CHAPTER 2

Decision Support for Air Quality

Use of CMAQ as a Decision Support Tool for Air Quality to Climate Change

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1. Introduction

Our ability to understand and forecast the quality of the air we breathe, as well as our ability to understand the science of chemical and physical atmospheric interactions, is at the heart of models of air quality. The quality of air is affected by and has implications for the topics presented in our other chapters. Air quality is affected by energy management and agricultural practices, for instance, and is a major factor in public health. Models of air quality also provide a means of evaluating the effectiveness of air pollution and emission control policies and regulations.

While numerous studies examine the potential impact of climate change on forests and vegetation, agriculture, water resources, and human health (examples are found in Brown et al., 2004; Mearns, 2003; Leung and Wigmosta, 1999; Kalkstein and Valimont, 1987), attempts to project the response of air quality to changes in global and regional climates have long been hampered by the absence of proper tools that can transcend the different spatial and temporal scales involved in climate predictions and air quality assessment and by the uncertainties in climate change predictions and associated air quality changes.

One of the popular modeling tools to study air quality as a whole, including tropospheric ozone, fine particles, toxics, acid deposition, and visibility degradation, is the United States (U.S.) Environmental Protection Agency's (EPA) Community Multiscale Air Quality (CMAQ) modeling system. CMAQ's primary objectives are to (1) improve the ability of environmental managers to evaluate the impact of air quality management practices for multiple pollutants at multiple scales, (2) enhance scientific ability to understand and model chemical and physical atmospheric interactions (http://www.epa.gov/asmdnerl/CMAQ/), and (3) guide the development of air quality regulations and standards and to create state implementation plans. It has been also used to evaluate longer-term pollutant climatology as well as short-term transport from localized sources, and it can be used to perform simulations using downscaled regional climate from global climate change scenarios listed in Intergovernmental Panel on Climate Change (IPCC) (2000). Various observations from the ground and in-situ and from aircrafts and satellite platforms can be used at almost every step of the processing of this Decision-Support Tool (DST) for air quality.

Although there are significant effects of long-range transport, most of the serious air pollution problems are caused by meteorological and chemical processes and their changes at regional and local areas—scales much smaller than those resolved by global climate models (GCM), which are typically applied at a resolution of several hundred kilometers. Current-day regional climate simulations, which typically employ horizontal resolutions of 30 to 60 kilometers (km), are insufficient to resolve small-scale processes that are important for regional air quality, including low-level jets, land-sea breezes, local wind shears, and urban heat island effects (Leung et al., 2006). In addition, climate simulations place enormous demands on computer storage. As a result, most climate simulations only archive a limited set of meteorological variables, the time interval for the archive is usually 6 to 24 hours (e.g., Liang et al., 2006), and some critical information required for air quality modeling is missing.

The interaction and feedback between climate and air chemistry is another issue. Climate and air quality are linked through atmospheric chemical, radiative, and dynamic processes at multiple scales. For instance, aerosols in the atmosphere may modify atmospheric energy fluxes by attenuating, scattering, and absorbing solar and infrared radiation and may also modify cloud formation by altering the growth and droplet size distribution in the clouds. The changes in energy fluxes and cloud fields may, in turn, alter the concentration and distribution of aerosols and other chemical species. Although a few attempts have been made to address these issues, our understanding of climate change is based largely on modeling studies that have neglected these feedback mechanisms.

The impact of climate change on air emissions is also of concern. Changes in temperature, precipitation, soil moisture patterns, and clouds associated with global warming may directly alter emissions, including biogenic emissions (e.g., isoprene and terpenes). Isoprene, an important natural precursor of ozone, is emitted mainly by deciduous tree species. Emission rates are dependent on the availability of solar radiation in the visual range and are highly temperature sensitive. Emissions of terpenes (semi-volatile organic species) may induce formation of secondary organic aerosols. The accompanying changes in the soil moisture, atmospheric stability, and flow patterns complicate these effects, and it is difficult to predict whether climatic change will eventually lead to increased degradation of air quality.

This chapter discusses how CMAQ is used as the DST for studying climate change impact on air quality to address the focus areas required by the Synthesis and Assessment Product (SAP) 5.1 Prospectus: (1) observational capabilities used in the DST, (2) agencies and organizations responsible, (3) characterization of interactions between users and the DST information producers, (4) sources of uncertainties with observation and the decision-support tools, and (5) description of the relation between the DST and climate change information.

