

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 US Environmental Protection Agency's (EPA) Community Multiscale Air Quality (CMAQ) modeling system. CMAQ has as its primary objectives 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 climatologies 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 IPCC (2000). Various observations from the ground and from *in-situ*,

751 aircrafts, and satellite platforms can be used at almost at every step of the processing of this Decision Support System
752 (DSS) for air quality.

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

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

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

776 This chapter discusses how CMAQ is used as the DSS for studying climate change impact on air quality addressing
777 the focus areas required by the *SAP 5.1 Prospectus*: (1) observational capabilities used in the DSS, (2) agencies and
778 organizations responsible, (3) characterization of interactions between users and the DSS information producers, (4)

779 sources of uncertainties with observation and the decision support tools, and (5) description of the relation between the
780 DSS and climate change information.

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783 **2. Description of CMAQ**

784 The US EPA CMAQ modeling system (Byun and Ching, 1999; Byun and Schere, 2006) has the capability to
785 evaluate relationships between emitted precursor species and ozone at urban/regional scales (Appendix W to Part 51 of
786 40CFR: Guideline on Air Quality Models in “[http://www.epa.gov/fedrgstr/EPA-AIR/1995/August/Day-09/pr-
787 912.html](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
788 transport, transformation, and deposition of atmospheric pollutants. The primary modeling components in the CMAQ
789 modeling system include (1) a meteorological modeling system (e.g., The Fifth-Generation NCAR/Penn State
790 Mesoscale Model, MM5) or a Regional Climate Model (RCM) for the description of atmospheric states and motions,
791 (2) inventories of man-made and natural emissions of precursors that are injected into the atmosphere, and (3) the
792 CMAQ Chemistry Transport Modeling (CTM) system for the simulation of the chemical transformation and fate of the
793 emissions. The model can operate on a large range of time scales from minutes to days to weeks as well as on numerous
794 spatial (geographic) scales ranging from local to regional to continental.

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

802 Within this overall DSS structure as shown in Table 1, CMAQ is an emission-based, three-dimensional (3-D) air
803 quality model that does not utilize daily observational data directly for the model simulations. The databases utilized in
804 the system represent typical surface conditions, and demographic distributions. An example is the EPA’s Biogenic
805 Emissions Land Use Database, version 3 (BELD3) database (<http://www.epa.gov/ttn/chief/emch/biogenic/>) that
806 contains land use and land cover as well as the demographic and socioeconomic information. At present the initial

807 conditions are not specified using observed data even for those species routinely measured as part of the controlled
808 criteria species listed in the National Clean Air Act and its Amendments (CAAA) in an urban area using a dense
809 measurement network. This is because of the difficulty in specifying the multi-species conditions that satisfy chemical
810 balance in the system, which is subject to the diurnal evolution of radiative conditions and of the atmospheric boundary
811 layer as well as temporal changes in the emissions that reflect constantly changing human activities.

812 The main output of the CMAQ and its DSS is the concentration and deposition amount of atmospheric trace gases
813 and particulates at the grid resolution of the model, usually at 36 km for the continental United States (CONUS)
814 domain, and 12 km or 4 km for regional or urban scale domains. The end users of the DSS want information on the
815 major scientific uncertainties and our ability to resolve them subject to the information on socioeconomic context and
816 impacts. They seek information on the implications at the national, regional, and local scales and on the baseline and
817 future air quality conditions subject to climate change to assess the effectiveness of current and planned environmental
818 policies. Local air quality managers would want to know if the DSS could help assess methods of attaining current and
819 future ambient air quality standards and evaluate opportunities to mitigate the climate change impacts. Decision makers
820 would ask modelers to simulate the air quality in the future for a few plausible variations in the model inputs that
821 represent plausible climate scenarios of regional implications. Through sensitivity simulations of the DSS with
822 different assumptions on the meteorological and emissions inputs, the effectiveness of such policies and uncertainties in
823 the system can be studied. The results can be also compared with the historic air quality observations with similar
824 ambient conditions to validate predictions of the DSS.

