Sensor-web Operations Explorer (SOX) for Earth Atmospheric Science Experiment

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Abstract— Future air quality missions will face significant measurement strategy design and implementation challenges. Characterizing the atmospheric state and its impact on air quality requires observations of trace gases (e.g., O_3, CO, NO_2, SO_2), aerosols (e.g., size and shape distributions, composition), clouds (e.g., type, height, sky coverage), and physical parameters (e.g., temperature, pressure, humidity) across temporal and spatial scales that range from minutes to days and from meters to >10,000 km. Validating satellite measurements is another major challenge, and it requires well organized and orchestrated sub-orbital sensor web deployments. No single sensor, instrument, platform, or network can provide all of the information necessary to address this issue. Constellations of spacecraft, integrated air-borne campaigns, and distributed sensor networks have been actively pursued to achieve the needed multi-dimensional observation coverage. However, these complicated sensor webs must address how to formulate the complex design trade space, how to explore the trade space rapidly, how to establish evaluation metrics, and how to coordinate observations optimally. The Sensor-web Operations Explorer (SOX) research task under NASA Earth Science Technology Office addresses these challenges by creating a virtual sensor-web experiment framework that can support orbital and sub-orbital observation system simulation experiment.

TABLE OF CONTENTS

1. INTRODUCTION

Understanding the chemical state and its impact on air quality requires observations of multiple trace gases (e.g., O_3, CO, NO_2, SO_2), as well as aerosols and their properties (e.g., particulate size and shape). In addition to the chemistry that relates these gases and aerosols, meteorological processes such as convection and transport affect the vertical and horizontal distribution of these gases and aerosols [1]. At the regional scale, urban and industrial regions can be sources of pollution that impact air quality on rural communities and ecosystems. At the global scale, intercontinental transport means that pollution generated on one continent can affect another thousands of kilometers away. For example, pollution generated over Asia can be transported across the Pacific to North America. Likewise, pollution generated in North America can be exported across the Atlantic to Europe.

Trace gases and aerosols cannot only affect air quality, but they may also impact regional and global climate through longer-lived greenhouse gases, e.g., ozone (O_3), CO_2, and CH_4. Aerosols can have a net cooling or heating effect depending on their type and vertical distribution. Each observational asset provides its own unique strengths and weaknesses in providing the data necessary to assess the chemical state. Satellite observations provide global coverage of multiple trace gases. However, these observations may be limited in vertical resolution and frequency of observation. As depicted in Figure 1, aircraft and sonde observations can complement the satellite data and provide additional measurement details, but they are limited in their spatial and temporal coverage compared to satellite observations [2]. Ultimately, operational scenarios that combine multiple satellite and sub-orbital observations in a coordinated sensor web will yield the greatest scientific value.

To explore operational scenarios of a complex sensor-web that answers science questions optimally requires an advanced design process that overcomes the limitations of the single-platform-oriented design paradigm. The goal of the Sensor-web Operations Explorer (SOX) is to provide an advanced observation system simulation experiment (OSSE) capability for the global Earth atmospheric science community. A three-step approach has been devised to achieve the goal. The first step is to develop a flexible concept design exploration space for sensor-web system architectures and operational scenarios. The second step is to develop a science impact metric that can be applied to quantitatively evaluate science-return from the explored system architectures and operational scenarios. The final step is to establish a process that coordinates inter-disciplinary collaboration between scientists and engineers to develop optimal observation scenarios.

This paper describes the technical approach and current capability of SOX. Section 2 describes modeling and simulation activities involved in developing a comprehensive observation system simulation experiment (OSSE) for global atmospheric study. Section 3 describes two types of metrics, the measurement quality metric and the prediction accuracy metric, which have been developed for quantitative science impact evaluation. Section 4 describes the design space exploration approach. Section 5 describes end-to-end OSSE process flow with respect to inter-disciplinary collaborative design exploration. Finally, Section 6 summarizes the current capabilities and technology readiness level (TRL) verification procedures.

