Synthesis of multiple observations using a regional aerosol assimilation/forecast model (RAQMS) and assessment of biomass burning emission estimates

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ABSTRACT

This study presents the synthesis of multiple observations using the regional component of the Real-time Air Quality Modeling System (RAQMS) to evaluate biomass burning emission estimates and assess consequent impacts on air quality. During the NOAA 2006 TexAQS II field study observations from different platforms, such as satellites, aircraft and ground network, are available. These combined resources provide an opportunity for detailed interpretation of factors influencing local air quality. However, their utilization is not straightforward due to difficulties in incorporating data that are at different temporal and spatial resolutions. A 3D aerosol assimilation/forecast model can be an effective tool for linking multiple observations. To demonstrate this we investigate aerosol loading due to wildfire emissions during Aug - Sept, 2006, and discuss how the assimilation system can be used to characterize biases in wildfire emission estimates. We assimilate MODIS aerosol optical depth (AOD) using RAQMS. RAQMS-MODIS AOD analysis increments are used to identify a bias in carbonaceous aerosol associated with biomass burning estimates. CALIPSO observations are used to evaluate the altitudes of aerosol layers. The ground-based measurements and the MODIS AOD retrieval are used to evaluate the model performance and to assess the impact of wildfire on local air quality in Houston, TX.

INTRODUCTION

Traditionally ground-based measurements are used to monitor and assess local air quality. Since 1960's, satellite observations deliver a global view of the atmospheric conditions. Among the satellite observations the MODIS instrument onboard the Terra and Aqua satellites provides aerosol optical depth (AOD) retrieval that represents column integrated aerosol loading. In June, 2006, a new satellite
CALIPSO started acquiring a vertical profile of aerosols and clouds as lidar backscatter signals. These satellite measurements add another dimension to the currently available datasets for use in air quality studies. Here we use a three-dimensional model in combination with the satellite observations to not only interpret the satellite retrieved quantity but also link the satellite measurements to surface networks in a systematic way.

In this study we assimilate MODIS AOD measurements using a three-dimensional regional aerosol model. The assimilation provides an observationally constrained 3D mass field of each speciated aerosol. The resulting aerosol mass distributions are used to interpret aerosol distributions over the continental US and within the Houston, TX metropolitan area during the TexAQS II field experiment deployed in Houston, TX, from mid August to mid October, 2006. This time period coincides with an aerosol event resulting from biomass burning over the Pacific Northwest. The near-real-time simulation results obtained during the field experiment is evaluated with respect to the MODIS AOD, the CALIPSO integrated attenuated backscatter retrieval and ground-based measurements. The evaluation is used to assess the performance of the assimilation/forecast model and the quality of biomass burning emission datasets. Finally an influence of smoke from biomass burning on local air quality in Houston is discussed.

PROCEDURES

Model Description

The regional aerosol model used for this study is the regional component of the Real-time Air Quality Modeling System (RAQMS) [Pierce et al, 2003, 2006], which incorporates on-line aerosol modules from GOCART [Chin et al., 2002, 2003 ] and a sulfate-nitrate-ammonium thermodynamic equilibrium model [Park et al., 2004]. The sulfate module is taken from Kittaka et al. [2004], which explicitly associates sulfate with four different types of water substances, cloud, rain, pristine ice and snow. The aerosol component of RAQMS is not coupled with gaseous chemistry, which is provided by the global component of RAQMS in this study. The model predicts concentrations of two gases (SO$_2$, NH$_3$), nine aerosol species (SO$_4$, NO$_3$, NH$_4$, hydrophobic OC, hydrophilic OC, hydrophobic BC, hydrophilic BC, dust, sea-salt). Figure 1 illustrates chemical constituents and physical processes associated with aerosol sources and sinks included in the model. The concentrations of three aerosol precursors such as hydrogen peroxide, nitric acid and hydroxyl radicals are prescribed by interpolating 6-hourly results of the global component of RAQMS in time and space. The model domain includes the entire continental US with an 80km spatial resolution. A time step used in this study is 180 seconds. The NASA Global Modeling and Assimilation Office (GMAO) global aerosol product provides the lateral boundary condition of aerosol distributions for the regional model studies.