2. Description of CMAQ

The U.S. EPA CMAQ modeling system (Byun and Ching, 1999; Byun and Schere, 2006) has the capability to evaluate relationships between emitted precursor species and ozone at urban/regional scales (Appendix W to Part 51 of 40 Code of Federal Regulations: Guideline on Air Quality Models in "http://www.epa.gov/fedrgstr/EPA-AIR/1995/August/Day-09/pr-912.html"). CMAQ uses state-of-the-science techniques for simulating all atmospheric and land processes that affect the transport, transformation, and deposition of atmospheric pollutants. The primary modeling components in the CMAQ modeling system include (1) a meteorological modeling system (e.g., the National Center for Atmospheric Research [NCAR]/Penn State mesoscale model version 5 [MM5]) or a Regional Climate Model (RCM) for the description of atmospheric states and motions, (2) inventories of man-made and natural emissions of precursors that are injected into the atmosphere, and (3) the CMAQ Chemistry Transport Modeling system for the simulation of the chemical transformation and fate of the emissions. The model can operate on a large range of time scales from minutes to days to weeks as well as on numerous spatial (geographic) scales ranging from local to regional to continental.

The base CMAQ system is maintained by the U.S. EPA. The Center for Environmental Modeling for Policy Development, University of North Carolina at Chapel Hill, is contracted to establish a Community Modeling and Analysis System (CMAS) (http://www.cmascenter.org/) for supporting community-based air quality modeling. CMAS helps development, application, and analysis of environmental models and helps distribution of the DST and related tools to the modeling community. The model performance has been evaluated for various applications (e.g., Zhang et al., 2006; Eder et al., 2006; Tong and Mauzerall, 2006; Yu et al., 2007). Table 2-1 lists the Earth observations (of all types—remote sensing and in situ) presently used in the CMAQ DST.

Within this overall DST structure as shown in Table 2-1, CMAQ is an emission-based, three-dimensional (3-D) air quality model that does not utilize daily observational data directly for the model simulations. The databases utilized in the system represent typical surface conditions and demographic distributions. An example is the EPA's Biogenic Emissions Land Use Database, version 3 (BELD3) database (http://www.epa.gov/ttn/chief/emch/biogenic/) that contains land use and land cover as well as demographic and socioeconomic information. At present, the initial conditions are not specified using observed data even for those species routinely measured as part of the controlled criteria species listed in the National Clean Air Act and its Amendments in an urban area using a dense measurement network. This is because of the difficulty in specifying multi-species conditions that satisfy chemical balance in the system, which is subject to the diurnal evolution of radiative conditions and the atmospheric boundary layer as well as temporal changes in the emissions that reflect constantly changing human activities.

The outputs of the CMAQ and its DST are the concentration and deposition amount of atmospheric trace gases and particulates at the grid resolution of the model, usually at 36 km for the continental U.S. domain and 12 km or 4 km for regional or urban scale domains. The end users of the DST want information on the major scientific uncertainties and our ability to resolve them subject to the information on socioeconomic context and impacts. They seek information on the implications at the national, regional, and local scales and on the baseline and future air quality conditions subject to climate change to assess the effectiveness of current and planned environmental

Table 2-1 Input Data Used for Operating the CMAQ-based DST.

Dataset	Type of Information	Source	Usage
Regional climate model output	Simulation results from an RCM used as a driver for CMAQ modeling; processed through meteorology-chemistry interface processor	RCM modeling team; Pacific Northwest National Laboratory (PNNL), University of Illinois at Urbana Champaign (UIUC), National Center for Environmental Prediction (NCEP), EPA, and universities	Regional climate characterization, driver data for air quality simulations, and emissions processing
Land use, land cover, subsoil category, and topography data; topography for meteorological modeling	Describes land surface conditions and vegetation distribution for surface exchange processes	Various sources from U.S. Geological Survey (USGS), National Astronautics and Space Agency (NASA), NCEP EPA, states, etc.	Usually the data are associated with RCMs land surface module; need to be consistent with vegetation information, such as BELD3 if possible
Biogenic emissions land use database version 3 (BELD3)	Land use and biomass data and vegetation/tree species fractions	EPA	Processing of biogenic emissions; used to provide activity data for county-based emission estimates; now also used for land surface modeling in RCM
Air emissions inventories: national emissions inventories and state/special inventories; often called “bottom-up” inventories	Amount and type of pollutants into the atmosphere: Chemical or physical identity of pollutants Geographic area covered Institutional entities Time period over which the emissions are estimated Types of activities that cause emissions	EPA, regional program organizations, state and local government, and foreign governments	Preparation of model-ready emission inputs; perform speciation for the chemical mechanism used; used to evaluate “top-down” emissions (i.e., from inversion of satellite observations though air chemistry models)
Chemical species initial and boundary conditions	Clean species concentration profiles initial input and boundary conditions used for CMAQ simulations; originally from observations from clean background locations	EPA (fixed profiles), Goddard Earth Observing System (GEOS)-Chemical (GEOS-Chem) (Harvard and University of Houston), Model of Ozone and Related Chemical Tracers (MOZART) (NCAR); dynamic concentrations with diurnal variations (daily, monthly or seasonal)	CMAQ simulations; fixed profiles are used for outer domains where no significant emissions sources are located
Archived databases: Air Quality System (AQS)/ AIRNow	Near real-time (AIRNow) and AQSs for ozone, particulate matter, and some toxic species	Joint partnership between EPA and state and local air quality agencies	Measurement data used for model evaluations; report and communicate national air quality conditions for emissions control decision support