825

826 **3. Potential Future Uses and Limits**

827 Although one of the major strengths of CMAQ is its reliance on the first principles of physics and chemistry, a few
828 modeling components, such as cloud processes, fine scale turbulence, radiative processes, etc., rely on
829 parameterizations or phenomenological concepts to represent intricate and less-well known atmospheric processes. The
830 present limitations in science parameterizations and modeling difficulties will continuously be improved as new
831 understanding of these phenomena are obtained through various measurements and model evaluation/verification. The
832 development of the chemical mechanism, Carbon Bond 05 (CB05), which recently replaced CB-4 is a case in point.
833 The reliability of the CMAQ simulation result is subject to quality of the emission inputs, both at the global and
834 regional scales, which depend heavily on socio-economic conditions. Because such estimates are obtained using

835 projection models in relevant socio-economic disciplinary areas, their accuracy must be scrutinized when used for the
836 decision-making process. The CMAQ DSS users/operators may not always have domain expertise to discern the
837 validity of such results.

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

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842 Table 1. Input data used for operating the CMAQ-based DSS.

843 <<footnotes: PNNL, UIUC, NCEP, EPA, USGS, NASA>>

844 PNNL: Pacific Northwest National Laboratory

845 UIUC: University of Illinois at at Urbana-Champaign

846 NCEP: National Center for Environmental Prediction

847 EPA: Environmental Protection Agency

848 USGS: US Geological Survey

849 NASA: National Astronautics and Space Agency

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851 For example, research has been undertaken to use satellite remote sensing data products together with high-
852 resolution land use and land cover (LULC) data to improve the land-surface parameterizations and boundary layer
853 schemes in the RCMs (e.g., Pour-Biazar *et al.*, 2007). Active research in chemical data assimilation (e.g.,
854 Constantinescu *et al.*, 2007a and b) is currently conducted with models such as STEM-II (Carmichael *et al.*, 1991) and
855 Goddard Earth Observing System (GEOS)-Chem (Bey *et al.*, 2001) , which utilize both *in situ* and satellite observations
856 (e.g., Sandu *et al.*, 2005; Kopacz *et al.*, 2007; Fu *et al.*, 2007). Because of the coarse spatial and temporal resolutions of
857 the satellite data collected in the 1960s through the 1980s, and gas measurements through the launch of EOS Aura in
858 2004, most research in this area has been performed with global chemistry-transport models. As the horizontal
859 footprints of modern satellite instruments reach the resolution suitable for regional air quality modeling, these data can
860 be used to evaluate and then improve the bottom-up emissions inputs in the regional air quality models. However, they
861 do not provide required vertical information. The exception is occultation instruments, but these do not measure low

862 enough in altitude for air quality applications. In-*situ* and remote sensing measurements from ground and aircraft
863 platforms could be used to augment the satellite data in these data assimilation experiments.

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

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

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

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902 **4. Uncertainty**

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

915 measurements), as discussed in Russell and Dennis (2000) and NARSTO (2000), need to be addressed. These factors
916 are the principal cause of simulation/prediction errors.

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

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

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

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945 **5. Global Change Information and CMAQ**

946 CMAQ could be used to help answer several questions about the relationship between air quality and climate
947 change. For instance:

948

949 1) How will global warming affect air quality in a region?

950 2) How will land use change due to climate, urbanization, or intentional management decisions affect air quality?

951 3) How much will climate change alter the frequency, seasonal distribution, and intensity of synoptic weather patterns
952 that influence pollution in a region?

953 4) How sensitive are air quality simulations to uncertainty in wildfire projections and to potential land management
954 scenarios?

955 5) How might the contribution of the local production and long-range transport of pollutants differ due to different
956 climate change scenarios?

957 6) Will future emissions scenarios or climate changes affect the frequency and magnitude of high pollution events?