The SO$_2$ 1°x1° emission data for year 1985 is taken from GEIA. This SO$_2$ emission dataset is scaled by a factor of 0.7 to account for the reduction of SO$_2$ emission resulting from control program associated with Title IV of the Clean Air Act Amendments of 1990. 2.5% of sulfur is assumed to be primary sulfate aerosol. Black and organic carbonaceous aerosol emissions from anthropogenic sources are provided by Bond et al. [2004]. The estimate of carbonaceous aerosol emissions from biomass burning is described in Al-Saadi et al. [2007]. In short, total carbon amount emitted from biomass burning is estimated using the MODIS fire count product, a set of static available fuel data bases for low, medium, and severe fires [Soja et al., 2007] and fire severity, which is based on the prevailing meteorological conditions.

MODIS Aerosol Optical Depth Assimilation

Aerosol optical depth (AOD) retrieval from the MODIS instrument onboard the Terra satellite is used to constrain vertically integrated total aerosol masses within RAQMS. MODIS AOD is assimilated at the MODIS observation time (to within the model time step) as illustrated in Figure 2. MODIS on the Terra satellite makes an observation over the continental US in three separate orbits within five hours,
from the eastern US at ~16Z to the western US at ~21Z. These three orbits cover almost the entire continental US on a daily basis. AOD within RAQMS is computed based on masses of all of modeled aerosol species and relative humidity and can be written as:

$$AOD = \sum_i \sum_k q_{ik} \beta_{ik} dz$$  \hspace{1cm} (1)$$

where $q_{ik}$ is the mixing ratio and $\beta_{ik}$ is the mass specific extinction of aerosol species $i$ at the vertical level $k$. $dz$ is the thickness of the layer. The mass specific extinction is a function of the local relative humidity. The assimilation method used here is optimal interpolation. The observational error (obs_err) is assumed to be 0.2, while the model error is assumed to be same as obs_err except where the ratio of sulfate AOD to total carbonaceous AOD is greater than 5 and the model error is 2_obs_err elsewhere. This is introduced to account for larger first guess errors associated with uncertainties in the biomass burning carbon emission dataset. The assimilated AOD is converted to aerosol masses using the equation (1) and vertically redistributed based on the relative contribution of each species at each vertical layer of the first guess. Figure 3 illustrates an effect of the AOD assimilation on aerosol distributions. Figure 3 (a) is the MODIS AOD distribution for Sept. 7, 2006. It shows significantly elevated AOD values over the Northwestern US region and moderately elevated AOD over the Midwest and the Southeast. The first guess AOD distribution calculated based on modeled aerosol masses and relative humidity is shown in Figure 3 (b). The calculated AOD distribution underestimates AOD over the Northwestern, Midwest and Southeastern regions. This AOD distribution is incorporated into the AOD assimilation as the first guess. The analyzed AOD distribution is shown in Figure (c). As a result of the assimilation, the underestimated AOD values are adjusted toward the MODIS AOD retrieval. Subsequently the aerosol masses are corrected to be consistent with the corresponding AOD values.

**Simulation of Smoke Injection Height**

The heat generated by biomass burning can introduce local temperature anomalies that may generate convection. The convection can lead to transport smoke to a higher altitude. To simulate a convective transport, the surface heat flux anomaly associated with the fire is approximated based on total carbon burned and the conversion factor 8000 BTU/lb [bioenergy.ornl.gov/papers/misc/energy_conv.html]. The heat flux is partitioned into two components, sensible heat flux and radiative heat flux, and added to the soil layer of fire locations. Relative humidity is assumed to be 100% where a fire location is. This gives additional convective energy to the layer above a fire location through latent heating.