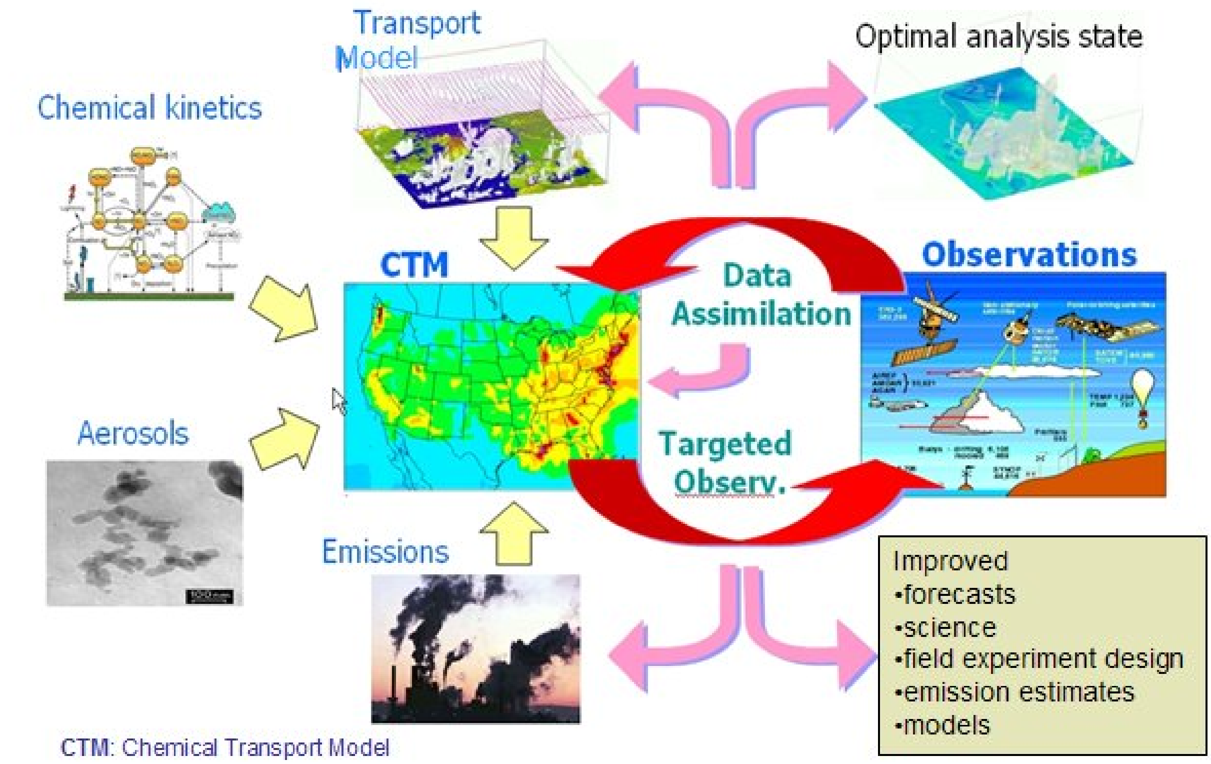

Figure 1 –Relationship between Models, Observations, Data Assimilation, and Observation Scenario Design

2. Modeling and Simulation

SOX integrates models from multiple disciplines into an end-to-end process that flows from science objective definition through science return evaluation. Figure 2 illustrates the SOX model categorization, the science requirements flow, and the SOX information and process flow. The development activities are divided into three areas: sensor-web information modeling; virtual-mission operation and measurement simulation; and science impact evaluation.

A sensor-web in this context is defined to be a system composed of multiple sensors (instruments) deployed on multiple orbital/sub-orbital platforms. The number and type of each sensor/platform combination defines a specific sensor-web measurement design strategy, and the optimal strategy varies with the science question(s) to be addressed and available resources. SOX provides an adaptive sensor-web measurement strategy design tool for rapid air-quality assessment in which the sensor-web system architecture and integrated campaign planner are modeled, and the observation process and measurement products are simulated. SOX can also support measurement requirement validation by quantifying the sensitivity of a given measurement to simulated retrieval uncertainty.

