClONO2, N2O, CH4

Transported Species:
Ox, NOy, HNO3, N2O5, HNO4, H2O, NO3, NO2, CO, H2O2, CH2O, CH3OOH

Task 1. RAQMS reduced (strat/trop) chemistry

(12 species/families explicitly transported, PCE assumptions for “fast” species)

1) Ox
2) NOy
3) HNO3
4) N2O5
5) H2O2
6) HNO4
7) H2O
8) NO3
9) NO2
10) CH2O
11) CH3OOH
12) CO
13) CH4
14) ClONO2
15) N2O

Ox-HOx-NOx+CH4+CO oxidation

NOy partitioning relies on climatological ClNO3*

Stratospheric Bromine and Chlorine Ozone P-L from model* climatology

Chemical families

Ox=O(1D)+O(3P)+O3+NO2+HNO3+2(NO3)+3(N2O5)+HNO4

NOy=N+NO+NO2+NO3+2(N2O5)+HNO3+HNO4+ClNO3

Transported Species:

Ox, NOy, HNO3, N2O5, HNO4, H2O, NO3, NO2, CO, H2O2, CH2O, CH3OOH

Climatological Species:

ClONO2, N2O, CH4

***LaRC IMPACT coupled chemistry/dynamics model (Al-Saadi et al., 2004, Pierce et al., 2000)**

Regression Analysis using IMPACT Model Results

- Long lived species (CH4 and N2O)
  - Mixing ratio as function of potential temperature and potential vorticity
  - Bi-weekly, separate regressions for northern and southern hemispheres

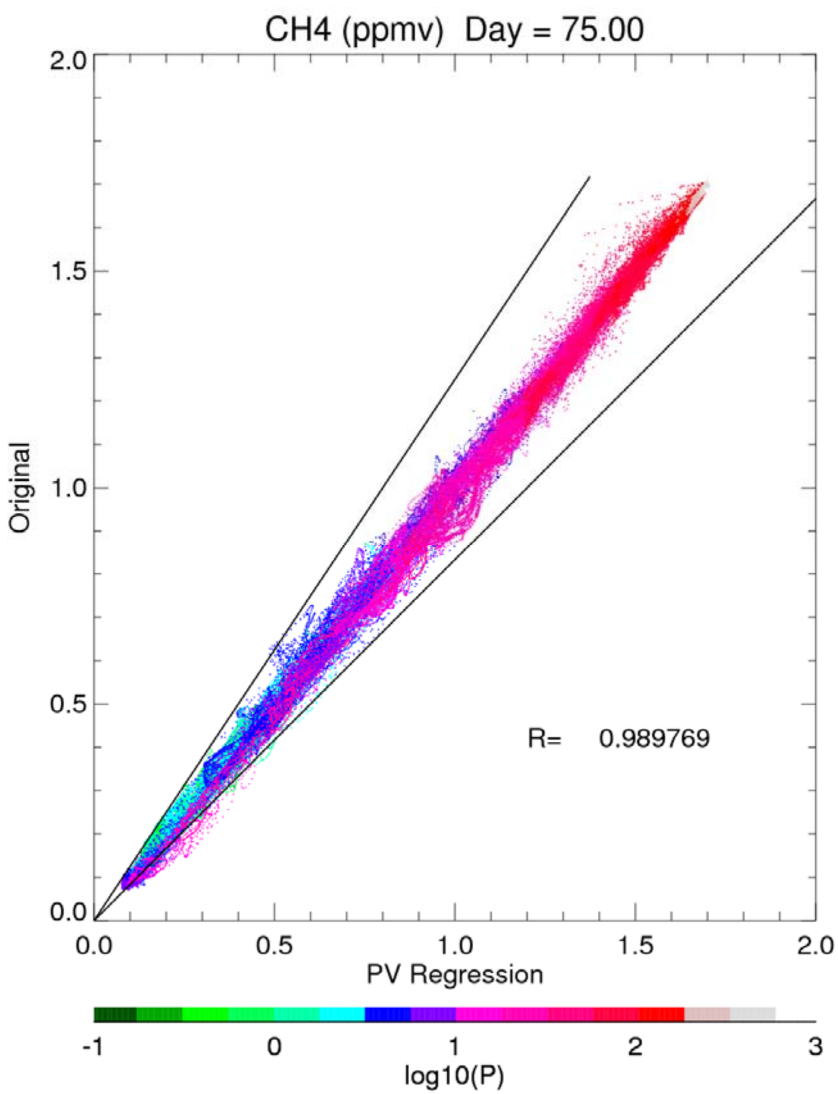
- Short lived species (ClONO2)
  - Mixing ratio as function of potential temperature and potential vorticity, followed by adjustment of the residual as a function of zenith angle
  - Bi-weekly, separate regressions for northern and southern hemisphere, morning (midnight to noon) and evening (noon to midnight)
  - Polar vortex region treated separately