**Aerosol Event in September, 2006**

EPA AIRNow hourly PM$_{2.5}$ concentrations show air quality over the southeastern US started deteriorating on Sept. 2, 2006. It continued until Sept. 9, 2006 with a widespread AQI of “Moderate”, with 24 hour average PM$_{2.5}$ concentrations ranging from 15 µg/m$^3$ to 40 µg/m$^3$. During the same time period, Eastern Washington and western Montana reported an AQI of "Moderate" with an occasional AQI of "Unhealthy", which indicates a range of 24 hour average PM$_{2.5}$ concentrations of 65 µg/m$^3$ to 150 µg/m$^3$. Figure 4 shows the monthly average MODIS AOD retrieval for September, 2006. AOD values of 0.4 to 0.8 are seen over the southeastern states. Significantly elevated AOD values of greater than 0.8 are seen over eastern Washington, eastern Montana and British Columbia, Canada. These high PM$_{2.5}$ concentrations and high AOD values over the Pacific Northwest are attributed to smoke emitted from biomass burning in Columbia Complex fires in Washington. In 2006 the US wildland fire season broke records in the number of large fire incidents and acres burned with a total of 9,873,429 acres burned reported nationally. Fires in the Pacific Northwest were one of the biggest contributors to the national acre burned with more than 386,000 acres burned in September (http://www.nifc.gov/information.html). Figure 5 shows time series plots of our estimates of total carbon
emissions from biomass burning over three different regions, the Pacific Northwest, California and the South Central regions. The biomass burning emissions in the Pacific Northwest are dominant in early September and the emissions in the California region become comparable on Sept. 11, 2006.

RESULTS

Model Evaluation

During the August-October, 2006 TexAQS II field experiment in Houston, TX, we assimilated MODIS AOD in near-real-time and used the assimilated AOD to forecast aerosol distributions for the following 72 hours for flight planning. The near-real-time analyses are evaluated with respect to MODIS AOD retrieval and ground-based measurements. Figure 6 is the average AOD distribution calculated based on the RAQMS assimilated mass fields of sulfate, carbonaceous and nitrate aerosol for the same time period. It generally agrees with the monthly average MODIS AOD distribution shown in Figure 4 over the east coast. Both show AOD values of greater than 0.3 to the east of the Ohio River Valley and a relatively higher value to the south of Lake Erie. Both AOD distributions show an area of elevated AOD along the coast of the Gulf of Mexico. In contrast to the east coast, a significant discrepancy is found over the western US where MODIS AOD values of greater than 0.4 are seen in confined areas in western Washington, Idaho, Utah, California and Northern Mexico, whereas the RAQMS AOD distribution does not show such elevated values. Figure 7 shows an AOD fraction associated with carbonaceous aerosol. In general, more than 60% of simulated aerosol over the Pacific Northwest and off the coast of California is carbonaceous aerosol. This suggests that the discrepancy found in Figure 7 is attributed to carbonaceous aerosol.

Next, the model results are compared with ground-based measurements. Figure 8 (a) shows two time series plots of carbonaceous aerosol concentrations measured (black line) and analyzed (red line) at the Deer Park site, southeast of Houston, TX. Figure 8 (b) is the same plots except for sulfate aerosol concentrations. In September, 2006, particle air pollution, with sulfate concentrations of 15 - 20 µg/m³ and carbonaceous aerosol concentrations of 3 - 5 µg/m³, took place in the Houston area until September 15 and relatively clear days were persisted for the rest of the month. The RAQMS simulation is generally in a good agreement with measured sulfate concentrations whereas it overestimates carbonaceous aerosol by a factor of 2 - 2.5. Both simulated carbonaceous and sulfate aerosol concentrations are low with respect to the measurements on Sept. 5 - 6. During this time period, a frontal system came through the Texas area and brought clouds and precipitation. The lower concentration of measured sulfate and meteorological conditions on Sept. 5 - 6 suggest that sulfate aerosol of about 5 µg/m³ is removed from the boundary layer. The model overestimates the wet removal processes of carbonaceous and sulfate aerosol. The AOD assimilation does not adjust the sulfate masses since cloud cover over Texas resulted in no AOD retrieval at this time.

