Status of Data Assimilation for GEMS
(Ozone Data Assimilation with WRF-CHEM model)

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Overview:

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

Problem and Motivation

- 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.
- **Modeling interaction of trace gases and aerosols with climate and weather** requires employing coupled chemistry-atmosphere models, preferable at cloud-resolving scales**.**
- **Satellite observations** of trace gases and aerosols bring important new information.
- **Advanced data assimilation** is best suited to blend information from satellite chemistry observations and from coupled chemistry-atmosphere models.
- **Regional coupled chemistry-atmosphere data assimilation** has additional complexity due to the interaction between cloud microphysics and trace gases and aerosols, implying high nonlinearity and flow-dependent forecast errors.

The benefits of regional coupled chemistry-atmosphere data assimilation, however are considerable:

- Air quality and long-range pollution transport
- 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**

- **Second year goals**:

  1- Prepare for synthetic chemistry observations
  2- Preliminary assimilation of synthetic chemistry observations
  3- Preliminary system assimilation of combined synthetic chemistry and real atmospheric observations.

- **Following years**:

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

Data assimilation considerations

- The method of choice is a **hybrid variational-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 as well as chemistry observations**.

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

- Assimilation of *synthetic* data helps in early development of the assimilation-forecasting system.

- Assimilation of *real* data is the ultimate test of data assimilation.

- Important to understand **how data assimilation disseminates information from atmospheric and chemistry observations**.

Year 2 (2013)

Research content

- Develop capability to assimilate synthetic chemistry observations: prepare data, observation operator and connect with data assimilation
- Evaluate the preliminary system in assimilation of synthetic chemistry observations
- Perform assessment of the preliminary system in assimilation of combined chemistry and real atmospheric observations.

Research tasks

1- Include trace gases in data assimilation control variable

2- Setup the augmented system for assimilation experiments

3- Evaluate the impact of chemistry pseudo observations on error covariance

Coupled chemistry-atmosphere system design

- Focus on developing the capability to assimilate and predict trace gases responsible for air pollution (e.g., O_3, NO, NO_2, NO_3, SO_2).
- Make initial preparation for assimilation of real observations (chemistry and atmosphere)

  - use forward component of the NCEP Gridpoint Statistical Interpolation (GSI) system to access atmosphere and chemistry observations

- Pay attention to error covariance structure:

  - atmosphere-atmosphere and chemistry-chemistry auto-covariance

  - atmosphere-chemistry cross-covariance

- Make necessary adjustments that facilitate the final goal of assimilating real GEMS satellite observations

  - make the use of observation operator transparent, i.e. minimal impact on the rest of the codes

  - modular code design to allow adding GEMS observation operator in future

Challenges of chemistry Data Assimilation

- Nonlinearity

  - ozone observation operator can be highly nonlinear

  - atmospheric chemistry is nonlinear

- Flow-dependent uncertainties

  - time-dependent, regional and local impact

  - required time-dependent forecast error covariance

- Complexity

  - a chemical interacts with other chemical constituents

  - a chemical interacts with dynamical model variables

  - cross-covariances are important

- Computation

  - high-dimensional regional data assimilation

  - requires MPI and high-performance parallel computing

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

Challenge of coupled chemistry-atmosphere data assimilation: Forecast error covariance

- Proper structure (e.g., correlations) of forecast error covariance is fundamental for data assimilation.
- Dynamical relations between model variables have to be adequately represented in error covariance.

$$P_f = \begin{bmatrix} P_{atm,atm} & P_{atm,chem} \\ P_{atm,chem}^T & P_{chem,chem} \end{bmatrix}$$

Example: (Ensemble) Kalman filter

$$x^a - x^f = P_f H^T \left(H P_f H^T + R \right)^{-1} \left(y - H x^f \right)$$

$$P_f = \sum_i \lambda_i u_i u_i^T \qquad \boxed{x^a - x^f = \sum_i \alpha_i u_i}$$

