Ozone Data Assimilation with WRF-CHEM model: Year 1 Midterm Status

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Overview:

- Goals and necessity of research
- Research content
- Status and accomplishments
- Future plan

Problem

Atmospheric gases and aerosols have complex interactions that are impacted by natural and human source such as traffic, power generation, industry and agriculture

Trace gases and aerosols interact with climate and weather by their direct impact on radiation, and by indirect impacts on clouds

- Implications on air quality and long-range pollution transport
- Need to develop a system for prediction of transboundary air-pollution at regional scales

Necessity of research

- Prepare for utilizing new high-resolution atmospheric chemistry observations from the Korean environmental satellite GEMS
- Employ a coupled atmosphere-chemistry model with explicitly resolved microphysics to account for high-resolution transboundary interactions
- Prediction model and observations are optimally combined in data assimilation, which provides an optimal estimate of the state of the atmosphere-chemistry system and its uncertainty.
- Advanced data assimilation is required due to

  - Complexity of processes at high-resolution,
  - Nonlinear atmosphere-chemistry interactions and satellite observations, and
  - Flow-dependent nature of uncertainties

- The choice of prediction model is WRF-CHEM
  - includes interaction between atmospheric conditions and chemistry at scales relevant to transboundary air-pollution

- The choice of data assimilation is MLEF (Maximum Likelihood Ensemble Filter)
  - Hybrid ensemble-variational method
  - Suitable for nonlinear observations and high-resolution applications

Research goals

- **Main goal of this multi-year project is to develop a chemical transport data assimilation system for assimilation of data from the new Korean environmental satellite GEMS**

- **First year goals**:

  1- Preliminary design of WRF-CHEM-MLEF data assimilation
  2- Prepare the system for data assimilation of synthetic ozone
  3- Complete design of the preliminary system

- **Following years**:

  - Continue by adding a capability for real ozone observations assimilation and eventually for assimilation of GEMS observations.

Data assimilation considerations

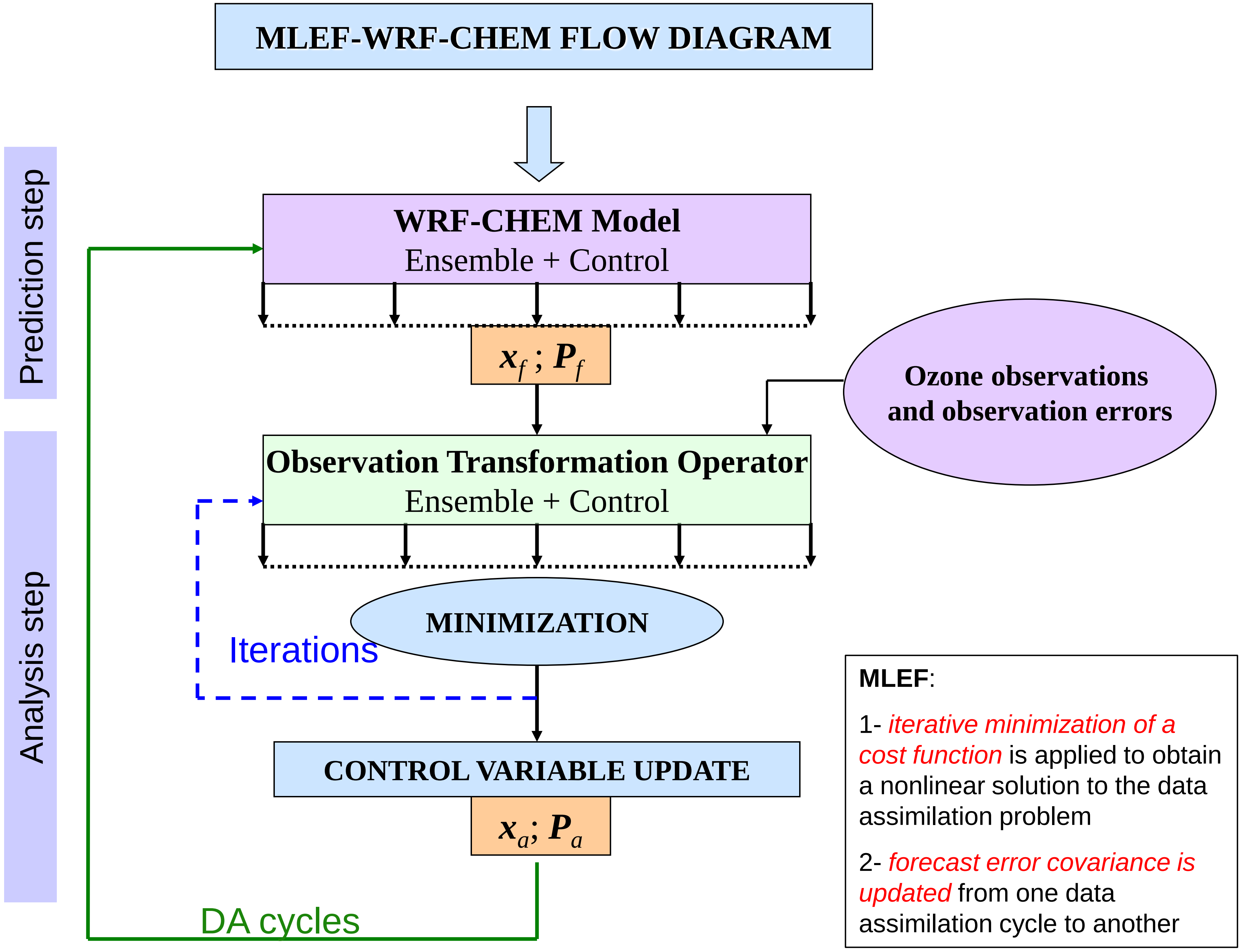
- The method of choice is likely a **hybrid between variational and ensemble methods** since it is preferable that data assimilation system for future GEMS observations has a nonlinear capability and a flow-dependent error covariance.

