National Aeronautics and Space Administration

Strategic Advances in Air Quality Research and Technology Development

Principal Investigator: Jonathan H. Jiang (329J)

Co-Is: Meemong Lee (329I), Zhijin Li (329B), Marcin Witek (329J), Masashi Minamide (329E), Yuan Wang (Caltech), Vivienne Payne (329I), Jessica Neu (329I), Hui Su (329D), John Worden (329), Kristen Fahy (329I)

Program: Strategic Initiative

Project Objective:

Develop the capability to provide surface aerosol and trace gas concentrations at spatial scales (between 100 m and 2 km) needed to support human and ecosystem health studies identified as a Most Important (MI) objective by the Decadal Survey (DS). We will utilize measurements from the Program of Record and evaluate requirements for upcoming DS missions.

Science Questions: How do local and remote anthropogenic and natural emissions affect regional air quality? How does air quality affect public health, ecosystem health and the economy?

Link to Earth Science Grand Challenges and DS: Air Quality Hazard, Carbon, and improve our capabilities for hazard response and preparedness.

Application Aspiration: Integrate and advance the Lab's observing and modeling capabilities and provide comprehensive technical capabilities to assess air quality from global to neighborhood scales in order to enhance the scientific return from current and identified future missions.

Formulation Targets: MAIA, HYSPIRI, EV-S ECHO (Ecological Health and Ozone), and DS Atmospheric Composition mission(s) to measure gaseous and particle pollutants.

FY19 Highlight

1. A GEOS-Chem 4D variational assimilation (4DVAR) system and the Emission information system were implemented and the Observation information system was extended to integrate the observations from MOPITT and MISR missions.
2. Performed a comprehensive evaluation of the aerosol tracer and AOD model simulation and a successful 4DVAR assimilation of the MISR-AOD observation.
3. An interface between the GEOS-Chem and the WRF-Chem models has been developed within the GC-DA system employing the convention of the MOZBC, a tool that the WRF-Chem model currently employs to interface with the MOZART chemistry transport model system.
4. An fully functional regional WRF-Chem data simulation system has been developed and running successfully using the GEOS-Chem–WRF-Chem interface with IC/BC provided by GEOS-Chem.
5. Implemented boundary conditions for complex geometries (topography and buildings) in the LES; Performed simulations with point and distributed pollution sources for various meteorological conditions.
6. Validation using laminar (non-turbulent) flow around sphere works as expected; Validation for turbulent geophysical flows works as expected; Simulations with idealized terrain works as expected

GEOS-Chem Data Assimilation System

The GEOS-Chem Data Assimilation System (GC-DA) is a global atmospheric composition forecasting system that optimally integrates the model forecast and the satellite observations. For the model forecast, the GC-DA employs the GEOS-Chem model system managed at Harvard University. For the satellite observations, the GC-DA generates a unified, "mission independent" representation of satellite observations prior to assimilating the level-2 data products to enable a joint assimilation of multiple tracers (e.g. O_3, CO, NH_3), which can be retrieved from multiple satellite missions.

During the FY19, the GC-DA system has developed the following capabilities on schedule:

1) A 4D variational assimilation (4DVAR) system and the Emission information system were implemented and the Observation information system was extended to integrate the observations from MOPITT and MISR missions. The GC-DA employs the 4DVAR system to compute the observation forces (forward process), to integrate their sensitivity to the emissions backing out the dynamics impact (adjoint process), and to estimate the optimal emission scale factor (optimize process). The GC-DA successfully performed assimilation of the MISR-AOD observations which provide the total column AOD and the AOD fractions of four types of particulate matter (small, medium, large, and non-spherical). Figure 2 shows the iterative 4DVAR assimilation process flow during the MISR-AOD assimilation with the integration of the observation information and the emission inventories.
2) Significant achievements include a comprehensive evaluation of the aerosol tracer and AOD model simulation and a successful 4DVAR assimilation of the MISR-AOD observation. The MISR-AOD observation provides the total column AOD and fractions of four particulate matter (PM) groups, a small PM (less than 0.4 um), a medium PM group (between 0.4 and 0.7 um), a large PM group (greater than 0.7 um), and a dust PM group (non-spherical shape). However, the GEOS-Chem computes the total AOD by integrating the four types of AODs, a carbon AOD, a sulfate AOD, a sea salt AOD and a dust AOD. Table 1 list the AOD types with respect to the aerosol tracers, effective radius, and mass density. Figures 1 and 2 show the spatial distribution of the MISR-AOD and the GEOS-Chem AOD respectively.

