Workshop on
"Data Assimilation in WRF-Chem: Application to Chemical Weather Studies"

This workshop was held from January 6-7, 2009 at NCAR in Boulder, CO. The motivation behind the workshop was to bring together colleagues interested in developing and applying data assimilation capabilities for WRF-Chem and to facilitate the formation of a chemical data assimilation community. The list of participants included atmospheric chemists, mathematicians, and meteorologists, modelers as well as satellite retrieval scientists to cover the complexity in chemical data assimilation and also to take advantage of the expertise existing in meteorological data assimilation.

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The agenda and presentations from the workshop are posted on WEBSITE TBD.

The main target points for discussion included:

- Status and development of data assimilation tools for WRF-Chem and other widely used chemical transport models such as Geos-chem, CAM-chem, STEM and MOZART.
- Challenges in Chemical Data Assimilation
  - Assimilation of data from different observing platforms (in-situ/remote sensing)
    - Mismatch in model/observation spatial and temporal scales and inclusion of observation operators
    - Assimilation of observed radiances versus retrieved geophysical products
- Treatment of systematic and random errors in observations and models
  - Assimilation of chemically active species
- Priority science applications and possibilities for joint projects and proposals

The three main areas of research directions involved in data assimilation are: Models/Observations / Assimilation Schemes.

**Models**

Even though special focus was put on the WRF-Chem model, a large part of the discussions dealt with the general challenges in chemical data assimilation and are thus applicable to a variety of models. Current and future research will have to bridge across different scales – the global scale coming down, the regional scale going up. Thus applications involve models and observations on a range of scales and research will benefit from increased consistency between different scale models in regard to chemical schemes and physics. In addition, simultaneous assimilation of the same observations into both global and regional models helps achieve consistency at the boundary (e.g. adjoint for Geos-Chem and WRF-Chem; EnKf for CAM-Chem and WRF-Chem).

Model imperfections remain a main issue in data assimilation (e.g. representation of PBL, parameterization of convection).

The evolving nature of models necessitates the need to develop a consistent software engineering framework, in order to allow easier modifications and implementation of the data assimilation schemes. This will facilitate the updating of adjoints for new model versions.

**Assimilation Schemes**

Two schemes are being explored for inclusion into WRF-Chem: The Ensemble Kalman Filter (EnKf) and the Adjoint/4D-Var. Both schemes need to be considered in future directions as they complement each other and together allow a wide range of science questions to be explored. For example, in the chemical forecast application the EnKf may be a more practical solution, whereas in source-receptor analysis the adjoint approach is a powerful way to investigate dependences. In addition, the development of hybrid systems is being considered to make use of the complementarities between the EnKf and 4D Var. This includes a framework consisting of 4D-Var to constrain emission sources and subsequent application of EnKf to update species concentrations.

**EnKf**

The NCAR Data Assimilation Research Testbed (DART) has been used to incorporate data assimilation capabilities into the CAM-Chem model. Currently the DART/CAM-
The Chem framework is set up for joint assimilation of meteorological observations, MOPITT CO and MODIS AOD and is being explored for the assimilation of OMI NO2. These capabilities will be included into a DART/WRF-Chem framework, and in future works both frameworks will be extended for the assimilation of other satellite products. The coupling of a global model to a regional model and the use of one data assimilation framework for both assimilation activities provides a more consistent and flexible framework in dealing with different scales (up/downscaling). This can also be used as a prototype for nesting global and regional models - as an interim solution to global WRF (global WRF-Chem) applications.

Ensuring sufficient model spread across the ensemble is an important requirement in the EnKf approach. To this end, multi-physics and multi-chemical scheme ensembles are being explored.

**Adjoint and 4-D Var**

There is a strong desire in the community to develop the adjoint of WRF-Chem, including the adjoints of both the transport and chemistry schemes. Looking further ahead, the development of a 4D-Var system is desirable. As a starting point, the existing adjoint of the meteorological WRF model will be examined for compatibility with the current WRF-Chem version with the goal of developing an adjoint for WRF-Chem to treat initially chemical tracers and aerosols. The latter will build on existing capability with the GOCART adjoint. The meeting stressed the importance of developing adjoints in a manner that allows for a fairly easy update as new model versions become available.

Issues common to both data assimilation approaches include appropriate and practical methods to determine correlations and covariances and the treatment of chemical non-linearities. The impact of assimilating data sets that update one or more constituents in coupled chemical systems, ozone and its precursors for instance, required further work. It was felt that OSSE-type studies might be a good way to explore these issues.

**Observations**

The designed systems will be applied to a range of observations made from different platforms including ground-based and aircraft in-situ instruments and satellite remote sensors. Satellite products of chemical species present an additional challenge with regard to data assimilation because of:

- The influence of retrieval prior constraints
- Correlated errors for profile data assimilation
- Data often represent columns or partial columns with limited vertical information instead of point parameters
• Possible biases introduced through the instrument and/or retrieval technique

When assimilating satellite retrievals, the appropriate use of observation characteristics (i.e. transformation and correct observation operators) is crucial and if properly represented in the data assimilation setup, several of these issues will be minimized. One potential way to consider observation characteristics properly is the use of a singular value decomposition of the averaging kernels and this will be explored. Assimilation of radiances instead of retrieved products would avoid many of these problems, but is hard to achieve from a practical point of view when the range of quite different satellite observations needed for chemical weather applications is considered. This would require the inclusion of very different observation characteristics and forward models and put it beyond the scope of likely resources.

Science Applications:
Chemical Data Assimilation is a powerful way to address current and future research questions. Some of the research topics that will significantly benefit from the developed frameworks and that will be addressed include:

• Chemical Weather: Air quality analysis and prediction, the impact of transported versus local pollution and source-receptor analysis
• Feedbacks between chemical weather and meteorology and climate
• Observation System Simulation Experiments (OSSE) Studies: Assessing the information content of current observing systems and the design of future instruments/platforms, monitoring networks and observing strategies
• Design and analysis of field campaigns

Development Goal: Chemical Data Assimilation Testbed
The development of a framework consisting of a variety of data assimilation tools (EnKf, Adjoint/4D-Var and hybrid systems) around WRF-Chem (and possibly other models) was discussed as a goal for this community. This framework could share a number of efforts common to all data assimilation schemes such as acquiring observations and converting them to a common format, analysis tools, etc. After an initial development phase the framework would be shared with the community and community involvement encouraged.

The testbed would significantly support a wide range of research directions and the capability of parallel experiments between different assimilation schemes is crucial for advances in chemical data assimilation.
Considerations for the development: Funding (specific funds for full development and/or individual small proposals that each contribute to parts of the Testbed) and leadership. A next workshop dedicated specifically to the design of a such a community facility will be considered.

Other Actions:

- Possible collaboration in developing common proposals will be taken (NSF/CMG, NASA ROSES 2009).

- Test cases for development/applications have been selected: TEXAQS 2006, ARCTAS-CARB 2008