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Global scale model performance evaluation and source attribution tools

Background

The modeling domains of regional and urban-scale photochemical models used in air quality planning for O_3, $PM_{2.5}$, and regional haze are usually defined to encompass the majority of sources and receptors of interest. However, sources outside the modeling domain, such as long-range, international transport or stratospheric intrusion, may affect concentrations within the domain. To quantify the contribution of these extra-regional sources to concentrations within the domain, global-scale chemical transport models are being used increasingly to define time-varying boundary conditions for regional and urban scale modeling, as opposed to the past practice of assuming static conditions based on climatological averages.

The global chemical transport models being used for this purpose include GEOS-Chem, MOZART, RAQMS, CAM-Chem, AM3, UKCM, C-IFS, EMEP, OsloCTM3, and others. These models have been developed primarily as research tools to examine issues related to global atmospheric chemistry, stratospheric chemistry, and climate change. Most of these models have relatively coarse spatial (0.5-2.0 degrees)), and thus, are not useful for directly evaluating air quality impacts on a regional or local scale for which higher resolution is needed. To extend our in-house capabilities, EPA has developed a hemispheric-scale version of the CMAQ model that can be run at relatively coarse resolution to provide boundary conditions for a finer resolution regional sub-domain.

Understanding these extra-regional sources is especially important in the western United States because international transport and natural background often are the largest contributor to O_3 and regional haze in model simulations for rural and high altitude regions in western states. Further, the Clean Air Act includes provisions that enable consideration of non-local contributions when considering mitigation. Several upcoming regional scale air quality modeling simulations intended to support regulatory actions (e.g., ozone SIPs, regional haze SIPs, PM NAAQS review) would benefit from near-term research aimed at improving global scale model performance and developing tools that would enable detailed attribution of the impacts of these extra-regional sources. Additional background information is provided at the end of this document.

Problem Statement

In some cases, biases and errors in global models limit the ability of the global-regional modeling system to reproduce observed spatial or temporal O_3/PM patterns on either an episodic or seasonal scale. Furthermore, the global modeling results that are currently available for use as boundary conditions to regional models do not provide source attribution information for the contributions from international anthropogenic emissions versus international natural emissions, and this distinction is important for regional haze in which planning requirements differ for natural and anthropogenic sources of haze.

Research Topics

- Identify a set of continuing observations, including ground based monitoring and vertical profiles using sondes, lidar, aircraft and satellite data that can be used to evaluate performance of global and nested regional models.
- Facilitate model evaluation studies by creating a mechanism for publishing up-to-date benchmark data sets as additional observations become available (building upon HTAP2, AQMEII3, and TOAR).
- Quantify errors and biases, through model-to-observation (including satellite data) and model-to-model comparisons, due to the use of different global model simulations for defining boundary conditions for regional model simulations of conditions where extra-regional sources are expected to be significant contributors to exceedances of NAAQS or regional haze objectives (building upon HTAP2 and AQMEII3).
- Evaluate, through model-to-model comparisons, the role of global model resolution, chemistry schemes, vertical transport, stratosphere/troposphere exchange, deposition, emissions, and meteorological drivers on errors and biases to identify best modeling practices and assumptions and key uncertainties for future model development (building upon HTAP2, AQMEII, CCMI and AerChemMIP).
- Evaluate the role of observational data assimilation (from satellites, surface networks, and other available sources) in defining regional boundary conditions and develop guidance on best practices.
- Develop and evaluate approaches for updating global emissions inventories for anthropogenic sources as well as wildfires and wind-blown dust. (building upon HTAP2)
- Develop and evaluate approaches for defining 10-30 year global emissions scenarios for O_3 and $PM_{2.5}$ precursors. (building upon HTAP2)
- Perform global model emissions sector zero-out sensitivity simulations to provide source attribution estimates and to evaluate global model performance for natural condition estimates for O_3 and regional haze. (building upon HTAP2)
- Compare zero-out and incremental emissions perturbations to other methods for assessing source-receptor relationships including DDM forward sensitivity analyses, adjoint backwards sensitivity methods, and tagged tracer methods. (building upon HTAP2 and AQMEII3)
- Evaluate the use of source-receptor parameterizations to adjust regional boundary conditions to account for expected or potential changes in global emissions and for use in screening-level analyses of international flows of air pollution such as those required in NEPA analyses or analyses of trade agreements (building upon HTAP2).
- Continue research and development on hemispheric CMAQ and next generation models that represent transport from the global to local scale.

Desired Outcomes

- Identify needs that must be met through a specific investment of EPA resources and needs that can be met through the community efforts of TF HTAP and AQMEII.

- Inform a protocol for "best practice" global air quality modeling (emissions, chemistry, transport, and meteorology) and evaluation, including the identification of specific model outputs needed for diagnostic evaluation and source apportionment.
- Based on the "best practice" protocol, enable EPA/stakeholder development of improved boundary condition data for regional AQ modeling analyses;
- Develop/enhance source attribution tools for hemispheric CMAQ and other global models for potential use in regulatory applications (e.g., NAAQS, Regional Haze, NEPA, etc.).
- Strengthen the community of practice bridging the global and regional modeling communities established through TF HTAP and AQMEII to provide support to EPA/stakeholder needs.