The sensor-web architecture modeling (SWAM) module provides implementation-independent parametric representations for instruments and platforms. This yields a uniform representation of a wide range of sensor-web system configurations, thus enabling rapid virtual prototyping of many sensor-web system architectures. SWAM also handles import protocols and automatic property translators for external model integration. Currently, SWAM models low-Earth-orbit satellites using a Keplerian orbit parameter set (i.e., altitude, incidence angle, ascending node, argument of periapse, and epoch) and scan platform property descriptors (e.g., cross track angle, along track angle, track rate). Each instrument is modeled employing the property descriptors of an imager, a spectrometer, and a radiometer, defining spatial, spectral, and intensity relationships between the observed phenomena and the measurements.

The sensor-web integrated campaign planner (SWIP) generates data acquisition strategies that account for the operational constraints unique to each asset in the sensor-web. Each data-acquisition strategy specifies sample location (longitude & latitude), sample coverage (footprint resolution), altitude (orbit trajectory, flight path), time (Sun direction, duration, sampling frequency), and wavelength. The multi-dimensional aspect of the data acquisition strategy is mapped to a target signal generation process whereby the physical content (e.g., temperature, pressure, humidity, chemical species) of the input to the Radiative Transfer Model (RTM) is defined [3].

The Measurement Simulation and Distribution Service (MSDS) integrates instrument models and platform models and simulates the observation process. The observation process simulation includes implementation of a virtual signal, a virtual sensor-web, and virtual measurement. The virtual signal is defined to be a radiance spectrum estimated from the sample location at the observation time. The virtual sensor-web is a system of virtual sensors on virtual orbiters as defined by SWAM. The virtual measurement is an output spectrum from a virtual sensor with the virtual signal as an input. The measurements are used to evaluate science impact of sensor-web architecture designs and/or observation scenarios on a specific sensor-web. Figure 2 depicts the process flow among SWAM, SWIP, and MSDS.