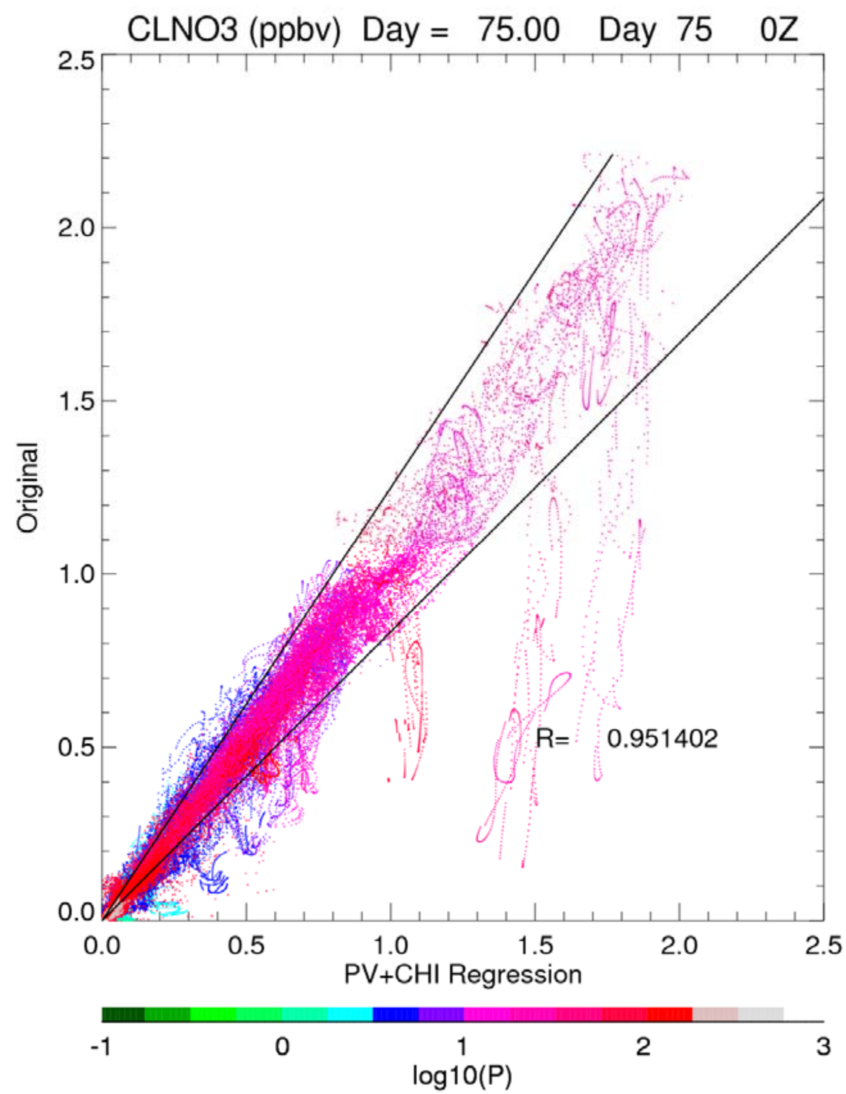
- Production and loss rates of odd oxygen due to chlorine and bromine cycles
  - Rate as a function of potential temperature and zenith angle
  - Bi-weekly, Northern/Southern hemispheres, Morning/Evening
  - Polar vortex region treated separately

Evaluation of regressions: mid-March

Solid lines show +/-20%

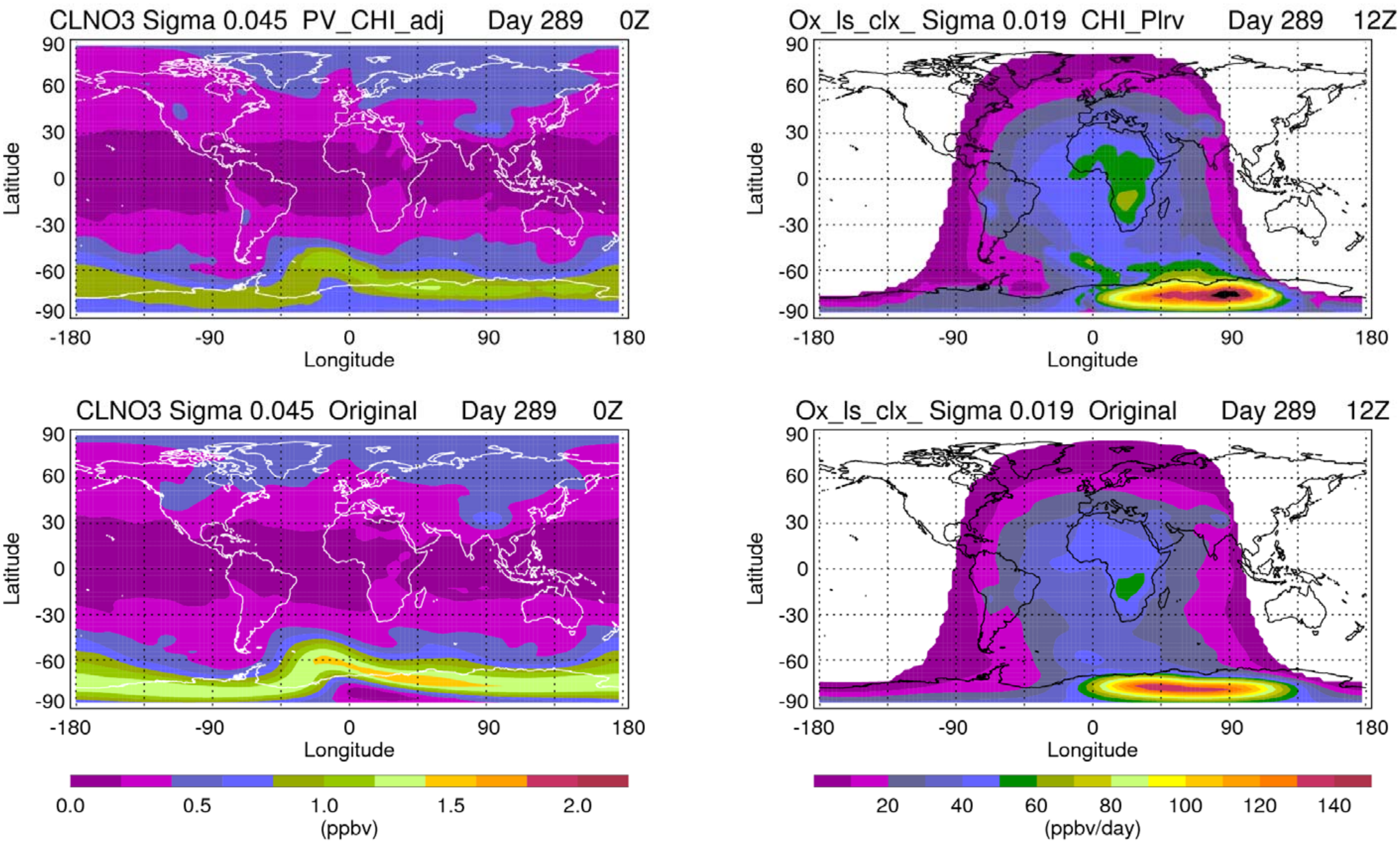
Reconstructions are highly correlated with reference values for both long- and short-lived species





Evaluation of regressions: mid-October

Structure associated with Antarctic polar vortex and spring ozone loss is reproduced