policies. Local air quality managers would want to know if the DST could help assess methods of attaining current and future ambient air quality standards and evaluate opportunities to mitigate the climate change impacts. Decision makers would ask modelers to simulate the air quality in the future for a few plausible variations in the model inputs that represent plausible climate scenarios of regional implications. Through sensitivity simulations of the DST with different assumptions on the meteorological and emissions inputs, the effectiveness of such policies and uncertainties in the system can be studied. The results can be also compared with the historic air quality observations with similar ambient conditions to validate predictions of the DST.

3. Potential Future Uses and Limits

Although one of the major strengths of CMAQ is its reliance on the first principles of physics and chemistry, a few modeling components, such as cloud processes, fine scale turbulence, radiative processes, etc., rely on parameterizations or phenomenological concepts to represent intricate and less well known atmospheric processes. The present limitations in science parameterizations and modeling difficulties will continuously be improved as new understanding of these phenomena are obtained through various measurements and model evaluation/verification. The development of the chemical mechanism, Carbon Bond 05, which recently replaced Carbon Bond 04 is a case in point. The reliability of the CMAQ simulation result is subject to quality of the emission inputs, both at the global and regional scales, which depend heavily on socioeconomic conditions. Because such estimates are obtained using projection models in relevant socioeconomic disciplinary areas, their accuracy must be scrutinized when used for the decision-making process. The CMAQ DST users/operators may not always have domain expertise to discern the validity of such results.

CMAQ needs to have the capability to utilize available observations to specify more accurately the critical model inputs, although they have been chosen based on best available information and current experience. A data assimilation approach may be used to improve the system performance at different processing steps.

For example, research has been undertaken to use satellite remote-sensing data products together with high-resolution land use and land cover data to improve the land-surface parameterizations and boundary layer schemes in the RCMs (e.g., Pour-Biazar et al., 2007). Active research in chemical data assimilation (e.g., Constantinescu et al., 2007a and b) is currently conducted with models such as Sulfur Transport Eulerian Model (STEM)-II (Carmichael et al., 1991) and GEOS-Chem (Bey et al., 2001) , which utilize both in-situ and satellite observations (e.g., Sandu et al., 2005; Kopacz et al., 2007; Fu et al., 2007). Because of the coarse spatial and temporal resolutions of the satellite data collected in the 1960s through the 1980s and gas measurements through the launch of Earth Observing System (EOS) Aura in 2004, most research in this area has been performed with global chemistry-transport models. As the horizontal footprints of modern satellite instruments reach the resolution suitable for regional air quality modeling, these data can be used to evaluate and then improve the bottom-up emissions inputs in the regional air quality models. However, they do not provide required vertical information. The exception is occultation instruments, but these do not measure low enough in altitude for near-surface air quality applications. In-situ and remote-sensing measurements from ground and aircraft platforms could be used to augment the satellite data in these data assimilation experiments.

Utilization of the column-integrated satellite measurements in a high-resolution, 3-D grid model like CMAQ poses serious challenges in distributing the pollutants vertically and separating those within and above the atmospheric boundary layer. Because similar problems exist for the retrieval of meteorological profiles of moisture and temperature, experiences that include these can be adapted for a few well-behaved chemical species. A data assimilation tool can be used to improve the initial and boundary conditions using various in-situ and satellite measurements of atmospheric constituents. At present, however, an operational assimilation system for CMAQ is not yet available, although prototype assimilation codes have recently been generated (Hakami et al., 2007; Zhang et al., 2007). Should these data assimilation tools become part of the DST, various conventional and new satellite products, including Tropospheric Emission Spectrometer ozone profiles, Geostationary Operational Environmental Satellites (GOES) hourly total ozone column (GhTOC) data, Ozone Monitoring Instrument (OMI) total ozone column (TOC), the Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observation (CALIPSO) (http://www-calipso.larc.nasa.gov/) attenuated backscatter profiles, and OMI aerosol optical thickness (AOT) data, can be utilized to improve the urban-to-regional scale air quality predictions.