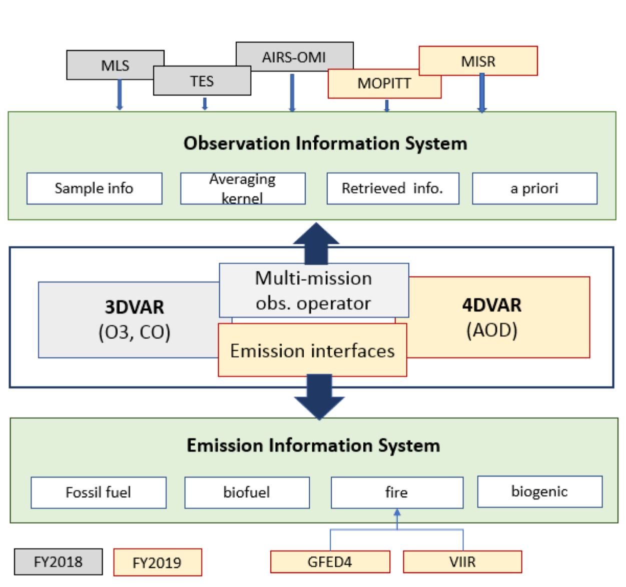


Figure 1: Inter-system collaboration infrastructure of the GEOS-Chem Data Assimilation System framework.

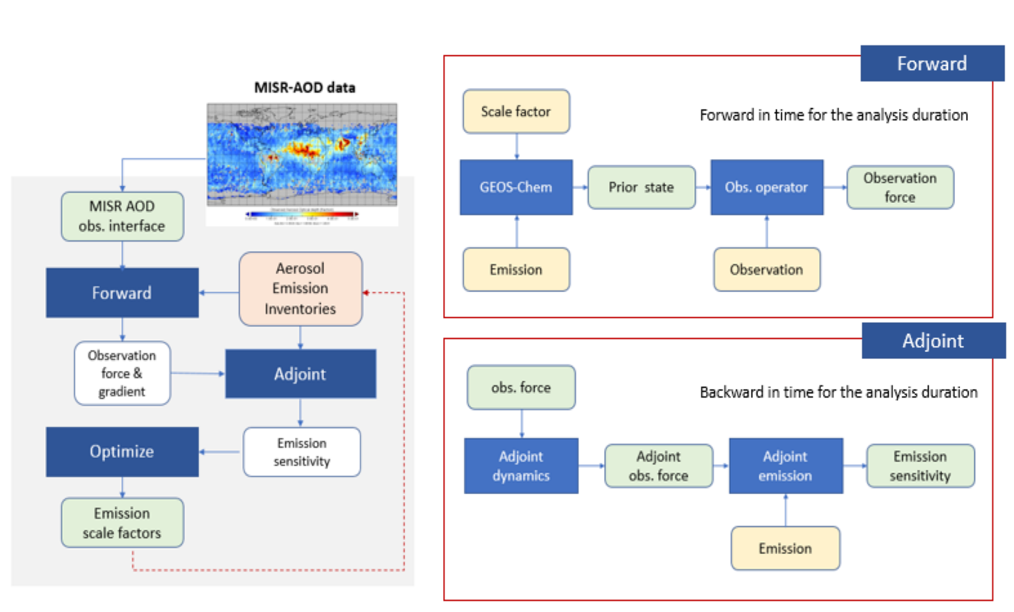


Figure 2: 4D variational assimilation (4DVAR): iterative emission scale factor estimation process flow involving the forward, adjoint, and optimize processes.