Analysis increment vector is a linear combination of eigenvectors of forecast error covariance

ASSIMILATION EXPERIMENTS WITH SYNTHETIC (PSEUDO) OBSERVATIONS

- Synoptic case: June 8, 2013
- WRF-CHEM model with CBMZ chemistry option, resolution 27 km / 28 layers
- 6-hour assimilation period
- 4 ensembles
- DA control variables:

  - *atmosphere*: wind, specific humidity, perturbation surface pressure, perturbation potential temperature, perturbation height

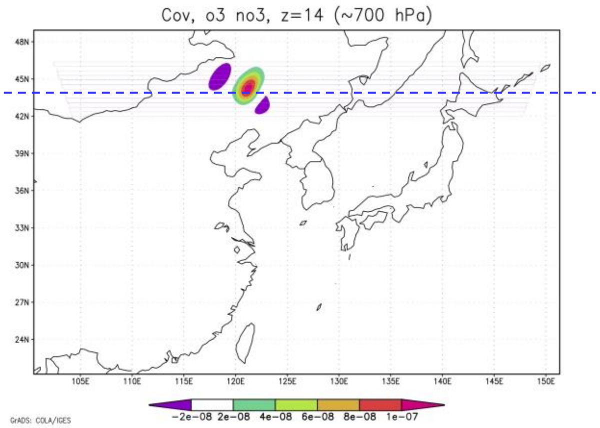
  - *chemistry*: concentrations of ozone (O_3), nitrates (NO, NO_2, NO_3) and sulfur dioxide (SO_2)
- Synthetic ozone (O_3) and nitrate (NO_3) observations
- Single observation experiments to examine the structure of forecast error covariance

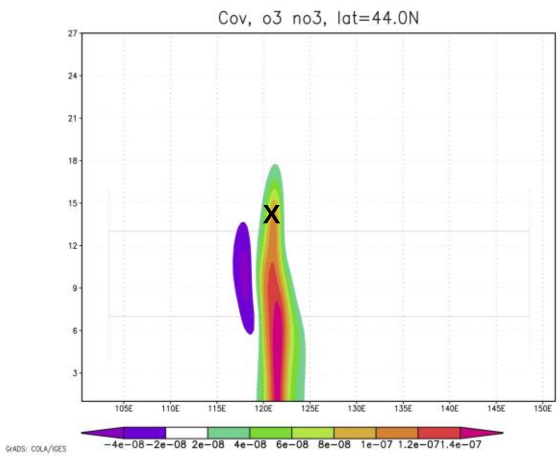
Analysis response (x^a-x^f) to single ozone (O_3) observation at 700 hPa

Horizontal (~700 hPa)

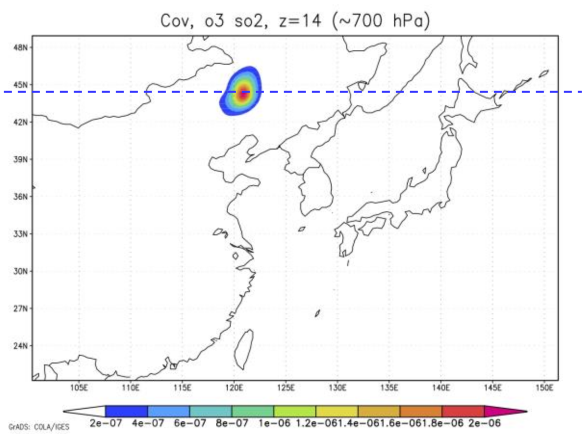
Vertical (~44 N)