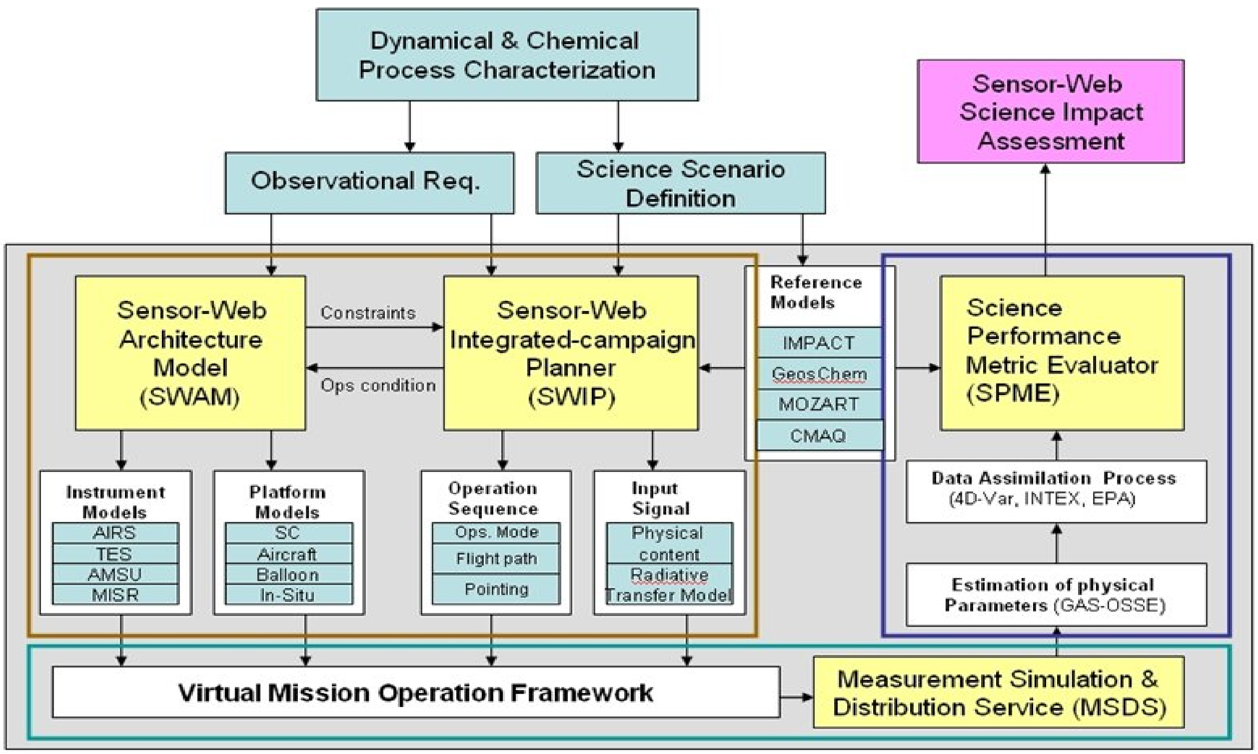

Figure 2 Sensor-web Operations Exploration Framework

3. Science Impact evaluation

The mission design and observation strategy must be considered together to optimize a given measurement. The criteria for defining the optimal measurement flow down from the science question to be addressed, as well as engineering and mission constraints. For example, optimization may maximize the margins for achieving the measurement requirements within a given performance parameter space. The optimization process establishes the "return on investment" where the design drivers can be quantitatively compared with respect to increased retrieval resolution. The Science Performance Metric Evaluator (SPME) addresses three topics: 1) Configuration of reference phenomena models that corresponds to science scenario definitions; 2) Configuration of a data assimilation system that integrates estimated physical parameters with the operational phenomena model; and 3) Composition of science performance metrics by evaluating reference phenomena models vs. assimilated models. The configuration of the data assimilation system includes: choice of assimilation algorithm (e.g., 4D-Var, Ensemble Kalman filtering), specification of the geophysical parameter state vector to be estimated (e.g., emissions, sources, ozone fields), and definition of assimilation algorithm parameters (e.g., background covariance matrices and scale lengths). The estimation of physical parameters from the simulated measurements is achieved by applying retrieval analysis and data assimilation.

The retrieval process involves three steps, 1) adding simulated noise to the atmospheric state profile and the Jacobean radiance; 2) performing a linear retrieval that computes the averaging kernel, retrieval gain, and vertical resolution; and 3) calculating the retrieval error statistics and distribution with respect to the measurement requirement parameters explored [4]. Figure 3 illustrates an example result of exploring the retrieved vertical resolution retrieval accuracy as a function of the signal-to-noise resolution (SNR) and spectral resolution for simulated atmospheric ozone measurement. These sensitivity analyses define requirement parameter ranges, as well as a design trade metric between the measurement requirement parameters [5].