958 To provide answers to these questions, CMAQ will rely heavily on climate-change-related information. In addition
959 to the influence of greenhouse gases and global warming, other forcing functions include population growth, land use
960 changes, new emission controls being implemented, and new energy sources to be available to replace the existing high-
961 carbon sources. Different scenarios can be chosen either to study potential impacts or to estimate the range of
962 uncertainties of the predictions. The two upstream climate models, GCMs and RCMs, generate the climate change data
963 that drive a GCTM and CMAQ. Both the GCMs and RCMs are expected to represent future climate change conditions
964 while simulating historic climate conditions that can be verified with comprehensive datasets such as the NCEP
965 Reanalysis data provided by the NOAA/OAR/ESRL PSD, Boulder, CO, from their Web site,
966 <http://www.cdc.noaa.gov/cdc/data.ncep.reanalysis.html> The meteorology simulated by the climate models represents

967 conditions in future year scenarios, reflecting changing atmospheric conditions. Furthermore, emissions inputs used for
968 the GCTM and CMAQ must reflect the natural changes and/or anthropogenic developments related to climate change
969 and other factors (e.g., population growth and geographical population shifts due to climate change).

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

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

984

985 Table 2. An illustrative example of the potential uses of the models and upstream and downstream tools for a CMAQ-
986 based Climate Change Impact Decision Support System.

987 <footnote: WRF-ARW, WRF-NMM, SLEUTH>>

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989 As shown in Table 2, for climate change studies, CMAQ is linked with upstream models such as a global climate
990 model (GCM), a global tropospheric chemistry model (GTCM), and a regional climate model (RCM) to provide
991 emissions sensitivity analysis, source apportionment, and data assimilation to assist policy and management decision-
992 making activities, including health impact analysis. Certain EPA STAR projects (Hogrefe *et al.*, 2004 and 2005;
993 Knowlton *et al.*, 2004; Civerolo *et al.*, 2007) have utilized the CMAQ-based DSS to assess whether climate change

994 would influence the effectiveness of current and future air pollution policy decisions subject to the potential changes in
995 local and regional meteorological conditions.

996 Other EPA STAR projects employ global climate change information from a GCM. For example, Tagaris *et al.*
997 (2007) and Liao *et al.* (2007a,b) use the results of GCM simulation with the well-mixed greenhouse gases—CO₂, CH₄,
998 N₂O, and halocarbons—updated yearly from observations for 1950 to 2000 (Hansen *et al.*, 2002) and for 2000 to 2052
999 following the A1B SRES scenario from the Intergovernmental Panel on Climate Change (IPCC 2001). The simulation
1000 used ozone and aerosol concentrations in the radiative scheme fixed at present-day climatological value provided in
1001 Mickley, *et al.* (2004).

1002
1003 To resolve the meteorological features affecting air pollution transport and transformation at a regional scale, the
1004 coarse scale meteorological data representing the climate change effects derived from a GCM are downscaled using an
1005 RCM. An RCM is often based on a limited-domain regional mesoscale model, such as MM5, the Regional
1006 Atmospheric Modeling System (RAMS), Eta, and WRF/ARW or WRF/NMM. An alternative method for constructing
1007 regional scale climate change data is through a statistical downscaling, which evaluates observed spatial and temporal
1008 relationships between large-scale (predictors) and local (predictands) climate variables over a specified training period
1009 and domain (Spak *et al.*, 2007). Because of the need to use a meteorological driver that satisfies constraints of dynamic
1010 consistency (i.e., mass and momentum conservations) for regional scale air quality modeling (e.g., Byun, 1999 a and b),
1011 the CMAQ modeling system relies exclusively on the dynamic downscaling method.

1012 Regional chemistry/transport models, like CMAQ, are better suited for regional air quality simulations than a
1013 GCTM because of the acute air pollution problems that are managed and controlled through policy decisions at specific
1014 geographic locations. Difficulty in prescribing proper boundary conditions (BC), especially in the upper troposphere, is
1015 one of the deficiencies of CMAQ simulations of air quality (e.g., Tarasick *et al.*, 2007; Tang *et al.*, 2007). Therefore,
1016 one of the main roles of the global CTM is to provide proper dynamic boundary conditions for CMAQ to represent
1017 temporal variation of chemical conditions that might be affected by the long-range transport of pollution (e.g., particle
1018 from large-scale biomass burnings) from outside the regional domain boundaries (Holloway, *et al.*, 2002; In *et al.*,
1019 2007). The contemporary EPA funded projects on climate change impact on air quality mainly use two 3-D GCTM
1020 models: the NASA/Harvard GEOS-Chem (Bey *et al.*, 2001) and the National Center for Atmospheric Research (NCAR)
1021 Model of Ozone and Related Chemical Tracers (MOZART) (Brasseur *et al.*, 1998; Horowitz *et al.*, 2003).