Because of the critical role of the RCM as the driver of CMAQ in climate change studies, RCM results for the long-term simulations must be verified thoroughly. To date, evaluation of the RCM has been performed for the air quality-related operations only for relatively short simulation periods. For example, the simulated surface temperature, pressure, and wind speed must be compared to surface observations to determine how well the model captures the mean land-ocean temperature and pressure gradients, the mean sea breeze wind speeds, the average inland penetration of sea breeze, the urban heat island effect, and the seasonal variations of these features. Comparisons with rawinsonde soundings and atmospheric profiler data would determine how well the model reproduces the averaged characteristics of the afternoon mixed layer heights and of the early morning temperature inversion as well as the speed and the vertical wind shears of the low-level jets. In addition to these mesoscale phenomena, changes in other factors can also alter the air pollution patterns in the future and need to be carefully examined. These factors include the diurnal maximum, minimum, and mean temperature; cloud cover; thunderstorm frequency; surface precipitation and soil moisture patterns; and boundary layer growth and nocturnal inversion strength.

In global model applications, it has been demonstrated that satellite measured biomass burning emissions data are necessary to enhance model predictability (e.g., Duncan et al., 2003; Hoelzemann et al., 2004). Duncan et al. (2003) presented a methodology for estimating the seasonal and interannual variation of biomass burning, which was designed for use in global chemical transport models using fire-count data from the Along Track Scanning Radiometer and the Advanced Very High Resolution Radiometer (AVHRR) World Fire Atlases. The Total Ozone Mapping Spectrometer (TOMS) Aerosol Index data product was used as a surrogate to estimate interannual variability in biomass burning. Also Spracklen et al. (2007) showed that the wildfire contribution to the interannual variability of organic carbon aerosol can be studied using the area-burned data and ecosystem specific fuel loading data. A similar fire emissions dataset at the regional scales could be developed for use in a study of climate impact on air quality. For retrospective application, a method similar to that used by the National Oceanic and Atmospheric Administration's (NOAA) Hazard Mapping System for Fire and Smoke (http://www.ssd.noaa.gov/PS/FIRE/hms.html) may be used to produce a long-term regional scale fire emissions inventory for climate impact analysis.

4. Uncertainty

The CMAQ modeling system as currently operated has several sources of uncertainty in addition to those associated with some of the limits described in the previous section. In particular, when CMAQ is used to study the effects of climate change and air quality, improvements in several areas are necessary to reduce uncertainty. First, the regional air quality models employ limited modeling domains and, as such, they are ignorant of air pollution events outside the domains unless proper dynamic boundary conditions are provided. Second, because the pollutant transport and chemical reactions are fundamentally affected by the meteorological conditions, improvement of both the global and regional climate models and the downscaling methods by evaluating and verifying physical algorithms that have been implemented with observations is necessary to improve the system's overall performance. Third, the basic model inputs, including land use/vegetation cover descriptions and emissions inputs must be improved. Fourth, the model representativeness issues, including grid resolution problems, compensating errors among the model components, and incommensurability of the model results compared with the dimensionality of the measurements (i.e., inherent differences in the modeled outputs that represent volume and time averaged quantities to the point or path-integrated measurements) as discussed in Russell and Dennis (2000) and NARSTO (2000), need to be addressed. These factors are the principal cause of simulation/prediction errors.

Although the models incorporated in this DST are first principle-based environmental models, they have difficulties in representing forcing terms in the system, particularly, the influence of the earth's surface, long-range transport, and uncertainties in the model inputs such as daily emissions changes due to anthropogenic and natural events. There is ample opportunity to reduce some uncertainties associated with CMAQ through model evaluation and verification using current and future meteorological and atmospheric chemistry observations. Satellite data products assimilated in the global chemical transport models (GCTM) could provide better dynamic lateral boundary conditions for the regional air quality modeling (e.g., Al-Saddi et al., 2005). Additional opportunities to reduce the model uncertainty include comparison of model results with observed data at different resolutions, quantification of effects of initial and boundary conditions and chemical mechanisms, application of CMAQ to estimate the uncertainty of input emissions data, and ensemble modeling (using a large pool of simulations among a variety of models) as a means to estimate model uncertainty.

