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
Objectives

- 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.
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
Background error covariance

NMC method application for GSI

- Parish and Derber (1992) - proxy for model errors
- Calculate difference between $\text{Forecast}_1(t=t_1+2dt)$ and $\text{Forecast}_2(t=t_2+dt)$ 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 $\exp\left(-\frac{x^2}{L^2}\right)$
Background error covariance

Hollingsworth-Lonnberg method

- Calculate differences between forecasts and observations
- Calculate covariances, correlations and variances
- Bin correlations according to the distance between gridpoints
- Find characteristic lengthscales 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 $dx=27\text{km}$, RADM and RACM gas phase chemistry and MADE/SORGAM as well as GOCART aerosols
Results

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

Mean bias
Results

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

RMSE
Results

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

Correlation
Results

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

PM2.5: 24-hour forecasts at 00 UTC, Aug 11-30, 2006
Results

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

Mean bias
Results

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

RMSE
Results

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

Correlation
Results

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