1022 The GEOS-Chem model (<http://www-as.harvard.edu/chemistry/trop>) is a global model for predicting tropospheric
1023 composition. The model was originally driven by the assimilated meteorological observation data from the GEOS of the
1024 NASA Global Modeling and Assimilation Office (GMAO). GEOS-Chem has been used as community assessment
1025 models for NASA Global Model Initiative, climate change studies with the NASA/GISS GCM, chemical data
1026 assimilation of tropospheric gaseous and aerosol species at NASA GMAO, and regulatory models for air pollution, in
1027 particular providing long-range transport information for regional air quality models. Long-term retrospective studies
1028 are possible with the GEOS data, which are available from 1985 to present at horizontal resolution of 2 degrees
1029 (latitude) by 2.5 degrees (longitude) until the end of 1999 and 1 degree by 1 degree afterward. For climate studies, the
1030 NASA GISS GCM meteorological outputs are used instead. Emission inventories include a satellite-based inventory of
1031 fire emissions (Duncan *et al.*, 2003) with expanded capability for daily temporal resolution (Heald *et al.*, 2003) and the
1032 National Emissions Inventory for 1999 (NEI 1999) for the US with monthly updates in order to achieve adequate
1033 consistency with the CMAQ fields at the GEOS-Chem/CMAQ interface.

1034 MOZART (<http://gctm.acd.ucar.edu/mozart/models/m3/index.shtml>) is built on the framework of the Model of
1035 Atmospheric Transport and Chemistry (MATCH) that can be driven with various meteorological inputs and at different
1036 resolutions such as meteorological reanalysis data from the National Centers for Environmental Prediction (NCEP),
1037 NASA GMAO, and the European Centre for Medium-Range Weather Forecasts (ECMWF). For climate change
1038 applications, meteorological inputs from the NCAR CCM3 are used. MOZART includes a detailed chemistry scheme
1039 for tropospheric ozone, nitrogen oxides, and hydrocarbon chemistry, semi-Lagrangian transport scheme, dry and wet
1040 removal processes, and emissions inputs. Emission inputs include sources from fossil fuel combustion, biofuel and
1041 biomass burning, biogenic and soil emissions, and oceanic emissions. The surface emissions of NO_x, CO, and NMHCs
1042 are based on the inventories described in Horowitz *et al.* (2003), aircraft emissions based on Friedl (1997), and lightning
1043 NO_x emissions that are distributed at the location of convective clouds.

1044 GCTMs are applied to investigate numerous tropospheric chemistry issues, involving gases – CO, CH₄, OH, NO_x,
1045 HCHO, and isoprene– and inorganic (sulfates and nitrates) and organic (elemental carbons, organic carbons)
1046 particulates. Various *in situ*, aircraft, and satellite-based measurements are used to provide the necessary inputs, to
1047 verify the science process algorithms, and to perform general model evaluations. They include vertical profiles from
1048 aircraft observations as compiled by Emmons *et al.* (2000), multiyear analysis of ozonesonde data (Logan, 1999), and
1049 those available at the Community Data Web site managed by the NCAR Earth and Sun Systems Laboratory (ESSL)

1050 Atmospheric Chemistry Division (ACD); and multiyear surface observations of CO reanalysis (Novelli *et al.*, 2003).
1051 Current and previous atmospheric measurement campaigns are listed in Web pages by NOAA Earth Systems Research
1052 Laboratory (ESRL), <http://www.esrl.noaa.gov/>; NASA, Tropospheric Integrated Chemistry Data Center, [http://www-](http://www-air.larc.nasa.gov/)
1053 [air.larc.nasa.gov/](http://www-air.larc.nasa.gov/); and NCAR ESSL (Earth and Sun Systems Laboratory) Atmospheric Chemistry Division (ACD)
1054 Community Data, <http://www.acd.ucar.edu/Data/>. These observations are used to set boundary conditions for the slow
1055 reacting species, including CH₄, N₂O, and CFCs, and to evaluate other modeled species, including CO, NO_x, PAN,
1056 HNO₃, HCHO, acetone, H₂O₂, and non-methane hydrocarbons. In addition, several satellite measurements of CO, NO₂,
1057 and HCHO from the Global Ozone Monitoring Experiment (GOME), The SCanning Imaging Absorption SpectroMeter
1058 for Atmospheric CHartographY (SCIAMACHY), and OMI instruments have been used extensively to verify the
1059 emissions inputs and performance of the GCTM.