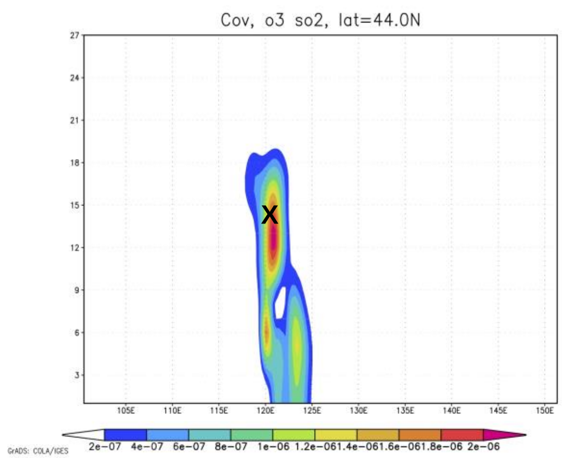
NO_3 analysis response





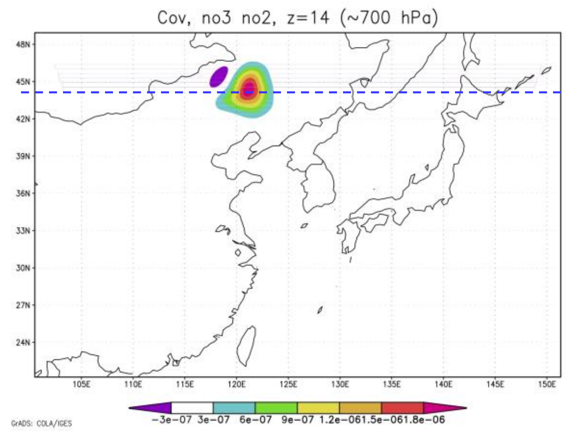
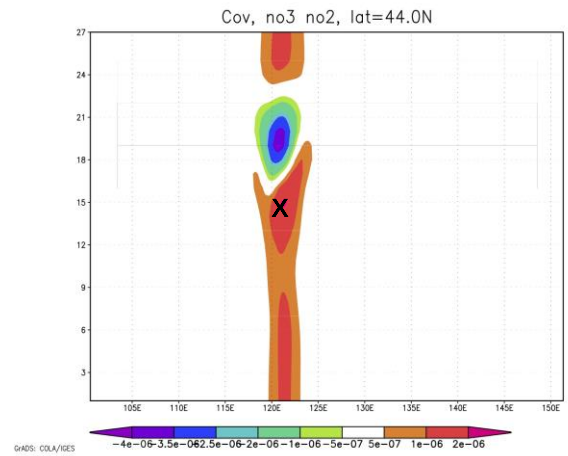
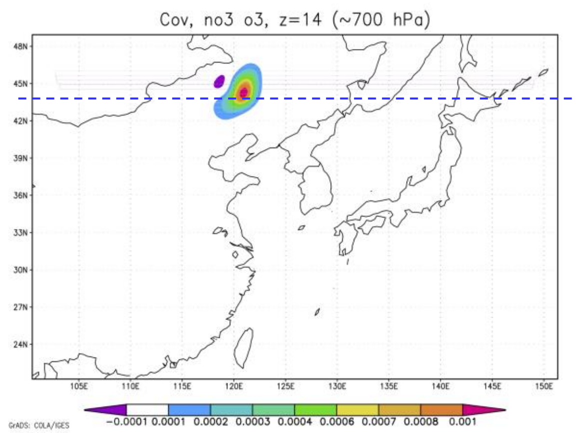
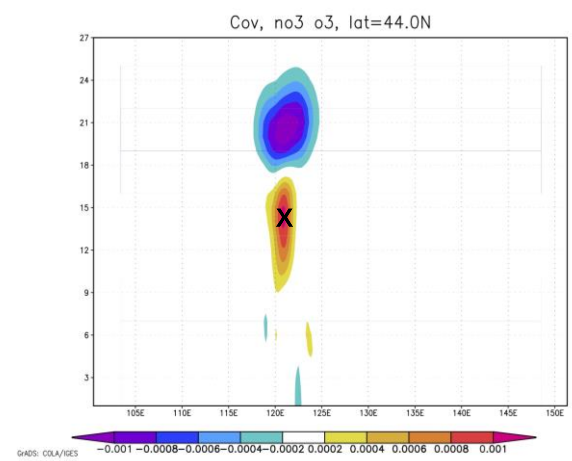
SO_2 analysis response





Ozone observations impact the NO_3 analysis at lower levels, and the SO_2 analysis at the observation level and below.