- The MLEF data assimilation system developed at Colorado State University has these two important components, and has been used in our previous collaborative research (e.g., Kim et al. 2008).

- Since the MLEF has been used with forward component of the NOAA GSI system as observation operator, it has a **capability to assimilate operational weather observations**. This considerably reduces the extent of required preliminary algorithmic development and allows us to focus on developing the capability to assimilate chemistry observations.

- The MLEF has a modular algorithmic structure that allows an **efficient adjustment of the code** in relation to possible chemistry assimilation requirements.

- The MLEF code is also **fully parallelized** using Message Passing Interface (MPI) as well as an additional script-driven parallelization of ensemble calculations.


MLEF-WRF-CHEM FLOW DIAGRAM
Prediction step
WRF-CHEM Model
Ensemble + Control
x_f ; P_f
Ozone observations and observation errors
Analysis step
Observation Transformation Operator
Ensemble + Control
MINIMIZATION
Iterations
CONTROL VARIABLE UPDATE
x_a; P_a
DA cycles
MLEF:
1- iterative minimization of a cost function is applied to obtain a nonlinear solution to the data assimilation problem
2- forecast error covariance is updated from one data assimilation cycle to another

Year 1 (2012)

Research content

- Preliminary development of the MLEF-WRF-CHEM system (first half)
- Preliminary system evaluation in assimilation of synthetic ozone (second half)

Research tasks

1- Preliminary system design

2- Prepare the system for assimilation experiments

3- Complete design of the preliminary system

Preliminary system design

- Focus on developing the capability to assimilate and predict tropospheric ozone.
- Use it as a foundation for the future complete system for assimilation of GEMS observations.
- Pay attention to algorithmic details that will be relevant in the final system:
  - Cycling of data assimilation and automatized data flow
  - Transferability to various computing systems, scalability
- Automatic access to global operational data sets from NOAA (at http://nomads.ncdc.noaa.gov)
  - GFS model data
  - observations (conventional, satellite, ozone)
  - use ‘wget’ to access data files online

Prepare the system for assimilation experiments

- Install WRF-CHEM model on EWHA University computers
- Install MLEF on EWHA University computers
- Install NOAA GSI (forward component) to access real observations
- Develop tropospheric ozone observation operator

  - treat synthetic observations as real, with irregular locations
  - use bilinear interpolation to get model guess
  - user-transparent for processing real or synthetic observations
- Create synthetic ozone observations

  - allow the WRF-CHEM model to be different when used for data assimilation and for creating observations (e.g., implicit representation of model error)
- Interface all above components into a single data assimilation system

Install new codes on EWHA University computers

- EWHA servers ‘weather’ and ‘feedback’
- Install WRF-CHEM model
  - download standard WRF-ARW model
  - download CHEM sub-directory
  - compile WRF with CHEM option
- Install MLEF
  - use the most recent version with improved capability and data flow
  - add PGI compiler option
  - add Little-Endian adjustments (e.g., re-blocking the BUFR input files)
- Install NOAA Gridpoint Statistical Interpolation (GSI) system
  - download GSI
  - add MLEF module for interfacing GSI and MLEF
  - compile the complete MLEF/GSI operator