Additional Background

In the United States, global models have been primarily developed and applied by academic or government researchers with funding from NSF, NOAA, and NASA. As with regional and urban-scale models, global chemistry transport models require emissions and meteorological information as inputs. Together, the global emissions inventory, meteorological data, and the chemistry and transport mechanisms define a simulation. Global meteorological data is available from NOAA and NASA for use in model simulations. However, global emissions inventories for air pollutants are not regularly produced by any U.S. agency. The global emissions inventories that are used for specific simulations of interest to U.S. air quality planners are typically built upon inventories constructed for international assessments or cooperative experiments for other years and may be modified on an ad hoc basis for the specific periods of interest.

In the United States, regional models are typically evaluated against observational data from AQS or one of the specific U.S. networks, such as CASTNet, IMPROVE, NADP, etc. Furthermore, performance is usually evaluated for policy-relevant metrics, such as maximum daily eight-hour average O_3 or 24 hour average $PM_{2.5}$, and common tools such as the Atmospheric Model Evaluation Tool (AMET) are used by the community. Thus, separate regional model evaluation results are often comparable. The same observational data are available for use in evaluating global model performance within the United States. However, outside the United States, evaluations include a varying combination of observations from surface networks, sondes, aircraft, and satellites. The inconsistency in the evaluation datasets and metrics used for evaluations makes it difficult to compare separate global model evaluation results. Global models have been compared to one another in a number of coordinated experiments, including those under TF HTAP, AeroCom, and CCMI. These intercomparisons have also included comparisons to observations. HTAP1 (which was focused on simulations of 2001) demonstrated that current global O_3 models vary significantly in their absolute estimates of seasonal average surface O_3 and can have significant biases compared to observations. Model differences and biases increase for estimates of O_3 aloft and at high elevation surface sites. The model spread and bias in HTAP2 results (which includes simulations of 2008-2010) are not significantly different from HTAP1.

For global aerosol models, the model differences and biases compared to observations are generally higher and vary by chemical component of PM. In HTAP1, the differences across models were about a factor of two for sulfate surface concentrations in the mid-latitude continental regions, whereas the model differences approach a factor of four for black carbon and particulate organic matter surface concentrations, and a factor of seven for soil dust surface concentrations. A detailed comparison across the HTAP1-participating models revealed a factor of four difference in the atmospheric lifetime of sulfate calculated by the different models.

As emissions (and climate) in the United States and other parts of the world change over time, the absolute and relative contributions of extra-regional sources to exceedances of NAAQSs and regional haze objectives will also change. To develop robust air quality management plans, expected changes in extra-regional contributions must be assessed. However, as with emissions inventories, global emissions scenarios for O_3 and $PM_{2.5}$ precursors are not produced by U.S. agencies. Meteorological inputs representative of future climate conditions are available, but the change in precursor emissions is likely to have a far greater impact on air quality in the United States over the next 20-50 years than will changes in meteorology.

Recent efforts under TF HTAP, AQMEII, MICS-Asia, TOR, CCMI and AerChemMIP continue to make incremental progress in addressing some of these issues. HTAP2 has produced a global emissions inventory and an ensemble of global model simulations for 2008-2010, as well as a set of future air pollutant emissions scenarios out to 2050. AQMEII-3 has produced a set of complimentary regional simulations for 2010 for North America and Europe that use boundary conditions from the HTAP2 global simulations. A focused comparison of the global and regional simulation results from HTAP2 and AQMEII to sonde and surface observations collected during the 2010 CalNex field campaign is being conducted. Furthermore, for purposes of AQMEII and HTAP, an extensive database of observational information for the North American and European domains has been compiled and systematic comparisons of the global and regional simulations to these data are being conducted. A similar set of regional simulations and observational data is being compiled under MICS-Asia, but the analysis of these simulations and data may lag behind that for North America and Europe. TOR has compiled a reference set of O_3 observations from around the world that may serve as a source of observations for model evaluation, although the relevance of specific sites and metrics must still be evaluated.

An objective of HTAP2 efforts in the coming years is to develop a recommended set of global model evaluation metrics and specifications for a benchmark data set. Given the coarse resolution of global models, care must be taken in comparing gridded model estimates to point observations, especially in locations of strong concentration gradients.

As part of the HTAP2-AQMEII3 effort, a suite of emissions perturbation simulations have been conducted to quantify model sensitivities and source-receptor relationships. The perturbations are defined based on combinations of source regions and pollutants or source regions and emission sector. The source receptor estimates developed from these simulations will be compared to estimates from adjoint and tagged tracer experiments. Parameterizations of the source-receptor relationships will also be developed and evaluated for use in policy analyses.

AerChemMIP is preparing to conduct global atmospheric chemistry simulations in support of CMIP6 and future IPCC assessments. Although the orientation of AerChemMIP is on very long-term trends, it represents an opportunity to leverage a coordinated activity engaging a large number of global models. The CCMI and AEROCOM communities conduct additional simulations designed for evaluation of global models with observations for chemistry-climate interactions including both gases and aerosols.

It is important to recognize that these community efforts are organized without dedicated research funding and are entirely dependent on the individual participants contributing research and analysis. Contributors are motivated to participate through a desire to make their research relevant to the policy community's needs and to make connections with the broader scientific community working on similar issues. For EPA, these efforts offer an important forum for interacting with the global atmospheric chemistry research community, which is not typically engaged in other forums in which EPA participates. For a small amount of investment, it is possible to instigate a large amount of research effort. In general, the efforts have produced far more data (both modeling and observation archives) than is ever analyzed and remain a significantly underutilized resource in a time of limited research funds.