Evaluation of a Smoke Plume Height Using CALIPSO Data

A smoke injection height is one of critical elements that determine the transport pathway of substances emitted from fires. A simulated smoke plume height is evaluated using a vertical profile of integrated attenuated backscatter at 532nm obtained from CALIPSO. Integrated attenuated backscatter (IAB) is a measure of aerosol loading. Unlike backscatter, an effect of the two-way transmittance for all overlying layers is not taken into account. A quantitative comparison of aerosol loading requires unattenuated backscatter. In this study, IAB is used to identify a smoke plume height only. From Sept. 1 to Sept. 9, when a considerable amount of smoke from fires was reported over the Pacific Northwest, CALIPSO acquired vertical profiles of the smoke layers. Three cases are considered as relatively fresh smoke emitted from fires and illustrated in Figures 9 - 11. Figure 9 (a) indicates the geo-location of the CALIPSO overpass (bold white line) superimposed on the MODIS AOD distribution for the day. Figure 9 (b) shows the CALIPSO vertical profile of IAB for the overpass. A white shaded block is a cloud layer
identified with the current CALIPSO aerosol-cloud discrimination algorithm [Liu, 2004]. Figure 9 (c) is a vertical profile of the total aerosol mixing ratio along the CALIPSO overpass. The white line indicates an area of greater than 80% relative humidity. The CALIPSO retrieval shows an aerosol layer with an IAB value of 0.005 1/sr at altitudes from 3km to 5km off the coast of Seattle whereas the RAQMS simulation shows an aerosol layer from the surface to 2.5km. Figure 10 and Figure 11 are same as Figure 9 except for a case observed on Sept. 6 and Sept. 7, respectively. The CALIPSO overpass over the Pacific Northwest on Sept. 6 is very close to an active fire location at about 45˚N (Figure 10 (a)). The smoke height at 45˚N obtained from the IAB retrieval is 3km (Figure 11 (b)), which is in a good agreement with the aerosol layer height from the RAQMS simulation (Figure 10 (c)). The CALIPSO IAB image shows the layer extending from 55˚N to 43˚N, whereas the layer obtained from the RAQMS results extends from 49˚N to 43˚N. Figure 11 shows a smoke plume about 600 miles downwind from an active fire location. The MODIS AOD distribution (Figure 11 (a)) depicts undiluted smoke plume being transported southeastward. The CALIPSO overpass intercepts the coherent thick smoke plume from north to south. The CALIPSO IAB retrieval shows a smoke plume extending from 2km to 4km at the northern edge of the plume. The height of the plume is higher at the southern portion of the plume and the top of the plume reaches 8km at 45˚N. The top of the simulated smoke plume is about 7km at 42˚N. All of three cases show a lower smoke plume height relative to the CALIPSO IAB retrieval. This indicates either a low bias in the wild fire heat anomaly or an underestimate of the convection associated with the wild fire anomalies.

Smoke Emission Estimates

Figure 12 shows the average AOD assimilation increment, which is the difference between the observation and the first guess, relative to the total AOD for September, 2006. It is an indicator of how much the AOD assimilation adjusts the AOD derived from simulated masses in order to match the MODIS AOD retrieval. A small adjustment is seen over the eastern US. A larger adjustment of AOD is made over the western US. A 20% reduction of AOD is seen over the Pacific Northwest (where most of the wild fires occurred), while a 40% reduction of AOD is seen over the Southern Rockies (where much of the smoke from the wild fires was transported). As suggested in Figure 7, these regions are significantly influenced by carbonaceous aerosol emitted from biomass burning during the study period. This indicates either a high bias in carbon emission dataset or an overestimate in the AOD transport. The disparate results of the plume height and analysis increment studies in terms of providing constraints on the wild fire emission estimates illustrates the difficulty in using satellite observations and models to constrain emission estimates. These difficulties arise due to the complexity of the transport processes responsible for the observed carbonaceous aerosol distributions during this time period. For example, underestimates in wild fire emissions or overestimates in loss of hydrophilic carbonaceous aerosols during pyro-convective transport could lead to underestimates in plume injection heights. Conversely, overestimates in wild fire emissions or underestimates in loss of hydrophilic carbonaceous aerosols during frontal precipitation could lead to overestimates on regional smoke transport.

Smoke Influences on Local Air Quality in Houston

The time evolution of AOD fraction associated with simulated carbonaceous aerosol is shown in Figure 13. Between Sept. 4 and Sept 7 carbonaceous aerosols are transported from wild fire sources over the Pacific Northwest southeastward to Texas. A zonal cross section of organic carbonaceous aerosol loading on Sept 7 at the longitude of 95˚W, which is approximately the longitude of Houston, is shown in Figure 14. Over the Houston area (29.77˚N and 95.39˚W), a maximum mixing ratio of greater than 10ppbv is seen near the surface and there is an aerosol layer at 8km with a mixing ratio of 4ppbv. The presence of lofted aerosol layer over the eastern TX is consistent with the measurement obtained from HSRL onboard the NASA Langley King Air on Sept. 7 and Sept. 8 (not shown). This indicates smoke emitted from biomass burning over the Pacific Northwest influenced air quality aloft and the surface over the Houston area on Sept. 7 and 8. However, the RAQMS surface carbonaceous aerosols are
overestimated relative to the Deer Park measurements.