Task 3: Incorporate reduced chemistry into the NOAA GFS

•Incorporation of grid-scale and sub-grid-scale chemical transport into GFS.
Test GFS O3 and CO predictions using P-L from RAQMS full-chemistry.
July-September 2004 (period of the NASA/NOAA ICARTT experiment)

•Collaboration with E. Kalnay and I. Syunyogh, UM College Park (UM-CP)
(Thesis work of Dave Kuhl, UM-College Park/NASA LaRC through NIA)

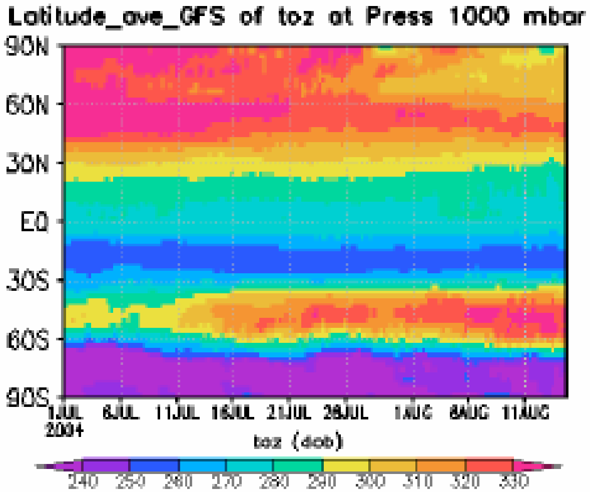
•GFS Resolution T62 with 28 levels in the vertical (frozen October, 2004) using
6hr averaged production and loss rates of ozone and CO from the RAQMS model

O3 and CO Forecasts

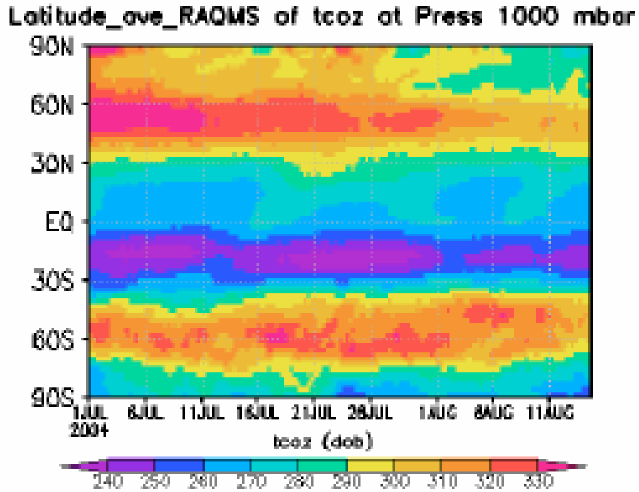
•6hr met forecast updated with NOAA GDAS meteorological fields
•O3 and CO IC from RAQMS
•Forecasted O3 and CO carried over to next meteorological forecast cycle.

Total Column Ozone (Analysis)

GFS Analysis
GFS O3 & Climate P/L



RAQMS Analysis
RAQMS O3 & RAQMS P/L

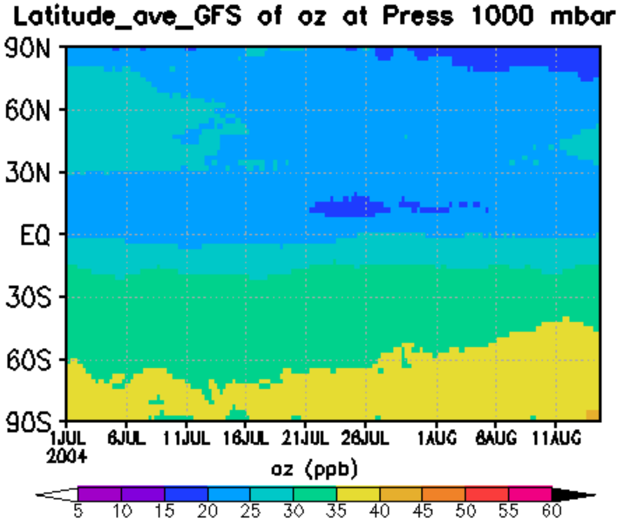


GFS Analysis: GFS ozone assimilated every 6 hours from SBUV/2 data.

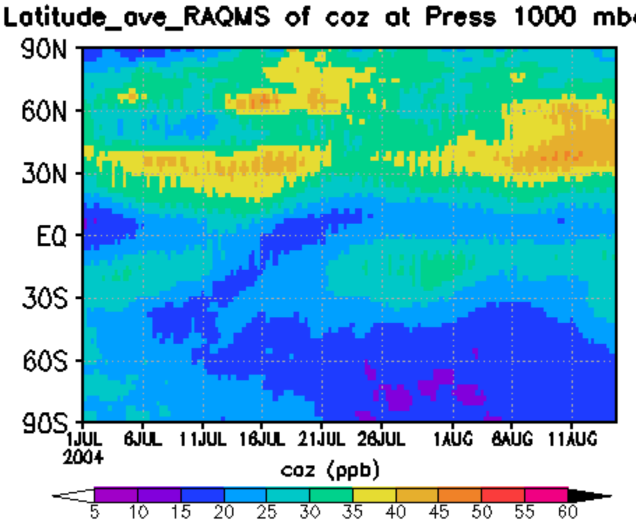
RAQMS Analysis: Ozone assimilated every 6 hours from TOMS, HALOE, SAGE II, and SAGE III.