Analysis response (x^a-x^f) to single nitrate (NO_3) observation at 700 hPa

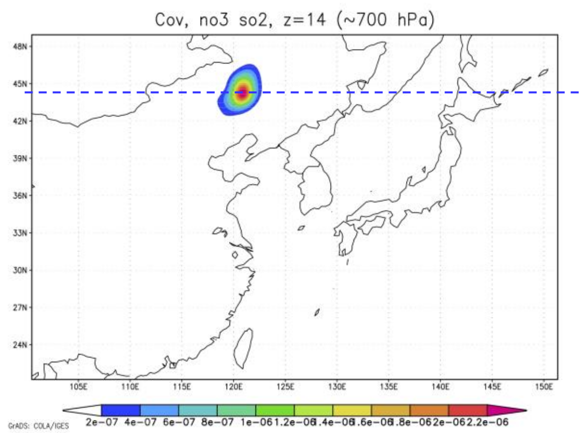
	Horizontal (~700 hPa)	Vertical (~44 N)
NO_2 analysis response		
O_3 analysis response		

Nitrate observations impact the NO_2 analysis at all levels, while the O_3 analysis at the observation level and above.

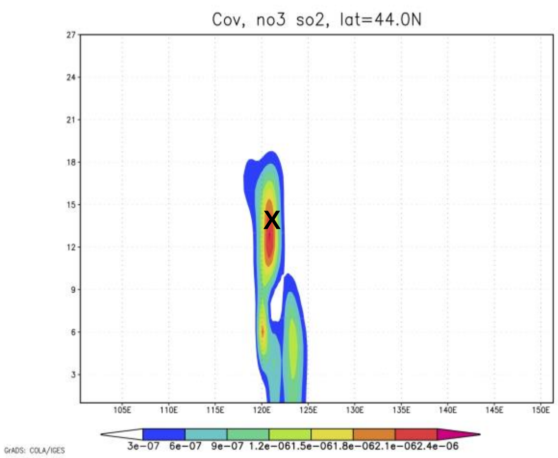
Analysis response (x^a-x^f) to single nitrate (no3) observation at 700 hPa

SO$_2$ analysis response

Horizontal (~700 hPa)



Vertical (~44 N)



Nitrate observations impact the SO$_2$ analysis at the observation level and below, indicating that future satellite observations of NO$_3$ at high levels would have an immediate impact on SO$_2$ at low levels due to data assimilation.

Summary of synthetic observation experiments

- WRF-CHEM-MLEF coupled data assimilation system is successfully tested with augmented chemistry-atmosphere control variable.
- Forecast error covariance structure reflects the complex dynamics of uncertainties.
- Analysis response to synthetic chemistry observations illustrates the coupled data assimilation system response to future real GEMS observations.

Coupled chemistry-atmosphere data assimilation with real atmospheric observations

- Synoptic case: June 8, 2013
- NCEP operational conventional observations (forward component of the GSI)
- WRF-CHEM model with CBMZ chemistry option, resolution 27 km / 28 layers
- 6-hour assimilation period
- 32 ensembles
- DA control variables:

  - *atmosphere*: wind, specific humidity, perturbation surface pressure, perturbation potential temperature, perturbation height

  - *chemistry*: concentrations of ozone (O_3), nitrates (NO, NO_2, NO_3) and sulfur dioxide (SO_2)