A limitation in CMAQ applications, and therefore a source of uncertainty, has been the establishment of initial conditions. The default initial conditions and lateral boundary conditions in CMAQ are provided under the assumption that after spin-up of the model, they no longer play a role, and in time, surface emissions govern the air quality found in the lower troposphere. Song et al. (2007) showed that the effects of the lateral boundary conditions differ for different latitudes and altitudes as well as seasons. In the future, dynamic boundary conditions can be provided by fully integrating the GCTMs as part of the system. Several research groups are actively working on this, but the simulation results are not yet available in open literature. A scientific cooperative forum, the Task Force on Hemispheric Transport of Air Pollution (http://www.htap.org/index.htm), is endeavoring to bring together the national and international research efforts at the regional, hemispheric, and global scales to develop a better understanding of air pollution transport in the Northern Hemisphere. This task force is currently preparing its 2007 Interim Report addressing various long-range transport of air pollutant issues (http://www.htap.org/activities/2007_Interim_Report.htm). Although the effort does not directly address climate change issues, many of findings and tools used are very relevant to meteorological and chemical downscaling issues.

Ultimately, CMAQ should consider all the uncertainties in the inputs. The system's response may be directly related to the model configuration and algorithms (e.g., structures, resolutions, and chemical and transport algorithms), compensating errors, and the incommensurability of modeling nature as suggested by Russell and Dennis (2000).

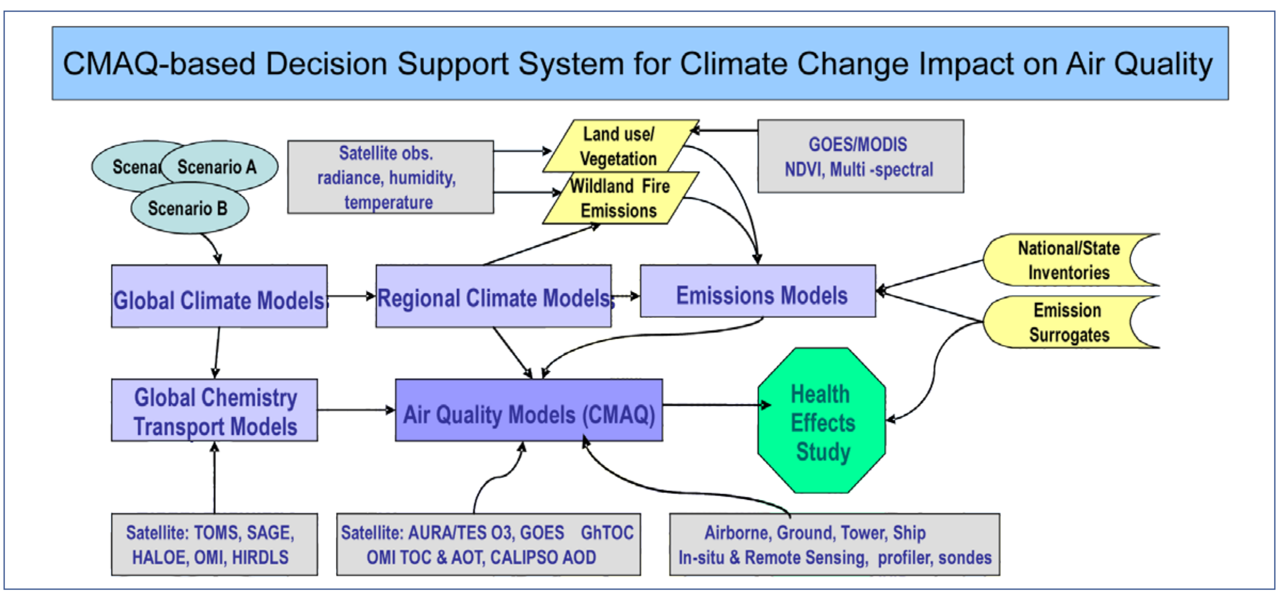
5. Global Change Information and CMAQ

CMAQ could be used to help answer several questions about the relationship between air quality and climate change, including the following:

1. How will global warming affect air quality in a region?
2. How will land use change due to climate change and urbanization, or how will intentional management decisions affect air quality?
3. How much will climate change alter the frequency, seasonal distribution, and intensity of synoptic weather patterns that influence pollution in a region?
4. How sensitive are air quality simulations to uncertainty in wildfire projections and to potential land management scenarios?
5. How might the contribution of the local production and long-range transport of pollutants differ due to different climate change scenarios?
6. Will future emissions scenarios or climate changes affect the frequency and magnitude of high pollution events?