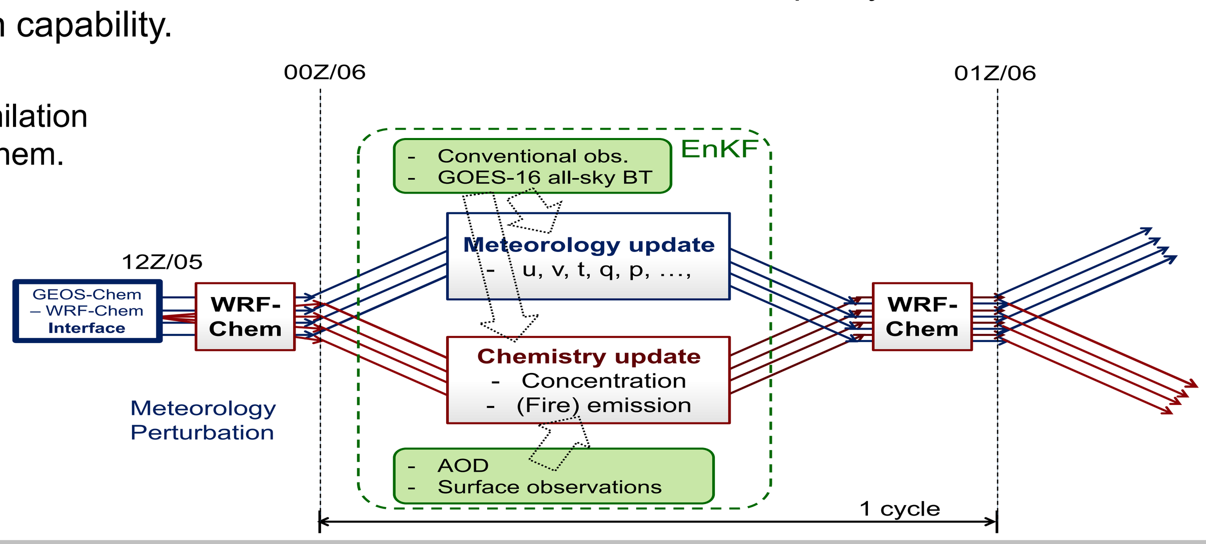
WRF-Chem Data Simulation System

An fully functional regional WRF-Chem data simulation system has been developed and running successfully using the GEOS-Chem–WRF-Chem interface with IC/BC provided by GEOS-Chem.

The WRF-Chem system has performed the following tasks on schedule:

1) Conducted ensemble forecast experiments using WRF-Chem to investigate the predictability of air-quality, as well as to design the data assimilation framework.
2) Developed quasi-real-time automatic system to initialize and run WRF-Chem simulation on southern California.
3) Developed EnKF data assimilation system built around WRF-Chem, which is able to assimilate satellite AOD and surface air-quality observations with strongly/weakly coupled data assimilation testbed among meteorology and chemistry variables.
4) Conducted preliminary experiment to assimilate satellite AOD and surface air-quality observations to demonstrate the assimilation capability.

Figure 3: The EnKF data assimilation framework built around WRF-Chem.



Large-Eddy Simulation (LES) Model

1) Implemented boundary conditions for complex geometries in LES, including topography and buildings
2) Performed simulations with point and distributed pollution sources for various meteorological conditions
3) Validation using laminar (non-turbulent) flow around sphere works as expected.
4) Validation for turbulent geophysical flows wors as expected.
5) Simulations with idealized terrain works as expected.
6) On going simulation with the actual LA basin topography.
7) Ongoing simulations with actual more detailed topography, realistic forcing and pollution sources.
8) Ongoing implementing physical interactions of momentum and tracers with the surface.