Surface Ozone (Analysis)

GFS Analysis (SBUV Assim)

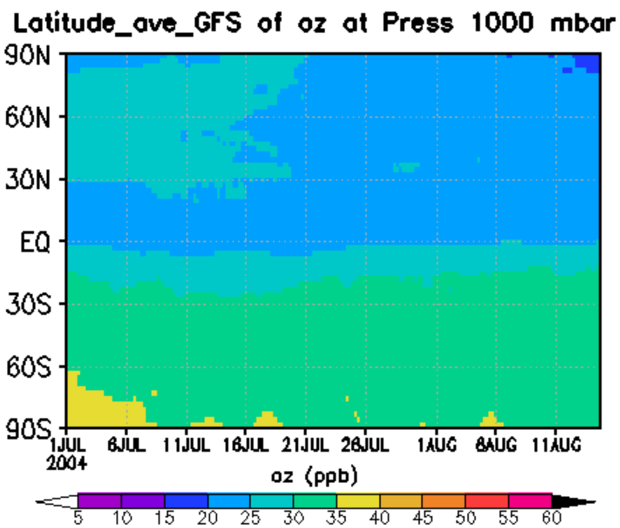


RAQMS Analysis (3D+TOMS Assim)

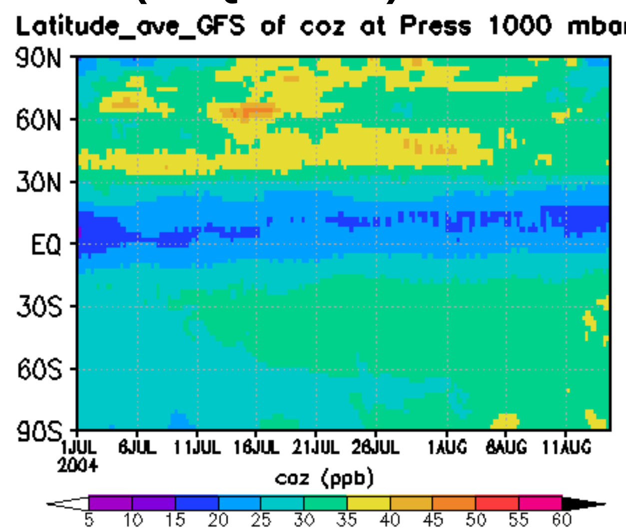


Surface Ozone (Forecast)

GFS Forecast
(Climatological P-L)

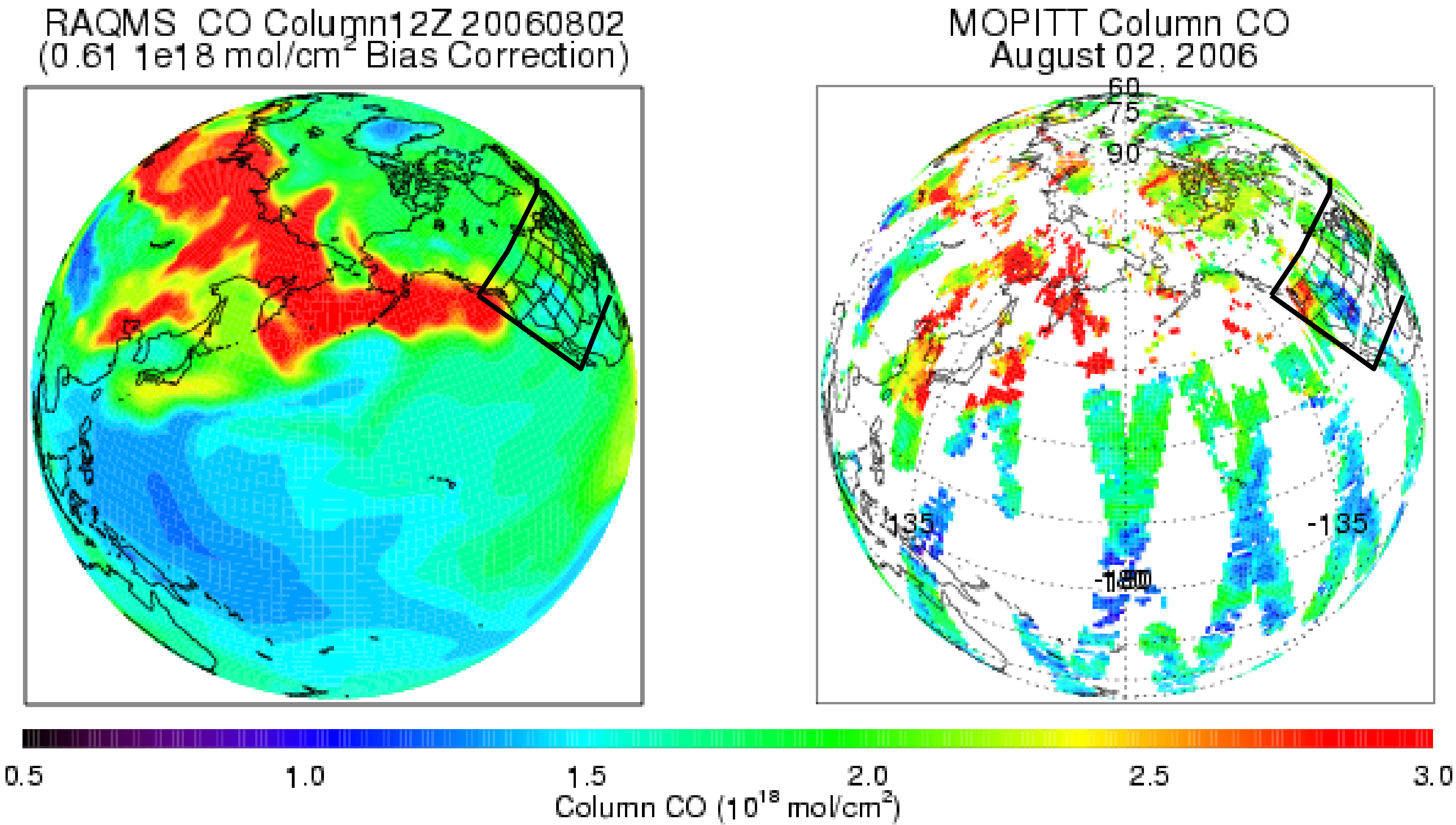


GFS Forecast
(RAQMS P-L)