To provide answers to these questions, CMAQ will rely heavily on climate change-related information. In addition to the influence of greenhouse gases and global warming, other forcing functions include population growth, land use changes, new emission controls being implemented, and the availability of new energy sources to replace the existing high-carbon sources. Different scenarios can be chosen either to study potential impacts or to estimate the range of uncertainties of the predictions. The two upstream climate models, GCMs and RCMs, generate the climate change data that drive a GCTM and CMAQ. Both the GCMs and RCMs are expected to represent future climate change conditions while simulating historic climate conditions that can be verified with comprehensive datasets such as the NCEP Reanalysis data provided by the NOAA/Oceanic and Atmospheric Research/Earth Systems Research Laboratory (ESRL) Physical Sciences Division, Boulder, Colorado, from their Web site, http://www.cdc.noaa.gov/cdc/data.ncep.reanalysis.html. The meteorology simulated by the climate models represents conditions in future year scenarios, reflecting changing atmospheric conditions. Furthermore, emissions inputs used for the GCTM and CMAQ must reflect the natural changes and/or anthropogenic developments related to climate change and other factors (e.g., population growth and geographical population shifts due to climate change).

In recent years, the EPA Science to Achieve Results (STAR) program has funded several projects on the possible effects of climate change on air quality and ecosystems. A majority of these projects have adopted CMAQ as the base study tool. Figure 2-1 provides a general schematic of the potential structure of a CMAQ-based climate change DST. The figure shows potential uses of CMAQ for climate study; most climate-related CMAQ applications are not yet configured as fully as indicated in the figure.



AOD = aerosol optical depth; HALOE = Halogen Occultation Experiment; HRDLS = High Resolution Dynamics Limb Sounder ; SAGE = Stratospheric Aerosol and Gas Experiment; TES = Tropospheric Emission Spectrometer

Figure 2-1 Configuration of CMAQ-based DST for Climate Change Impact Study

The projects linking CMAQ and climate study have used upstream models and downstream tools, including those identified in Table 2-1. Related projects that use regional air quality models other than CMAQ are also listed. For the GCMs, the NCAR Community Climate Model (CCM) (Kiehl et al., 1996), NASA Goddard Institute for Space Studies (GISS) model (e.g., Hansen et al., 2005), and NOAA Geophysical Fluid Dynamics Laboratory (GFDL) Climate Model 2 (CM2) (Delworth et al., 2006) are the most popular global models for providing meteorological inputs representing climate change events. A recent description for the GISS model can be found in Schmidt et al. (2006) (http://www.giss.nasa.gov/tools/) and for the CCM in Kiehl et al. (1996) (http://www.cgd.ucar.edu/cms/ccm3/). A newer version of the CCM was released on May 17, 2002 with a new name—the Community Atmosphere Model (http://www.ccsm.ucar.edu/models/atm-cam). The model is described in Hurrell et al. (2006).

As shown in Table 2-2, for climate change studies, CMAQ is linked with upstream models such as a GCM, a global tropospheric chemistry model (GTCM), and an RCM to provide emissions sensitivity analysis, source apportionment, and data assimilation to assist policy and management decision-making activities, including health impact analysis. Certain EPA STAR projects (Hogrefe et al., 2004 and 2005; Knowlton et al., 2004; Civerolo et al., 2007) have utilized the CMAQ-based DST to assess whether climate change would influence the effectiveness of current and future air pollution policy decisions subject to the potential changes in local and regional meteorological conditions.

Table 2-2 Illustrative Example of the Potential Uses of the Models and Upstream and Downstream Tools for a CMAQ-based Climate Change Impact DST

Component	Functions	Model Name: Owner	Users
GCM	Performs climate change simulations over the globe for different Special Report on Emissions Scenarios (SRES) climate scenarios; typical resolution for a long-term (50 year) simulation is at 4° x 5° latitude and longitude	CCM: NCAR Goddard Institute for Space Studies (GISS) GCM: NASA CM2: GFDL of NOAA	Climate research institutes, universities, and government institutions
GCTM	Computes global scale chemical states in the atmosphere; uses same resolution as GCM	GEOS-Chem: NASA, Harvard University MOZART: NCAR (Earth and Sun Systems Laboratory [ESSL]/Atmospheric Chemistry Division)	Global chemistry research organizations, universities, and government institutions
RCM	Simulates regional scale climate and meteorological conditions downscaling the GCM output; for U.S. application ~36-km resolution used	MM5-based: NCAR, PNNL, UIUC, and others The weather research and forecasting (WRF)/ advanced research WRF (ARW) core based: NCAR, UIUC Eta-based: NCEP (before June 2006) The WRF-nonhydrostatic mesoscale model (NMM) core based: NCEP (after June 2006)	Regional climate research groups, universities, and government institutions
Regional air quality models	Performs air quality simulations at regional and urban scales at the same resolution as the RCM	CMAQ: EPA Comprehensive air quality model with extensions: Environment WRF-Chemical (WRF-Chem): NOAA/NCAR STEM-II: University of Iowa	Regional, state, and local air quality organizations; universities; private industries; and consulting companies
Downstream tools for decision support	Performs additional computations to help decision support, such as sensitivity, source apportionment, and exposure studies	CMAQ/ Decoupled Direct Method: Georgia Institute of Technology CMAQ/4-dimensional variable: CalTech/Virginia Tech/University of Houston Stochastic human exposure and dose simulation: EPA Total risk integrated methodology: EPA	Universities and consulting companies
Upstream tools for representing climate change impacts on input data	Performs additional computations to generate model inputs that affect simulations	Land-surface models SLEUTH: USGS and University of California, Santa Barbara (captures urban patterns) Community land model: NCAR (used for RCM and biogenic emission estimates after growth)	Universities and consulting companies