1060 The grid resolutions used in the studies discussed above are much coarser than those used in the air quality models
1061 for studying emission control policy issues, such as evaluating state implementation plans (SIP). SIP modeling
1062 typically utilizes over 20 vertical layers at around 4-km horizontal grid spacing to reduce uncertainties in the model
1063 predictions near the ground and around high-emission source areas including urban and industrial centers. Although
1064 Civerolo *et al.*, (2007) applied CMAQ at a higher resolution, the duration of the CMAQ simulation was far too short a
1065 time scale to evaluate the regional climate impacts in detail.

1066 One of the additional key limitations of using the CMAQ for climate change studies is that the linkages between
1067 climate and air quality and from the global scale to regional scale models are only one-way (i.e., no feedback). Jacob
1068 and Gilliland (2005) stated that one-way assessment of the global change scenarios would be less useful for projection
1069 of air pollutant emissions because the evolution of regional air quality policies were not accounted for in these
1070 storylines. Also, to represent the interactions between atmospheric chemistry and meteorology, such as radiation and
1071 cloud/precipitation microphysics, particulates and heterogeneous chemistry, a two-way linkage must be established
1072 between the meteorology and chemistry models. An on-line modeling approach as implemented in WRF-chem is an
1073 example of such a linkage, but still there is a need to develop a link between the global and regional scales. A multi-
1074 resolution modeling system such as demonstrated by Jacobson (2001 a, b) might be necessary to address the true
1075 linkage between air pollution forcing and climate change and to provide the urban-to-global connection.

1076 In addition, there would be significant benefits to linking other multimedia models describing subsoil conditions,
1077 vegetation dynamics, hydrological processes, and ocean dynamics, including the physical/chemical interactions between

1078 the ocean micro-sublayer and atmospheric boundary layer to an air quality model. To generate such a megamodel under
1079 one computer coding structure would require handling of extremely different state variables in each multimedia model
1080 with substantially different data. Furthermore, interactions among the multimedia models need multidirectional data
1081 inputs, quality assurance checkpoints, and the decision-support entries. A more generalized on-line and two-way data
1082 exchange tools currently being developed under the Earth System Modeling Framework (ESMF)
1083 (<http://www.esmf.ucar.edu/>) may be a viable option.

1084 Observations not only represent the real changes in the climate but also provide a fundamental database to verify
1085 various modeling components in the DSS. The meteorological reanalysis data are available both in regional and global
1086 scales, but similar atmospheric chemistry database for air quality is lacking. An ozone database from ozonesonde
1087 system and other *in situ* measurements are useful for global scale studies. But for regional air quality studies, the
1088 availability of such measurements representing urban and local conditions in long-term is limited. Satellite or other
1089 remote sensing platform observations may provide additional data sources to build an atmospheric chemistry reanalysis
1090 database at global and regional scales, but these observations are mainly limited to ozone and aerosols. Such chemical
1091 reanalysis database can be utilized to study long-term air quality trends; to evaluate science process components in the
1092 air quality models, emissions, and other model inputs and configurations; and to improve model predictions through
1093 data assimilation approaches.

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1095 Figure 1. Configuration of CMAQ-based Decision Support System for climate change impact study