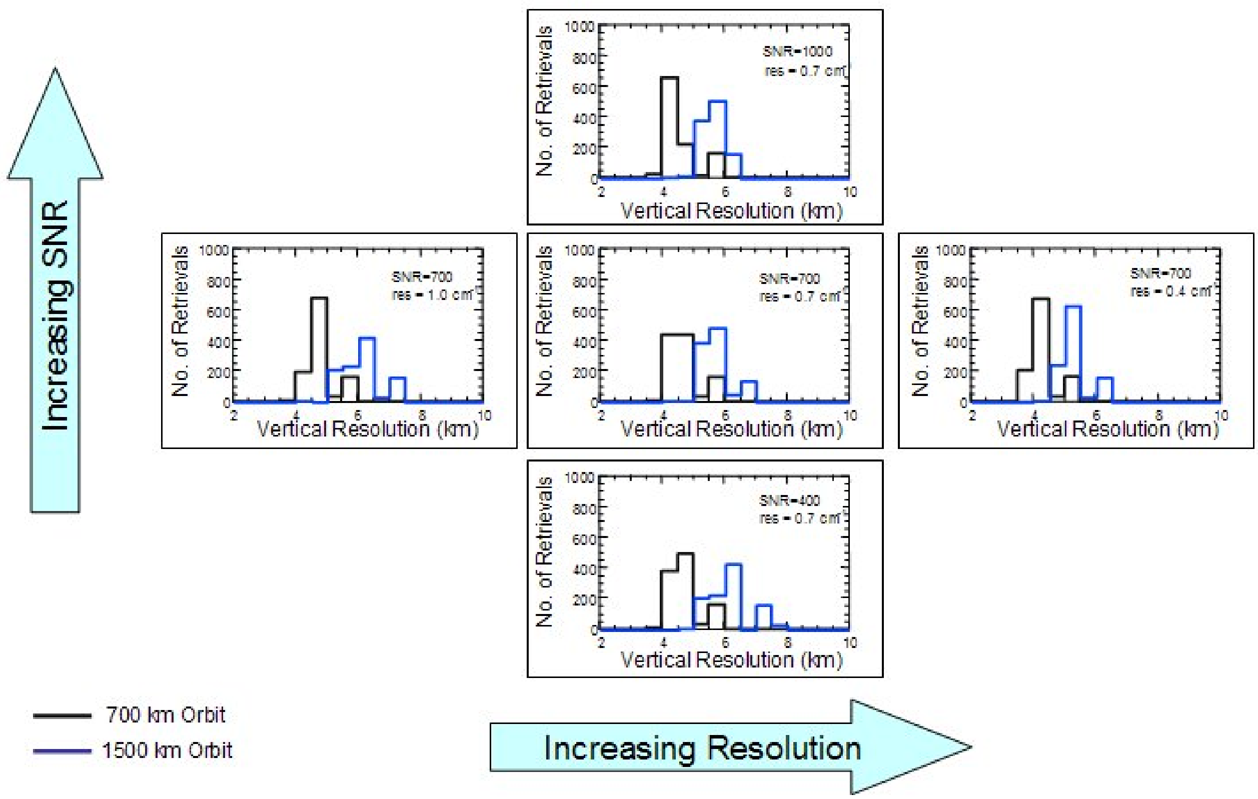

Figure 3 Sensitivity of Instrument Performance on Retrieval Analysis

The data assimilation process progressively incorporates the estimated physical phenomena and predicts the global distribution of the physical phenomena. The prediction error is expected to decrease as more observations are assimilated if the estimated physical phenomena were accurate. The accuracy of the physical phenomena estimation depends on the quality, quantity, and spatiotemporal distribution of the observations, which implies the dependency on instrument performance and observation scenario.

A display tool was developed to monitor the 4D data interactively in all dimensions by enabling the viewer to browse through each dimension (e.g., time, latitude, longitude, and altitude) of the data set. The display tool employs three two-dimensional maps of the dataset. The main map displays the atmospheric phenomenon over the entire latitude and longitude range at a fixed altitude. The top map displays data slices for longitude and altitude range at a fixed latitude. The side map displays data slices for latitude and altitude at a fixed longitude. The temporal dimension is controlled for all three maps simultaneously with the time slider at the bottom left.

Figure 4 presents two screen captures from the 4D display tool applied to the data assimilation results. The screen capture on the left presents the predicted atmospheric concentration error after seven orbits of observations. The red area over North America indicates the large error introduced as a result of the initial estimate conditions.