Other EPA STAR projects employ global climate change information from a GCM. For example, Tagaris et al. (2007) and Liao et al. (2007) use the results of GCM simulation with the well-mixed greenhouse gases—CO_2, CH_4, N_2O, and halocarbons—updated yearly from observations for 1950 to 2000 (Hansen et al., 2002) and for 2000 to 2052 following the A1B SRES scenario from the Intergovernmental Panel on Climate Change (IPCC) 2001. The simulation used ozone and aerosol concentrations in the radiative scheme fixed at present-day climatological value provided in Mickley et al. (2004).

To resolve the meteorological features affecting air pollution transport and transformation at a regional scale, the coarse scale meteorological data representing the climate change effects derived from a GCM are downscaled using an RCM. An RCM is often based on a limited-domain, regional mesoscale model (such as mesoscale model version 5 [MM5]), the Regional Atmospheric Modeling System, Eta, and the WRF-ARW or WRF-NMM. An alternative method for constructing regional scale climate change data is through statistical downscaling, which evaluates observed spatial and temporal relationships between large-scale (predictors) and local (predictands) climate variables over a specified training period and domain (Spak et al., 2007). Because of the need to use a meteorological driver that satisfies constraints of dynamic consistency (i.e., mass and momentum conservations) for regional scale air quality modeling (e.g., Byun, 1999 a and b), the CMAQ modeling system relies exclusively on the dynamic downscaling method.

Regional chemistry/transport models, like CMAQ, are better suited for regional air quality simulations than a GCTM because of the acute air pollution problems that are managed and controlled through policy decisions at specific geographic locations. Difficulty in prescribing proper boundary conditions, especially in the upper troposphere, is one of the deficiencies of CMAQ simulations of air quality (e.g., Tarasick et al., 2007; Tang et al., 2007). Therefore, one of the main roles of the GCTM is to provide proper dynamic boundary conditions for CMAQ to represent temporal variation of chemical conditions that might be affected by the long-range transport of pollution (e.g., particle from large-scale biomass burnings) from outside the regional domain boundaries (Holloway et al., 2002; In et al., 2007). The contemporary EPA-funded projects on climate change impact on air quality mainly use two 3-D GCTM models: the NASA/Harvard GEOS-Chem (Bey et al., 2001) and the NCAR MOZART (Brasseur et al., 1998; Horowitz et al., 2003).

The GEOS-Chem model (http://www-as.harvard.edu/chemistry/trop) is a global model for predicting tropospheric composition. The model was originally driven by the assimilated meteorological observation data from the GEOS of the NASA Global Modeling and Assimilation Office (GMAO). GEOS-Chem has been used as community assessment models for NASA Global Model Initiative, climate change studies with the NASA/GISS GCM, chemical data assimilation of tropospheric gaseous and aerosol species at NASA GMAO, and regulatory models for air pollution, particularly in providing long-range transport information for regional air quality models. Long-term retrospective studies are possible with GEOS data, which are available from 1985 to present at a horizontal resolution of 2 degrees (latitude) by 2.5 degrees (longitude) until the end of 1999 and 1 degree by 1 degree afterward. For climate studies, the NASA GISS GCM meteorological outputs are used instead. Emission inventories include a satellite-based inventory of fire emissions (Duncan et al., 2003) with expanded capability for daily temporal resolution (Heald et al., 2003) and the National Emissions Inventory for 1999 for the U.S. with monthly updates in order to achieve adequate consistency with the CMAQ fields at the GEOS-Chem/CMAQ interface.

MOZART (http://gctm.acd.ucar.edu/mozart/models/m3/index.shtml) is built on the framework of the Model of Atmospheric Transport and Chemistry that can be driven with various meteorological inputs and at different resolutions, such as meteorological reanalysis data from NCEP, NASA GMAO, and the European Centre for Medium-Range Weather Forecasts. For climate change applications, meteorological inputs from the NCAR Community Climate Model (CCM3) are used. MOZART includes a detailed chemistry scheme for tropospheric ozone, nitrogen oxides, and hydrocarbon chemistry; a semi-Lagrangian transport scheme; dry and wet removal processes; and emissions inputs. Emission inputs include sources from fossil fuel combustion, biofuel and biomass burning, biogenic and soil emissions, and oceanic emissions. The surface emissions of NOx, CO, and NMHCs are based on the inventories described in Horowitz et al. (2003), aircraft emissions based on Friedl (1997), and lightning NOx emissions that are distributed at the location of convective clouds.