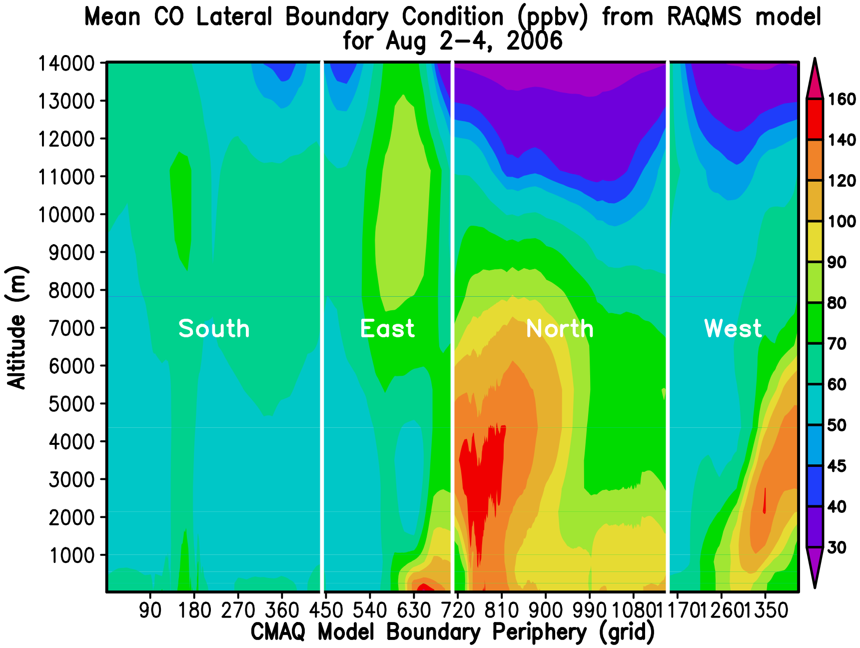


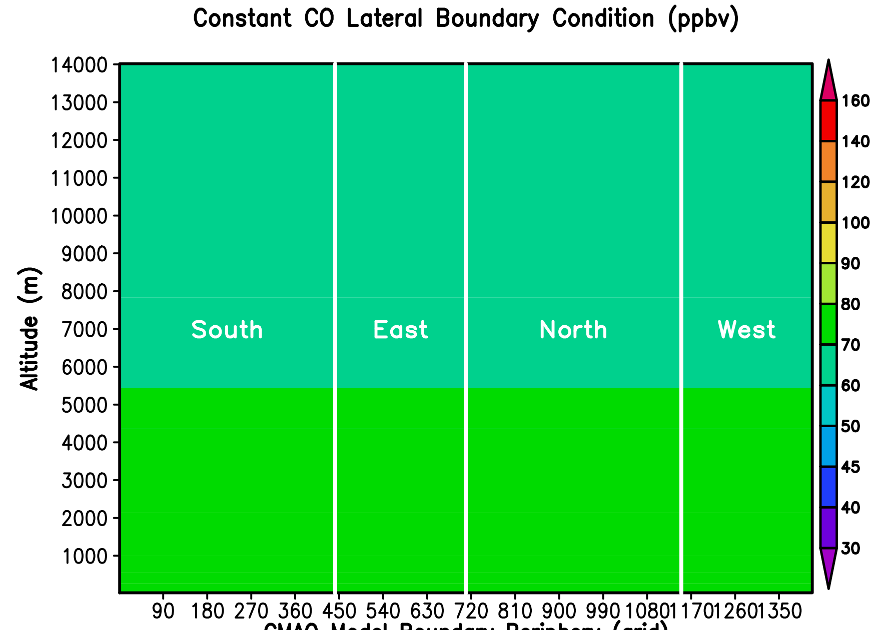
Task 2. Evaluation of chemical lateral boundary conditions on air quality forecast

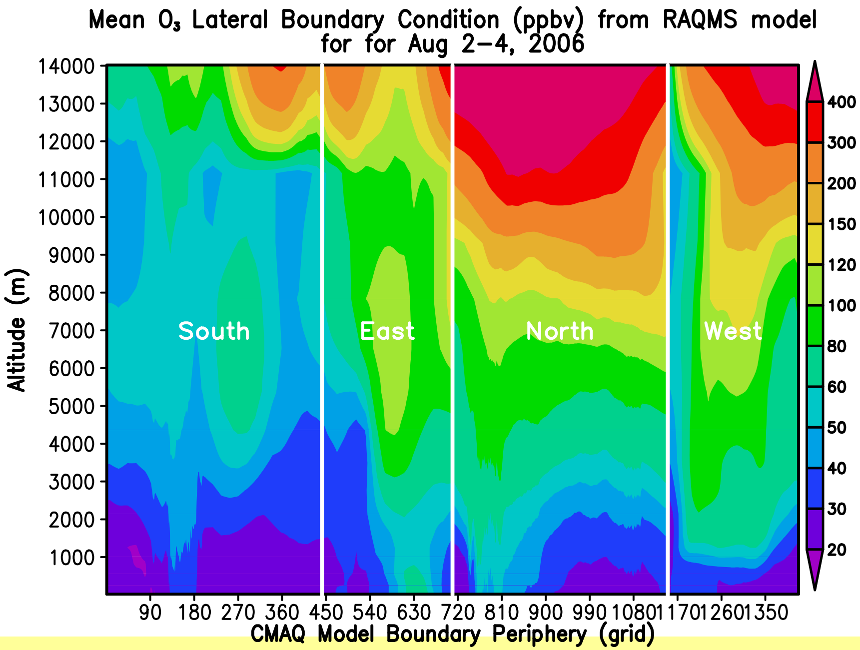
Case study analyzing whether long-range transport of Siberian wildfire emissions could impact Continental US (CONUS) Air Quality during forecast period