CONCLUSIONS

The RAQMS aerosol assimilation provides useful insight into the regional transport processes that give rise to the observed aerosol distributions over the continental US during September, 2006. Sulfate aerosols dominate the aerosol distribution over the eastern US in September, 2006. In contrast, an aerosol event associated with carbonaceous aerosol from biomass burning is dominant over the western US during the study period. An analysis of the AOD assimilation increment shows a significant reduction of AOD over the western US due to assimilation of MODIS AOD. This suggests an overestimate of carbonaceous aerosol loading from biomass burning in this region. The height of a simulated smoke plume near the wild fire source is evaluated for the first time. Vertical profiles of integrated attenuated backscatter obtained from CALIPSO allow us to evaluate the vertical structure of simulated aerosol plume from biomass burning. The comparisons with CALIPSO retrieval indicate the height of an aerosol layer simulated with RAQMS is 2km lower than that CALIPSO integrated attenuated backscatter shows. This suggests an underestimate in wild fire plume heights in the RAQMS analysis. The RAQMS simulation indicates an influence of smoke on air quality aloft over the Houston area on Sept. 7 and 8. However, an impact of smoke on the surface air quality is overestimated.

REFERENCES


FIGURES

Figure 1. Description of chemical constituents and physical processes associated with aerosol sources and sinks included in the model.

Figure 2. Schematic diagram illustrating a MODIS AOD assimilation procedure.
Figure 3. An example to illustrate an effect of the MODIS AOD assimilation on aerosol distributions on Sept. 7, 2006. a) the MODIS AOD distribution, b) predicted AOD distribution based on modeled aerosol masses and c) assimilated AOD.
Figure 4. Monthly average MODIS AOD for September, 2006.

Figure 5. Time series of total carbon emission from biomass burning in three regions (the Pacific Northwest in blue, California in green and the South Central in red) from August 1st to September 30, 2006 (a). The regions are indicated in (b).
Figure 6. Monthly average RAQMS AOD for September 2006.

Figure 7. Monthly average AOD fraction associated with carbonaceous aerosol for September 2006.
Figure 8. Time series plots of ground-based measurements (black) and RAQMS simulated (red) at Deer Park, TX. a) Carbonaceous aerosol mass concentrations. b) Sulfate aerosol mass concentrations.
Figure 9. Vertical profile comparison for Sept. 2, 2006. (a) CALIPSO ground track superimposed on the MODIS AOD distribution, (b) CALIPSO integrated attenuated backscatter retrieval and cloud distributions and (c) RAQMS total aerosol loading along the CALIPSO overpass.
Figure 10. Same as Figure 9 except for Sept. 6, 2006.

a) RAQMS Aerosol and CALIPSO Orbit

b) CALIOP_L2_05kmAloz-Prov-V1-10.2006-09-06T10-06-32Z,hdf 5km H-Ave

Log_{10}(Integrated Attenuated Backscatter [1/sr])

Cloud

C) RAQMS Total Aerosol (ppbv) along CALIPSO orbit on 2006 09 06

Latitude [deg]
Figure 11. Same as Figure 9 except for Sept. 7, 2006.

- **a)** RAQMS Aerosol and CALIPSO Orbit
- **b)** CALI-LID L2_05kmAlay-Proc-V1-10.2006-09-07T09-10-45ZN.hdf 5km H-Ave
- **c)** RAQMS Total Aerosol (ppbv) along CALIPSO orbit on 2006 09 07
Figure 12. Monthly average AOD assimilation increment for September, 2006.
Figure 13. AOD fraction associated with carbonaceous aerosol at 00Z on Sept. 4 (a), Sept. 6 (b), Sept. 7 (c) and Sept. 8 (d).
Figure 14. Zonal cross section of carbonaceous aerosol mixing ratio at 95°W for 18Z Sept. 7, 2006.