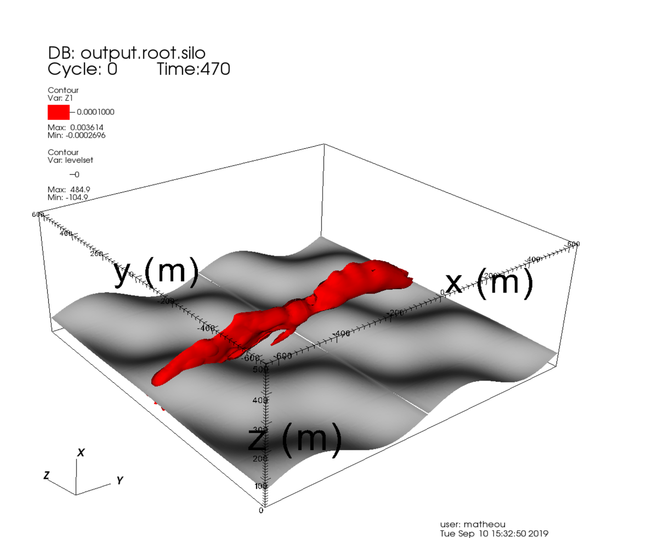


Figure 4: The LES simulated PM2.6 plums over with idealized terrain.

4. Benefits to NASA and JPL and Significance of Results

- We have coalesced in-house capabilities in aerosol, chemistry, and air quality research, and global and regional modeling.
- The unified modeling and data assimilation system will contribute critical information needed for assimilation of future space-borne air quality and chemical composition measurements and accelerate JPL's readiness in formulating future missions identified as high priority by 2007 DS and anticipated similarly for 2017 DS.
- The 2017 DS identified as a "Most important" Science and Application Question: What processes determine the spatial-temporal structure of important air pollutants and their concomitant adverse impact on human health, agriculture and ecosystems?
- The modeling and data assimilation system developed by this project provides a means to:
  - Address this question using the Program of Record
  - Establish observing system requirements for relevant DS targeted observables
  - Aerosol (designated)
  - PBL (incubation)

Sensitivity Experiment

The WRF-Chem system has been used to simulate a region of Northern California affected by the Camp Fire over the period of 7-21 Nov 2018 and evaluated the model performance using station observations of PM2.5.

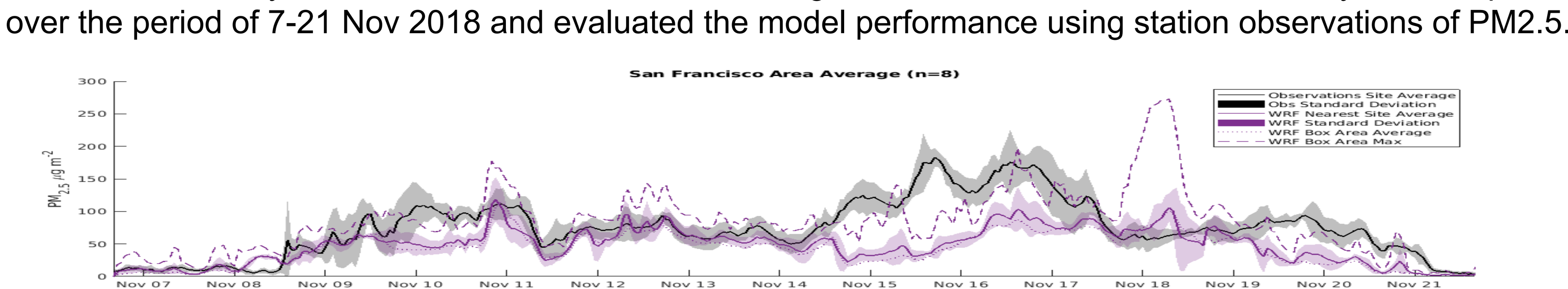


Figure 5: The WRF-Chem simulated average PM2.5 in μg m-3 (purple) and average surface observations (black) and standard deviation (shading) for the San Francisco area during the Camp Fire. The solid purple line indicates the average of the computational cells nearest the 8 observation sites. The dotted line indicates the average value of a box area encompassing the 8 stations, while the dashed line is the maximum of that area.

National Aeronautics and Space Administration

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, California

www.nasa.gov

PI/Task Mgr. Contact Info: 4-7135; email: Jonathan.H.Jiang@jpl.nasa.gov

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