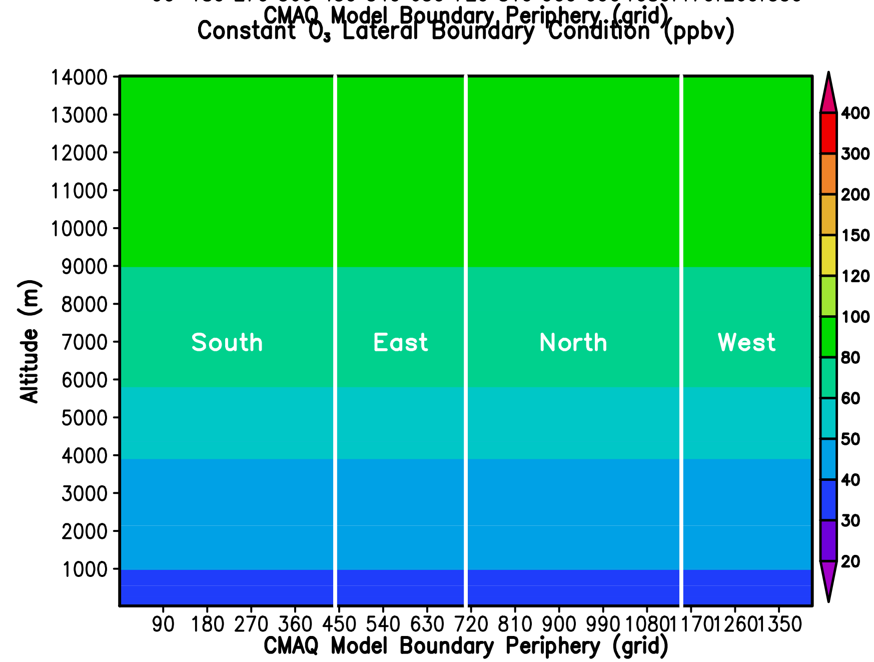


Both RAQMS and MOPITT show enhancements in column carbon monoxide (CO) across N. Pacific on August 02, 2006 due to eastward transport of emissions from Siberian wild fires. RAQMS tends to underestimate background CO concentrations relative to MOPITT. NOAA/NWS pre-operational NMM-CMAQ domain in black.





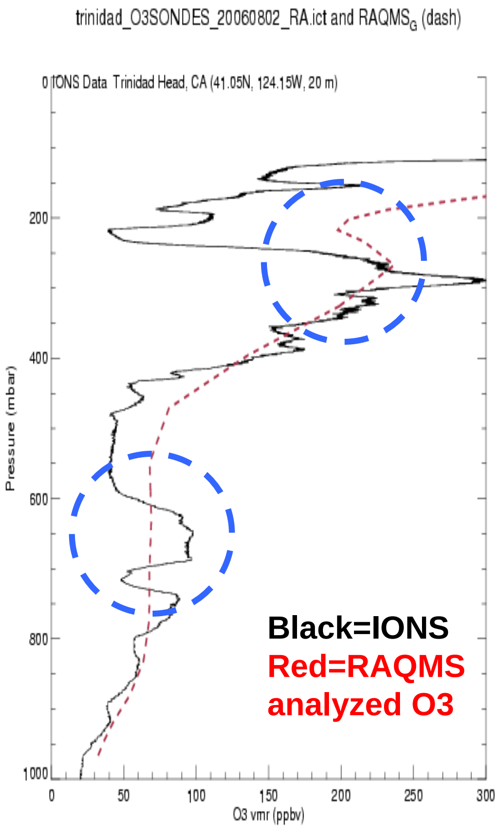


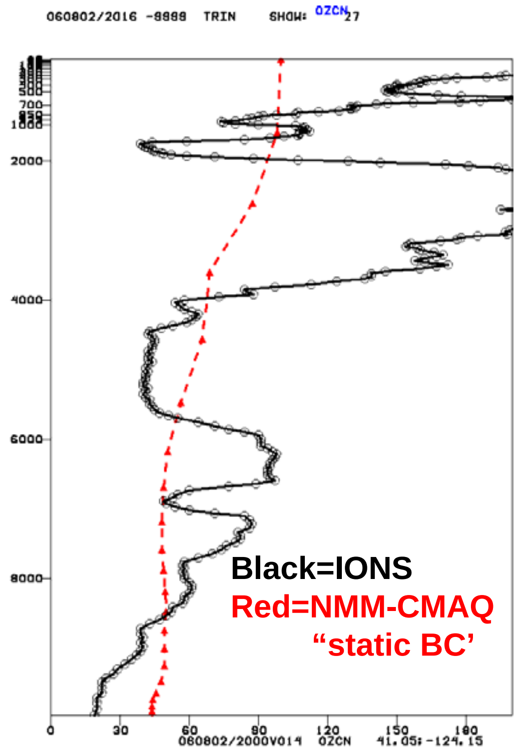


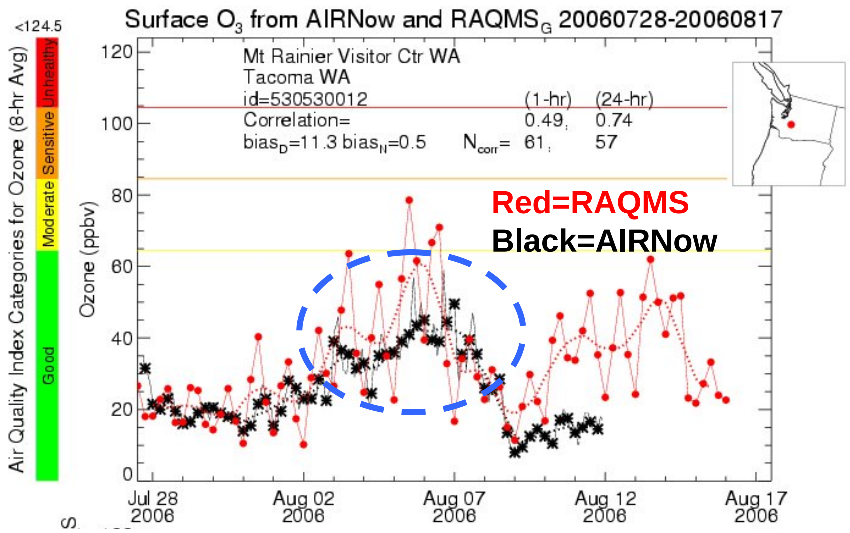
The global analysis provides large-scale information along inflow boundaries in horizontal and vertical directions for the NOAA/NWS pre-operational NMM-CMAQ.