The screen capture on the right represents the predicted atmospheric concentration error after 27 orbits of observations have been assimilated, showing significant error reduction. A Kalman filter based data assimilation algorithm was used for the illustration [5]

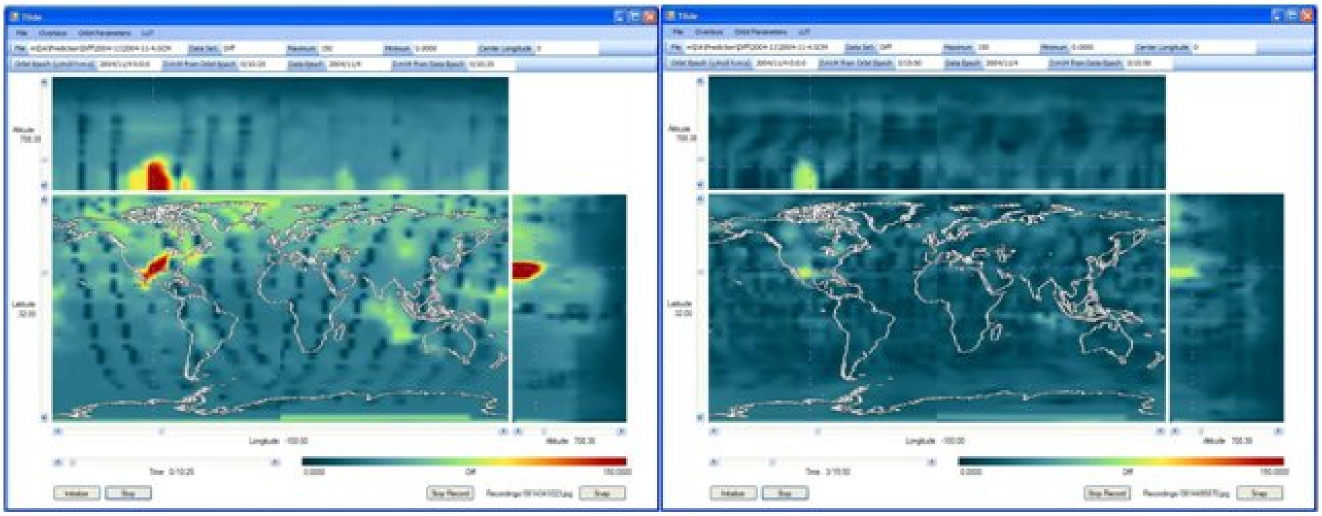

Figure 4 Post-data assimilation atmospheric concentration error uncertainty inferred after assimilation of observations from 7 orbits (left panel) and 28 orbits (right panel)

4. Design Space Exploration

Simulation of a given sensor-web followed by a quantitative science impact analysis enables the comprehensive validation of the sensor-web architecture and its operational scenario. The design validation process can explore a large number of candidate architectures and operational scenarios [6]. The SOX design space exploration exists can be performed on multiple levels (sensor-level, platform-level, operational scenario-level, and experiment-level). For example, a set of sensor options may be explored on the same platform using the same observational scenario. Alternatively, a set of operational scenarios may be explored for a single sensor on a single platform. Combining different sensor-web options in this manner, a rapid design space exploration capability is pursued by formulating two types of design spaces, an architecture design space and an observation scenario design space.

The architecture design space is formulated with parametric instrument and platform models. The exploration range and resolution of each parameter in the model is specified with a minimum value, a maximum value, and an increment value. The exploration tool automatically populates the design space with all of the possible parameter value combinations. The sensitivity of each parameter set is analyzed by applying the science impact evaluation process. For example, the SNR performance of a hypothetical instrument may be expressed as “SNR = 100, 1000, 50”. The populated design space will have 20 different instrument cases for which the SNR values vary from 100 to 1000 with an increment of 50.

The observation scenario design space is parameterized according to the operational constraints and measurement strategies. Each measurement strategy may be specified as a function of the viewing geometry, observation condition, sampling frequency, and observation duration. Parameter settings are used to identify target location and acquisition time. The virtual input signals are simulated by extracting the phenomena geophysical fields for the targeted location and time, calculating the corresponding radiance incident on the instrument aperture, and propogating this through the instrument model. The sensitivity of the measurement strategies can be analyzed by evaluating the prediction error obtained from the assimilation of the retrieved quantities from these simulated observations [7].

