Instrumented Models for Diagnostic Model Evaluation:
Decoupled Direct Method in 3-D, Carbon Apportionment, and Sulfur Tracking (2.3)

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It is often useful to determine not only the state of an environmental system, but also its response to perturbations in various parameters that define it. Instrumented models offer a unique interpretation of standard air quality model output and are useful to better understand the physical and chemical processes occurring in the atmosphere. In terms of diagnostic model evaluation, instrumented models can (1) identify model processes that require further attention, (2) complement operational model evaluation (which is important to establish a general level of confidence in modeling results), and (3) identify model outputs that require further attention. Three instrumented models are presented: Decoupled Direct Method in three dimensions (CMAQ-DDM-3D), Carbon Apportionment (CMAQ-CA), and Sulfur Tracking (CMAQ-ST).

- CMAQ-DDM-3D provides an efficient and accurate approach for calculating the sensitivity of atmospheric pollutant concentrations to changes in photochemical model parameters (emissions, chemical reaction rates, initial/boundary conditions, etc.).
- CMAQ-CA allows quantification of absolute contributions from different emission sources to primary organic carbon (OC) and elemental carbon (EC). Molecular tracer and radiocarbon techniques have been developed to measure source-specific contributions. The combination of these measurements and carbon apportionment allows evaluation of both the air quality model and the emissions inventory.
- CMAQ-ST allows for analysis of the sulfate production pathways. It tracks sulfate production from gas-phase and aqueous-phase chemical reactions, as well as contributions from emissions and initial and boundary conditions.

All of these models have been made available to the regulatory and academic communities. Each one has been used in a wide range of applications, and has extracted additional utility from model predictions. During the 2008 model release cycle, the models are being made available for the first time, via the Community Modeling and Analysis System (CMAS) Center.

Aside from diagnostic model evaluation, instrumented models are useful in regulatory applications in the areas of source apportionment, estimation of uncertainty, selection and evaluation of control strategies, and future projections. In the future, these instrumented models will continue to be updated to incorporate the latest scientific advancements contained in the base CMAQ model, and distributed to the user community. Furthermore, the Division plans to build additional instrumented model capabilities, including developing adjoint versions of the CMAQ model.