•Significant ozone enhancements observed aloft and in lower troposphere at Trinidad Head, CA on August 02, 2006

•Associated increase in RAQMS analyzed and observed surface ozone at downwind remote AIRNow sites (e.g., Mt. Rainier, WA) during forecast period



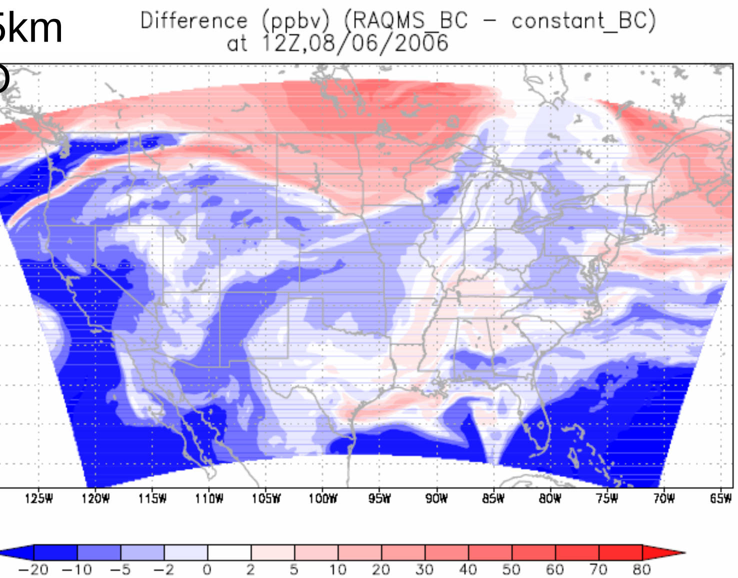




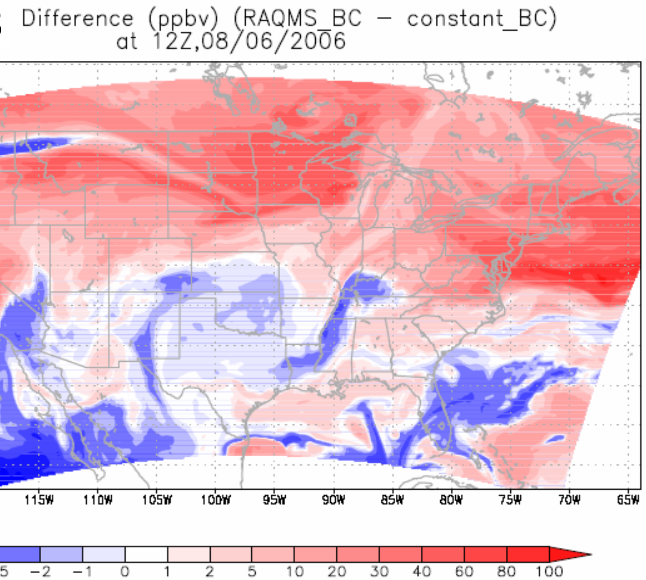
Both RAQMS analyzed O3 and IONS ozonesonde show enhancements in ozone (O3) along Pacific coast on August 02, 2006. The "static boundary condition" NMM-CMAQ profile does not account for these enhancements.

NOAA/NWS NMM-CMAQ 96hr FX (*pre-operational*): Effect of RAQMS BCs

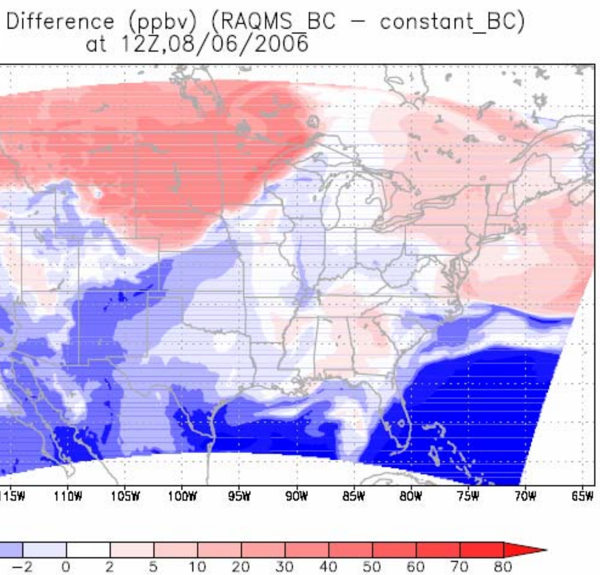
3.5km CO



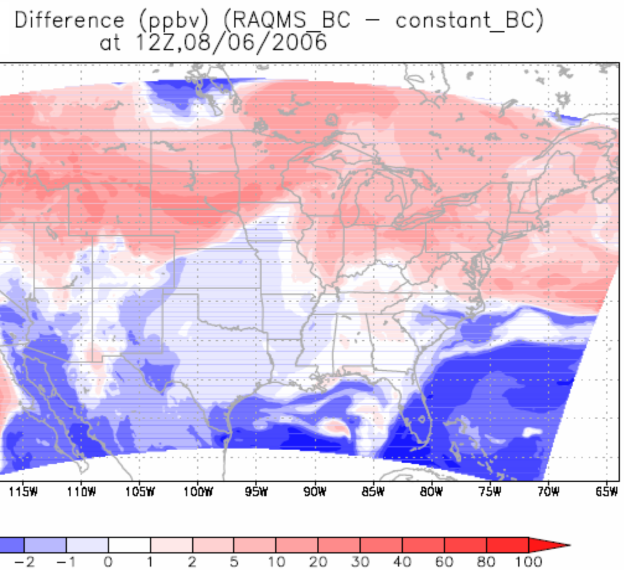
3.5km O3



Surface CO



Surface O3



Surface O_3 increased 5-20ppbv (10-60%) and surface CO increases 20-40ppbv (50-100%) north of 35°N. Forecasted O_3 and CO show slight decrease over Southern US and S.W. Atlantic.

Summary

•Ready to test reduced chemistry in RAQMS (2006 TexAQS case studies). Suitable regressions have been developed for all species and ozone-production tendencies that will not be explicitly represented.

•UM-CP GFS CO prediction (using RAQMS P-L) is in good agreement with RAQMS (verification of implementation of generalized 4-D P-L)

•UM-CP GFS O3 prediction (using RAQMS P-L) overestimates ozone in southern hemisphere marine boundary and underestimates stratospheric ozone maximum (insufficient stratospheric vertical resolution in UM-CP version GFS)

•Have prototyped linkage between global assimilation system (RAQMS) and NOAA/NWS CONUS forecast system (pre-operational) by leveraging TexAQS field mission activities

Decision points and suggested revisions to Task plan

Should we continue development and testing of reduced chemistry in UM-CP version of GFS (at LaRC) or should testing be conduced on more recent version of GFS?

Assimilation of TES + OMI ozone on Aura as proxy data set for AIRS or IASI + OMPS ozone for NPOESS risk mitigation.