Creating synthetic ozone observations

- Two setups required:
  1- “Truth”: used to create observations
  2- “DA”: used in data assimilation

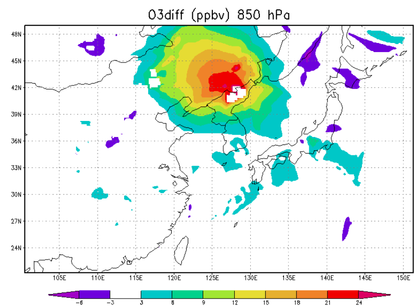
- Ozone observations are created by adding random perturbation to the “Truth” forecast

$$(O3)_{obs} = (O3)_{WRF\text{-}CHEM} + random \times e_{O3}$$

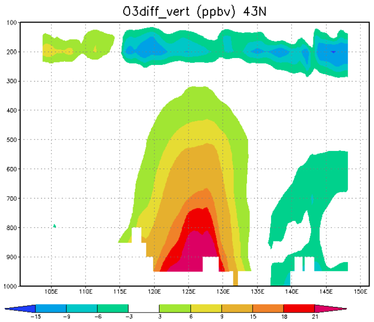
- Difference in initial conditions (IC) between “Truth” and “DA” for all variables
  (a) Atmos and Chem IC differ by choosing the input files lagging 12 hours
  (b) O3 IC additionally differ by a bell-shaped ozone perturbation

Ozone difference at initial time due to (a) and (b)

850 hPa



Vertical cross-section



- The above situation simulates an event characterized by a release of tropospheric ozone that was observed, but not predicted by the modeling system.
- Data assimilation has to be able to utilize ozone observations and re-create the ozone plume that was “observed”.

Complete the design of the preliminary system

- Evaluate the data assimilation performance in assimilation of synthetic ozone

  - Assimilation of synthetic ozone only

  - Assimilation of synthetic ozone and real atmospheric observations

  - Impact of combined atmospheric and chemistry observations allow a more direct exchange of information between atmospheric and chemistry components of the model

  - Choice of control variables includes both atmospheric and chemistry variables

  - Evaluation of data assimilation performance implicitly tests the cross-covariances between atmospheric and chemistry variables, which is fundamental for the future applications and development of the system

Forecast error covariance with WRF-CHEM

Complex inter-variable correlations:

$$P_f = \begin{bmatrix} P_{ATM,ATM} & P_{ATM,CH} \\ P^T_{ATM,CH} & P_{CH,CH} \end{bmatrix}$$

Correlations between **atmospheric** variables

Correlations between **chem** variables

Cross-correlations between Atmos (e.g., **p**, **t**, **v**) and Chem (e.g., **O3, CO2**) variables

$$P_{ATM,CH} = \begin{bmatrix} P_{p,\mathrm{O3}} & P_{t,\mathrm{O3}} & P_{v,\mathrm{O3}} \\ P_{p,\mathrm{CO2}} & P_{t,\mathrm{CO2}} & P_{v,\mathrm{CO2}} \end{bmatrix}$$

- Unknown correlations among chemistry variables and between Atmos and Chem variables
- Advantage for ensemble-based data assimilation since it does not require previous knowledge of correlations, being produced by an ensemble of WRF-CHEM models

Preliminary results: analysis

- Synthetic ozone observations
- WRF-CHEM model with CBMZ chemistry option, resolution 27 km / 28 layers
- 6-hour assimilation period
- DA control variables:

  - wind, specific humidity, perturbation surface pressure, perturbation potential temperature, perturbation height, and ozone concentration

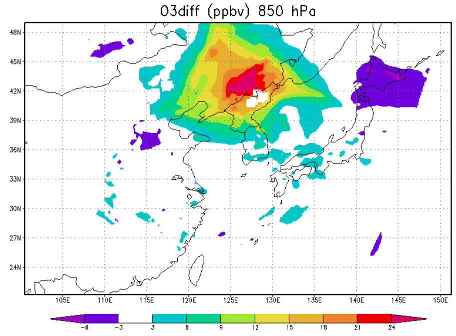
- Experiments:

  - CONTROL: No data assimilation
  - WRF-CHEM-MLEF: Assimilation of synthetic O3 observations with WRF-CHEM-MLEF