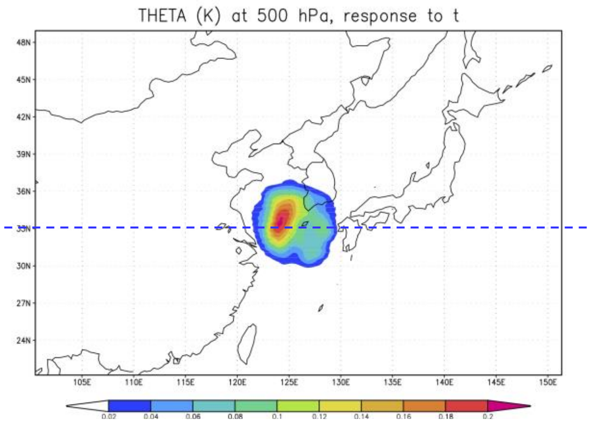
- Single real temperature observation at 500 hPa experiment to examine the cross-covariance between atmosphere and chemistry

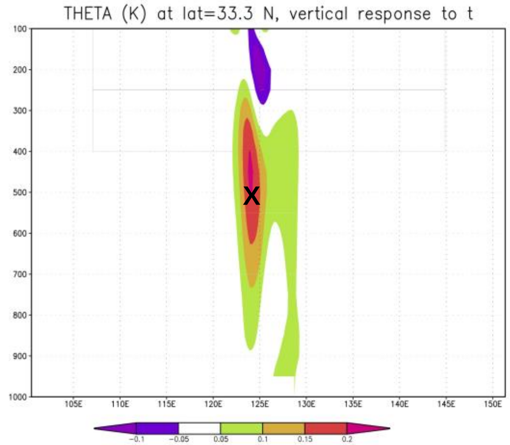
ANALYSIS RESPONSE (x^a-x^f) TO SINGLE TEMPERATURE OBSERVATION AT 500 HPA

Horizontal (~500 hPa)

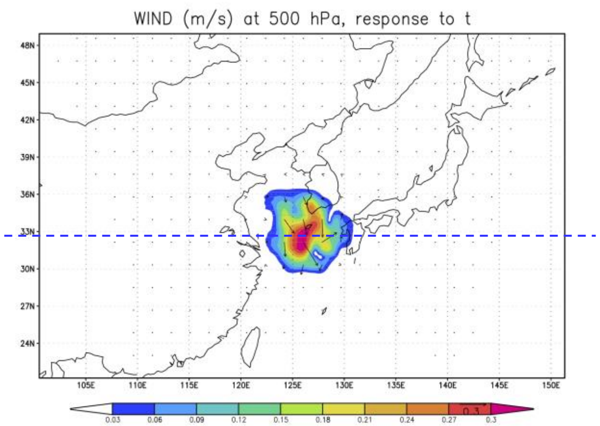
Vertical (~33 N)

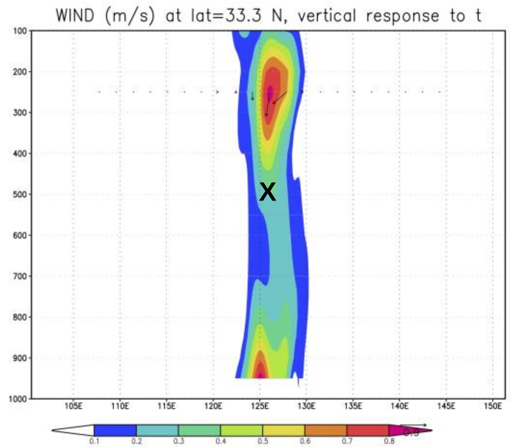
T





U,V





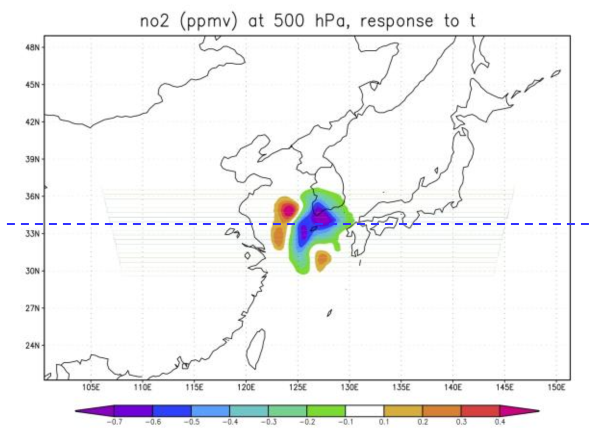
Reality check of data assimilation system: Temperature observations has the anticipated impact on its own analysis and on the wind analysis.