Focus on August-October 2006 for development time-period (NOAA TexAQS mission) to leverage current CMAQ-ETA, WRF-Chem, and RAQMS post mission analyses

- October 2006: Period of record Antarctic ozone hole
- August 2006: Extensive continental US ozonesondes for model verification

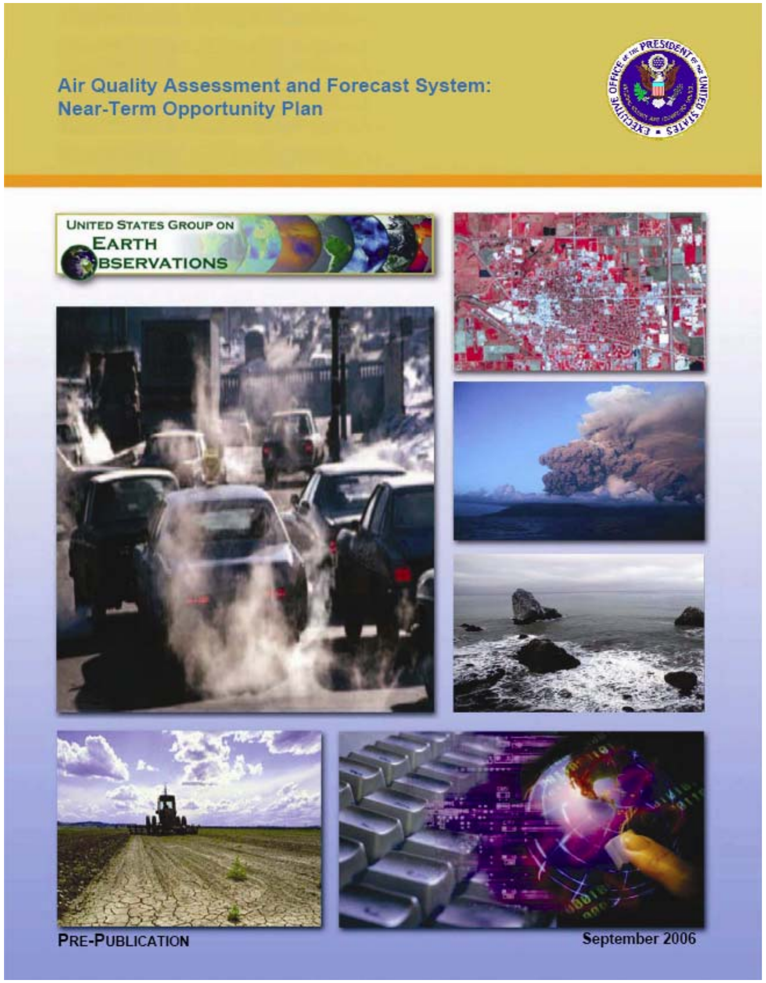
GFS Project Addresses National US-GEO Priorities

http://usgeo.gov/docs/nto/Air_Quality_NTO_2006-0925.pdf

1. PREFACE

This plan was prepared by the U.S. Group on Earth Observations[1] and is one of six near-term opportunities identified in the *Strategic Plan for the U.S. Integrated Earth Observation System.*[2] Near-term opportunities in this context are identifying observing systems or integration of components that meet high-priority societal needs, and making improvements to update existing systems that can be completed within 5 years and have tangible, measurable results. The near-term opportunities are:

- Improved Observations for Disaster Warnings (published September 2006);
- Global Land Observation System (in development);
- Sea Level Observation System (in development);
- National Integrated Drought Information System (published September 2006);
- Air Quality Assessment and Forecast System (published September 2006); and
- Architecture and Data Management (in development).



4. SYSTEMS FOR UTILIZING OBSERVATIONS TO IMPROVE AIR QUALITY FORECASTS

4.1 Need and Rationale

A number of state and local governments issue air quality forecasts and alerts to try to reduce the severity of poor air quality episodes (e.g., by urging residents to decrease driving) and to help the public protect themselves (e.g., by staying indoors or reducing physical activity). Air quality forecasters routinely use surface air quality observations to inform their forecasts; however, this approach does not adequately incorporate transport and other processes affecting air quality. NOAA's operational air quality forecast guidance provides prognostic information for forecasters, but the current operational model does not incorporate air quality observations. The air quality forecast system uses an emissions inventory and the chemical state of the atmosphere predicted by the last simulation as the chemical basis for predictions, which might not accurately represent the actual state of the atmosphere. Errors in one day's forecasts of the chemical state of the atmosphere may be propagated to a second day's forecasts.

Utilization of Real-Time Air Quality Observations in Regional Air Quality Models

Observations offer great potential for improving air quality forecasts by enabling air quality models to more accurately represent actual conditions. Observations can be used in several ways. Information about episodic and unpredictable emissions sources, such as biomass burning, can fill gaps in emissions inputs into air quality models. Observations of ambient conditions along a model's boundary can be used to improve information about pollutants such as intercontinental dust clouds flowing into the model's domain. Finally, air quality observations within the model's domain can be dynamically assimilated into the model to guide the initial state of a forecast to more closely match reality. In the future, improvements such as these will be incorporated into operational ozone and particulate matter forecast models.

Primary Existing Systems include:

- **HYbrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) Smoke Forecast Guidance Demo Project (NOAA).** Using biomass burning locations identified by the Hazard Mapping System, this prototype uses the USDA BlueSky fire emissions model and NOAA's HYSPLIT transport model to predict smoke plume locations.
- **IDEA AOD Trajectories (NASA, EPA, and NOAA).** The IDEA project also includes a prototype product that forecasts where areas of high PM may be transported.
- **Regional Air Quality Modeling System (RAQMS) (NASA).** This research system assimilates global satellite observations of ozone into a global model to provide improved boundary conditions for regional air quality models.
- **STEM-II Model (NSF and others).** This research air quality model assimilates surface air quality observations and has demonstrated that such assimilation can improve air quality forecasts, but this work is at an early stage.

Gaps include:

- **Prototype Air Quality Data Assimilation System (NOAA in consultation with EPA).** This will demonstrate the capabilities required to dynamically assimilate real-time air quality observations into operational regional air quality models. This will include enhanced observational data quality control, characterizing errors in observations and models, eliminating biases, and developing data assimilation algorithms and analysis software.