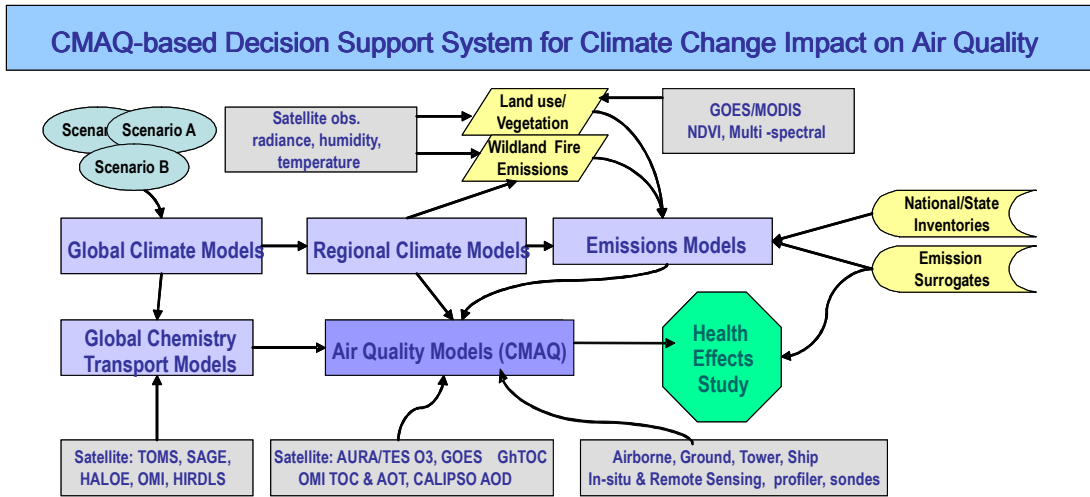


Figure 1. Configuration of CMAQ-based Decision Support System for climate change impact study

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1097 Table 1. Input data used for operating the CMAQ-based DSS.

Data Set	Type of Information	Source	Usage
Regional climate model output	Simulation results from a regional climate model (RCM) used as a driver for CMAQ modeling; processed through meteorology-chemistry interface processor (MCIP)	RCM modeling team; PNNL, UIUC, 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 USGS, NASA, NCEP EPA, states, etc.	Usually the data are associated with RCM's 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 (NEI) and state/special	Amount and type of pollutants into the atmosphere. Includes: - Chemical or physical identity of pollutants - Geographic area covered - Institutional entities	EPA, regional program organizations (RPO), states 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.,

inventories; often called as “bottom-up” inventories	<ul style="list-style-type: none"> - Time period over which the emissions are estimated - Types of activities that cause emissions 		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), GEOS-Chem (Harvard & Univ. Houston), 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
AQS/AIRNow	Near real-time (AIRNow) and archived datasets (AQS) for ozone, PM, and some toxics 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

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1099 Table 2. An illustrative example of the potential uses of the models and upstream and downstream tools for a CMAQ-
 1100 based Climate Change Impact Decision Support System.

Component	Functions	Model Name: Owner	Users
Global climate models (GCM)	Performs climate change simulations over the globe for different SRES climate scenarios. Typical resolution for a long-term (50 year) simulation is at 4° x 5° latitude and longitude	Community Climate Model (CCM): NCAR Goddard Institute for Space Studies (GISS) GCM: NASA CM2: Geophysical Fluid Dynamics Laboratory (GFDL) of NOAA	Climate research institutes, universities, and government institutions
Global chemistry transport models (GCTM)	Computes global scale chemical states in the atmosphere; uses same resolution as GCM	GEOS-Chem: NASA, Harvard University MOZART: NCAR (ESSL/Atmospheric Chemistry Division)	Global chemistry research organizations, universities, and government institutions
Regional climate models (RCM)	Simulates regional scale climate and meteorological conditions downscaling the GCM output; for US application ~36 km resolution used	MM5-based: NCAR, PNNL, UIUC, and others; the weather research and forecasting (WRF) model - advanced research WRF (WRF-ARW) core based: NCAR, UIUC Eta-based: NCEP (before June, 2006) The WRF- nonhydrostatic mesoscale model (WRF-NMM) core based: NCEP (after June,	Regional climate research groups, universities, and government institutions

		2006)	
Regional air quality models (AQM)	Performs air quality simulations at regional and urban scales at the same resolution as the RCM	Community multiscale air quality (CMAQ): EPA Comprehensive air quality model with extensions (CAMx): Environment 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 and source apportionment studies, exposure studies	CMAQ/DDM: GIT CMAQ/4Dvar: CalTech/VT/UH Stochastic human exposure and dose simulation (SHEDS): EPA Total risk integrated methodology (TRIM): 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, UC Santa Barbara (captures urban patterns) CLM (community land model): NCAR (used for RCM and biogenic emission estimates after growth)	Universities and consulting companies

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