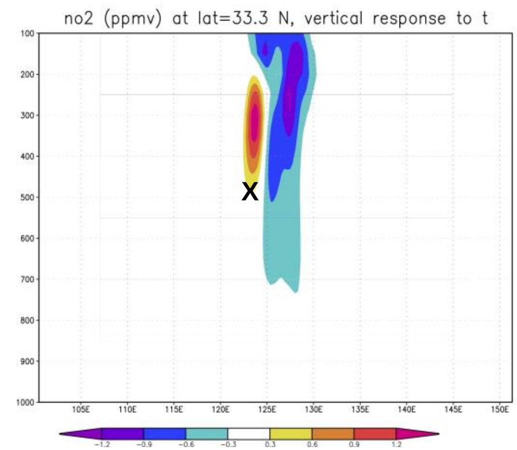
Analysis response (x^a-x^f) to single temperature observation at 500 hPa

Horizontal (~500 hPa)

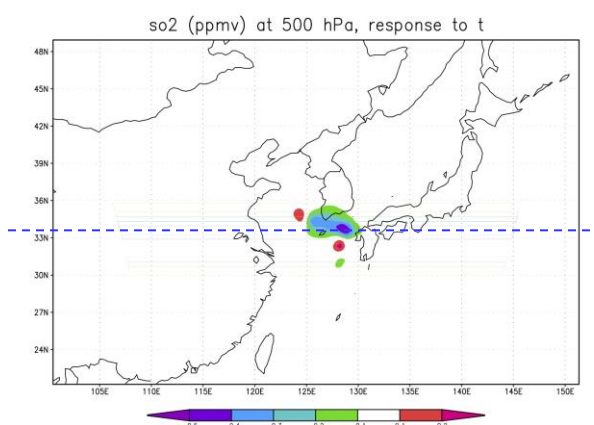
Vertical (~33 N)