The design space exploration is applied to mission concepts and/or instrument concepts as depicted in Figure 5. The end-to-end OSSE process of SOX is divided into two types of activities: database generation and design validation. The database-generation activity organizes a large number of design options, and the validation activity analyzes the sensitivity of each option, collectively achieving rapid design space exploration. The database-generation activity is subdivided into four databases: phenomena, input signal, measurement, and trace-gas profile. Each database generation process provides interface protocols to relevant community models; phenomena models for phenomena-database preparation, radiance transfer models for input-signal database generation, and instrument response models for measurement database generation.

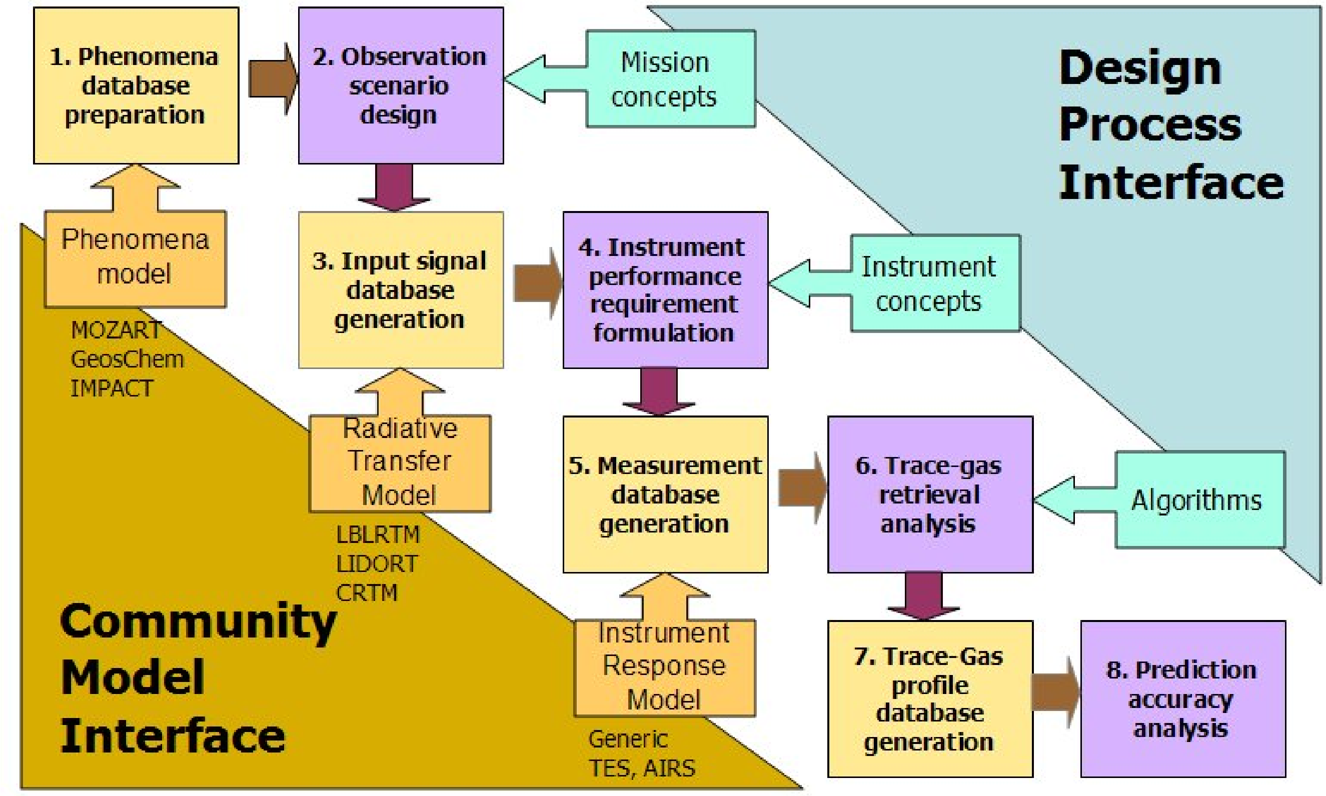

Figure 5 End-to-End Process Flow and Interfaces

5. SUMMARY

We have described our technical approach for developing the Sensor-web Operations Explorer (SOX), a virtual sensor-web experiment framework that can support orbital and sub-orbital OSSEs. A prototype system will be ready for TRL-3 verification in August of 2007. The prototype will simulate two satellites, one on the Aqua orbit and the other on the Aura orbit. The Aqua orbit satellite will be equipped with an AIRS-like instrument set (AIRS is Atmospheric Infrared Sounder) and the Aura orbit satellite will be equipped with TES-like instrument set (TES is Thermal Emission Spectrometer). Each instrument will be explored by varying 8 or more performance parameters. The verified prototype system will support observation system simulation experiment (OSSE) for global atmospheric mission concept study at JPL. The science scenario to be used for TRL verification is described below.

Scenario: Asian outflow thought to create unhealthful air quality conditions in Western United States.

Challenge: Track and assess the air quality risk.

Implementation: SOX simulations indicate that the optimal strategy is to assimilate data from targeted observations of

- TES-like nadir-viewing infrared (IR) data to characterize tropospheric O_3 levels
- Ultraviolet/visible (UV/VIS) O_3 data to provide additional constraints on tropospheric O_3 profiles
- UV/VIS NO_2 data to track fossil fuel combustion and related emissions
- UV/VIS data for formaldehyde (HCHO) (proxy for biogenic & non-methane hydrocarbon emissions)