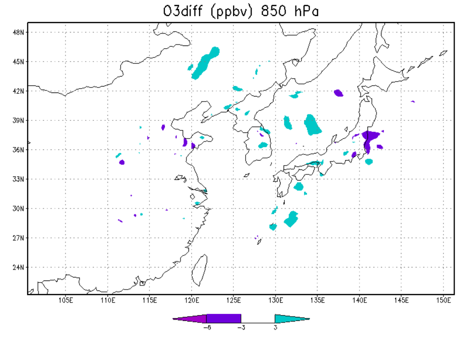
Analysis error

$$x_a - x_{true}$$

CONTROL



WRF-CHEM-MLEF



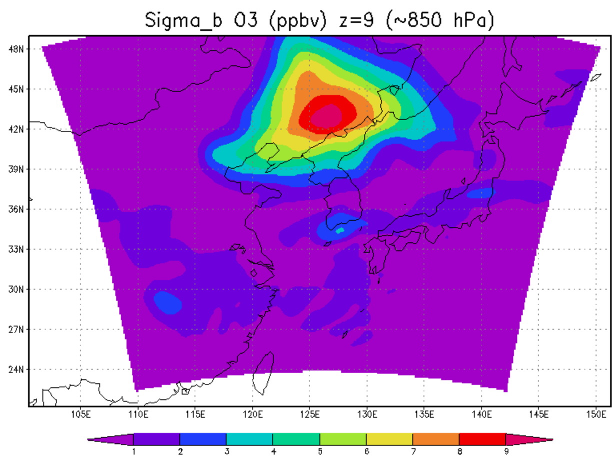
- Preliminary results suggest an improvement of ozone due to data assimilation
- Continue with new cases and observation distribution simulating satellite coverage

Preliminary results: ozone uncertainty

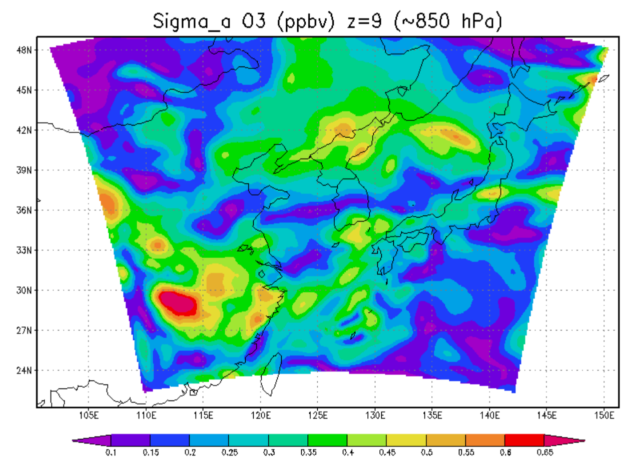
- WRF-CHEM-MLEF system can estimate uncertainties of forecast and analysis
- Important for assessing the confidence in trans-boundary air pollution forecast

Ozone uncertainty at 850 hPa
(valid at the end of the first DA cycle)

6-hour forecast uncertainty



Analysis uncertainty



Reliable estimate of uncertainties:

- Forecast uncertainty: The location of uncertainty coincides with the location of ozone perturbation, and with the actual difference $x_f - x_{true}$
- Analysis uncertainty: An order of magnitude smaller magnitude than forecast uncertainty

Midterm status and accomplishments (October 2012)

- The WRF-CHEM-MLEF system has been installed on EWHA servers ‘*feedback*’ and ‘*weather*’
- Installed MLEF on EWHA University computers
- Installed GSI operator
- The system has been adjusted for assimilation of synthetic ozone observations
- Preliminary tests of the WRF-CHEM-MLEF system have begun

  - results show the anticipated positive impact of synthetic ozone assimilation

  - positive impact of synthetic ozone observations maintained with additional assimilation of real atmospheric observations

Future plan

- Complete experiments with the current setup (e.g., synthetic ozone) using the updated WRF-ARW model (version 4.0) and updated GSI (version 3.1).

- Assimilation of synthetic ozone observations at higher resolution

  - Model used for “Truth” and for creating observations has higher resolution and different microphysics, compared to model used in “DA”
  - Synthetic observation coverage resembles satellite coverage
  - More realistic experiment due to observational coverage and implied model errors

- Preparation for assimilation of real ozone observations

  - GOME/OMI (Global Ozone Monitoring Experiment)
  - SBUV (Solar Backscattered Ultraviolet) ozone
  - initially use the observation operator developed in GSI
  - examine the value of these measurements for tropospheric ozone