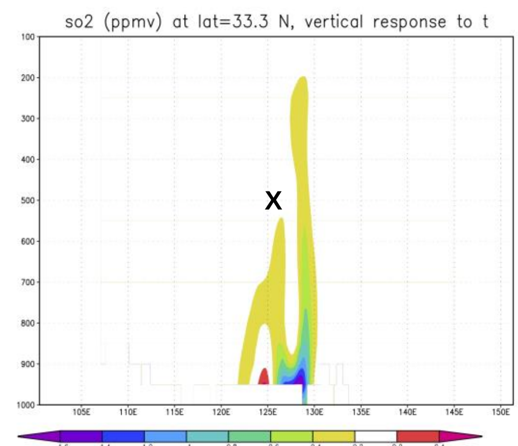
NO_2





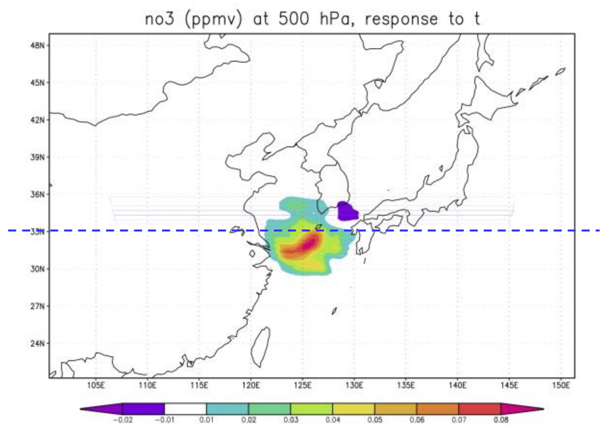
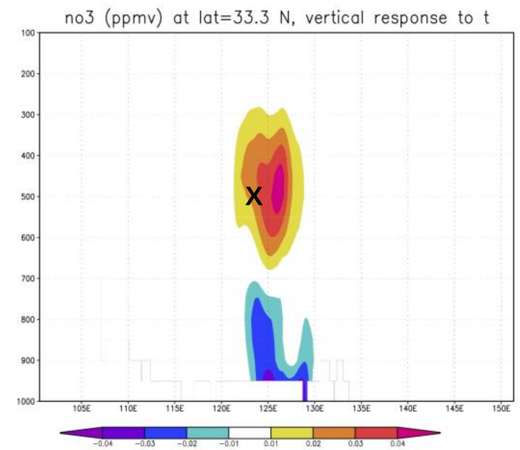
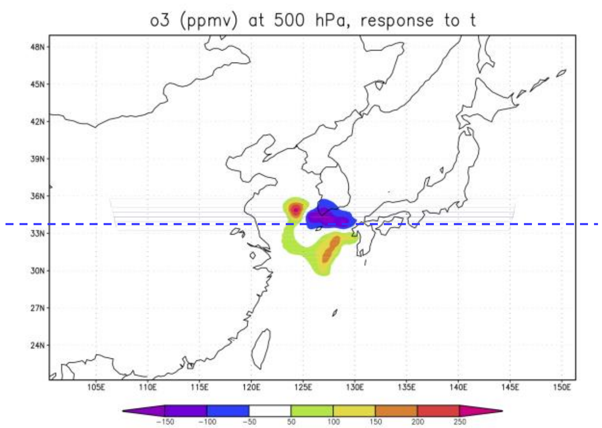
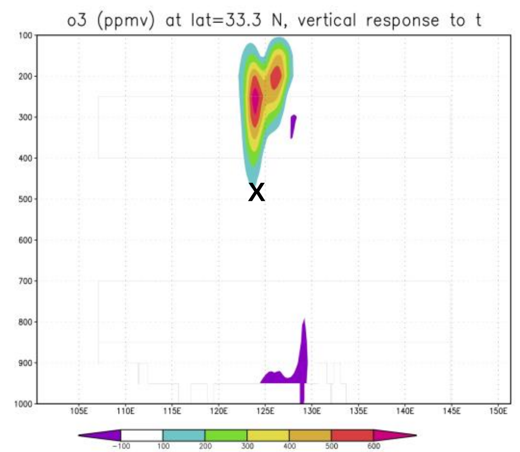
SO_2





Temperature observations impact the NO_2 analysis above the observation level, while the impact on the SO_2 analysis is mostly at surface

Analysis response (x^a-x^f) to single temperature observation at 500 hPa

	Horizontal (~500 hPa)	Vertical (~33 N)
NO_3		
O_3		

Temperature observations impact the NO_3 analysis at lower levels, and the O_3 analysis above the observation level and near surface.

Summary of real atmospheric observation experiments

- WRF-CHEM-MLEF coupled data assimilation system is successfully tested with augmented chemistry-atmosphere control variable and real observations.
- Using GSI as an interface to real observations has been successful. This is in preparation for assimilation of real ozone available through GSI.
- Analysis response to real temperature observations illustrates the complexity of atmosphere-chemistry cross-correlations and the forecast error covariance structure: non-centered analysis response.

Status and Accomplishments (October 2013)

- The WRF-CHEM-MLEF system with synthetic chemistry observations has been successfully tested.
- Forecast error covariance indicates dynamical uncertainty structure.
- Synthetic chemistry observation experiments indicate the capability of the coupled chemistry-atmosphere data assimilation system to assimilate future real GEMS observations.
- Single real atmosphere observation experiments represent first steps toward the assimilation of real atmosphere and chemistry observations.

Future plan

- Continue with assimilation of real atmospheric observations

- Examine further the impact of atmospheric observations on chemistry analysis

- 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