- Microwave radiometer surface temperature polarization resolving imager and UV/VIS backscatter measurements to track aerosol plume and quantify the particle-size distribution to determine potential particulate matter (PM 10 through PM 2.5) exceedances.

Upon a successful verification, a web-based exploration capability will be developed for on-line collaboration among the mission designers, instrument developers, and data-assimilation-algorithm developers NASA-wide.

During field campaigns, adaptive measurement strategies are essential to account for changing atmospheric and meteorological conditions as well as the number and type of sensors, instruments, and platforms available at any given time. Scientists plan measurement strategies that maximize science data return by identifying where and when specific measurements have the greatest impact. During FY'08 and FY'09, SOX will be extended to include airborne assets and in-situ assets to help optimize satellite and sub-orbital resource usage for both regional- and global-scale operations.

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REFERENCES

[1] M. Luo and R. Beer, "Simulated observation of tropospheric ozone and CO with the Tropospheric Emission Spectrometer (TES) satellite instrument," *J. Geophys. Re*s., **107**, D15, 2002.

[2] C.D. Rodgers, Vol. 2, *Inverse Methods for Atmospheric Sounding: Theory and Practice*, World Scientific Publishing, Series on Atmospheric, Oceanic and Planetary Physics, Singapore, 2000.

[3] S.A. Clough, M.W. Shephard, E.J. Mlawer, J.S. Delamere, M.J. Iacono, K. Cady-Pereira, S. Boukabara, and P.D. Brown: "Atmospheric radiative transfer modeling: a summary of the AER codes," *JQSRT*, **91**:233–244, 2005.

[4] M. Lee, A. Eldering, C. Miller, and Z. Qu, "Earth Science Mission Concept Design System," presented at *2007 IEEE Aerospace Conference*, Big Sky, MT, 2007.

[5] S.S. Kulawik, H. Worden, G. Osterman, L. Ming Luo, R. Beer, D.E. Kinnison, K.W. Bowman, J. Worden, A. Eldering, M. Lampel, T. Steck, and C.D. Rodgers, "TES atmospheric profile retrieval characterization: an orbit of simulated observations," *IEEE Transactions on Geoscience and Remote Sensing*, **44**:5, 2006.

[6] M. Lee and R. J. Weidner, "Virtual Mission Systems for Multi-disciplinary Engineering Design," presented at *AIAA SpaceOps-2005*, Long Beach, CA, 2005.

[7] M. Lee and R. J. Weidner, "Virtual Mission Operation Framework," presented at *IEEE Aerospace Conference*, Big Sky, MT, 2004.