GCTMs are applied to investigate numerous tropospheric chemistry issues involving gases—CO, CH_4, OH, NOx, HCHO, and isoprene—and inorganic (sulfates and nitrates) and organic (elemental and organic carbons) particulates. Various in-situ, aircraft, and satellite-based measurements are used to provide the necessary inputs to verify the science process algorithms and to perform general model evaluations. They include vertical profiles from aircraft observations as compiled by Emmons et al. (2000), multiyear analysis of ozonesonde data (Logan, 1999), and those available at the Community Data Web site managed by the NCAR ESSL Atmospheric Chemistry Division as well as multiyear surface observations of CO reanalysis (Novelli et al., 2003). Current and previous atmospheric measurement campaigns are listed in Web pages by NOAA ESRL (http://www.esrl.noaa.gov/); NASA, Tropospheric Integrated Chemistry Data Center (http://www-air.larc.nasa.gov/); and NCAR ESSL Atmospheric Chemistry Division Community Data (http://www.acd.ucar.edu/Data/). These observations are used to set boundary conditions for the slow reacting species, including CH4, N2O, and chlorofluorocarbons (CFC), and to evaluate other modeled species, including CO, NOx, peroxyacetyl nitrate (PAN), HNO3, HCHO, acetone, H2O2, and non-methane hydrocarbons. In addition, several satellite measurements of CO, NO2, and HCHO from the Global Ozone Monitoring Experiment, the Scanning Imaging Absorption Spectrometer for Atmospheric Chartography, and OMI instruments have been used extensively to verify the emissions inputs and performance of the GCTM.

The grid resolutions used in the studies discussed above are much coarser than those used in the air quality models for studying emission control policy issues, such as evaluating state implementation plans. State implementation plan modeling typically utilizes over 20 vertical layers with a 4-km horizontal grid spacing to reduce uncertainties in the model predictions near the ground and around high-emission source areas, including urban and industrial centers. Although Civerolo et al. (2007) applied CMAQ at a higher resolution, the duration of the CMAQ simulation was far too short a time scale to evaluate the regional climate impacts in detail.

One of the additional key limitations of using the CMAQ for climate change studies is that the linkages between climate and air quality and from the global scale to regional scale models are only one way (i.e., no feedback). Jacob and Gilliland (2005) stated that one-way assessment of the global change scenarios would be less useful for projection of air pollutant emissions because the evolution of regional air quality policies were not accounted for in these storylines. Also, to represent the interactions between atmospheric chemistry and meteorology, such as radiation and cloud/precipitation microphysics, particulates, and heterogeneous chemistry, a two-way linkage must be established between the meteorology and chemistry models. An online modeling approach as implemented in WRF-Chemistry (WRF-Chem) is an example of such a linkage, but still there is a need to develop a link between the global and regional scales. A multi-resolution modeling system, such as demonstrated by Jacobson (2001 a, b), might be necessary to address the true linkage between air pollution forcing and climate change and to provide the urban-to-global connection.

In addition, there would be significant benefits to linking other multimedia models describing subsoil conditions, vegetation dynamics, hydrological processes, and ocean dynamics, including the physical/chemical interactions between the ocean micro-sublayer and atmospheric boundary layer to an air quality model. To generate such a mega model under one computer coding structure would require handling of extremely different state variables in each multimedia model with substantially different data. Furthermore, interactions among the multimedia models need multidirectional data inputs, quality assurance checkpoints, and decision-support entries. A more generalized online and two-way data exchange tool currently being developed under the Earth System Modeling Framework (http://www.esmf.ucar.edu/) may be a viable option.

Observations not only represent the real changes in the climate but also provide a fundamental database to verify various modeling components in the DST. The meteorological reanalysis data are available both in regional and global scales, but a similar atmospheric chemistry database for air quality is lacking. An ozone database from the ozonesonde system and other in-situ measurements are useful for global-scale studies. But for regional air quality studies, the availability of such measurements representing long-term urban and local conditions is limited. Satellite or other remote-sensing platform observations may provide additional data sources to build an atmospheric chemistry reanalysis database at global and regional scales, but theses observations are mainly limited to ozone and aerosols. Such a chemical reanalysis database can be utilized to study long-term air quality trends; evaluate science process components in the air quality models, emissions, and other model inputs and configurations; and improve model predictions through data assimilation approaches.