Chemical data assimilation of ozone and fine aerosols. Some results using ARW-WRF/Chem and the GSI

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- Why and what
- Results
- Summary and future plans

- For air quality forecasting, the initial chemistry fields are usually forecasts from older runs, so errors will accumulate
- By using an online modeling system, producing an optimal initial state of weather and chemistry, forecasts of both may be improved
- A better analysis state for chemistry will also improve the meteorological analysis and therefore prediction of weather – better use of satellite data

#### From ECMWF: Operational Data Requirements: The Importance of Atmospheric Composition

In addition to reactive and greenhouse gases:

- Aerosols: Modelling and assimilation of aerosols is an emerging issue for accurate NWP. Neglect of aerosol in NWP can lead to errors of
  - 25W/m\*\*2 in clear-sky radiation calculations
  - 0.1-0.5K error in forward Radiation Transfer (RT, like CRTM) calculations in assimilation

The prediction and assimilation of aerosol is important for meteorological data assimilation

# What do you do?

- Get funding
- Get the analysis system to run that your funding agency wants you to use
  - GSI for us
- Hope that with some effort it can handle an additional variable
  - O3 and PM2.5 for us
- Using many runs to calculate statistics from your modeling system to provide background error covariances and length scales
  - NEAQS2004 test-bed data set
- Use a different test bed data set to explore the differences of runs with and without assimilation ("evaluation")
  - TEXAS 2006 field experiment
  - PM2.5 increments will be provided that have to be distributed among the pm species

### NMC method application for GSI

- Parish and Derber(1992) proxy for model errors
- Calculate difference between Forecast<sub>1</sub>(t=t<sub>1</sub>+2dt) and Forecast<sub>2</sub>(t=t<sub>2</sub>+dt) valid at the same time over a month/season (usually dt=12h or 24h)
- Calculate covariances, correlations and variances
- Bin correlations according to the distance between gridpoints
- Find characteristic lengthscale *L* of correlations by fitting a Gaussian curve exp  $(-x^2/L^2)$

Hollingsworth-Lonnberg method

- Calculate differences between forecasts and observations
- Calculate covariances, correlations and variances
- Bin correlations according to the distance between gridpoints
- Find characteristic lengthscale of correlations by fitting a function (here Gaussian curve)
- Can be used to compare/tune variances and lengthscales obtained with the NMC method
- In air quality measurements of species usually available only at the surface



### **Observations and model**







Real-time ozone and PM2.5 measurements network AIRNow

ARW WRF-Chem updated version 3.0 Grid length ~27 km, 34 vertical levels

Background error covariance derived from continuous forecasts issued at 00 UTC in August 2004 using NMC method (differences between forecasts at 24 and 48 hours)

24-hour assimilation cycles and evaluation performed in August of 2006

#### Currently rerunning this with V3.1.1,12h cycle, aircraft observations

### Length Scales

Horizontal and vertical length scales derived from the NEAQS2004 data set



WRF was run with dx=27km, RADM and RACM gas phase chemistry and MADE/SORGAM as well as GOCART aerosols

O3: forecast 8-hr maximum mixing ratios averaged over Aug 12-30, 2006



O3: forecast 8-hr maximum mixing ratios averaged over Aug 12-30, 2006



O3: next day 8-hr average maximum concentration, Aug 12-30, 2006



0.0

0.2

0.4

0.8

0.6

1.0

Correlation

O3: next day 8-hr average maximum concentration, Aug 12-30, 2006





PM2.5: 24-hr average concentration, Aug 11-30, 2006



PM2.5: 24-hr average concentration, Aug 11-30, 2006

4 to 8

>16

-80

-90

8 to 12

12 to 16

-70







#### PM2.5: 24-hr average concentration, Aug 11-30, 2006



# Summary

Experiments with 3DVAR chemical data assimilation show that even ozone forecasts may be improved. Results based on using NCEP's Grid Point Statistical Interpolation (GSI) analysis system and ARW-WRF/Chem

- For ozone this is somewhat surprising (because of strong dependence on time of day, sunlight, and chemistry
- PM forecasts are improved <u>drastically</u>

- Evaluation of effect of other in-situ observations (ozone soundings, aircraft observations of ozone and PM2.5) on forecasts as well as higher time resolution cycling when using 3DVAR and WRFV3.1.1
  - Initial results from 12hr cycle indicate no further improvement in ozone forecasts
- Kalman Filter with ensembles based on emissions
  - factors to account for uncertainty in emissions, sampling using logarithmic distributions with standard deviations ratios
- Use the Rapid Refresh with aerosol assimilation and aerosol forecasts
  - In the future maybe we can try to estimate the impact on meteorological assimilation
  - Produce not only PM2.5 forecasts but also more accurate visibility forecasts

## More Distant Future

- OSSE's ?
- Adjoint of simplified WRF/Chem
  - Start with Met-WRF adjoint and GOCART chemistry
- 4dvar, collaboration Greg Carmichael (U of Iowa), Daven Henze (CU), and Scott Spak (U of Iowa), and ESRL/GSD