7.3

DEVELOPMENT OF A MODULARISED AEROSOL MODULE IN CMAQ

Weimin Jiang * and Helmut Roth
Institute for Chemical Process and Environmental Technology
National Research Council of Canada
Ottawa, Ontario, Canada
e-mail: **weimin.jiang@nrc.ca**
Voice (613) 998-3992 Fax (613) 941-1571

1.0 INTRODUCTION

An effort is underway at the National Research Council of Canada to develop a new CMAQ aerosol module with modularity at the level of individual aerosol processes. The starting point of the project is the development of a new structure for the CMAQ aerosol module so that each aerosol process (e.g., primary particle emissions, condensation, secondary organic aerosols, etc) becomes an independent submodule of the aerosol module. Under the new structure, individual aerosol process submodules can be readily added, modified, removed and/or replaced without affecting or being affected by other parts of the model code.

Development of the new aerosol module is divided into two phases. In phase I, the AERO2 module released in Models-3 version 4.1 is completely restructured and substantially recoded to implement the new aerosol module structure. A detailed review and analysis of science, algorithms, and code in AERO2 has been completed in support of this effort (Jiang and Roth, 2002). In phase 2, individual aerosol process submodules will be modified and/or replaced to reflect new developments in aerosol science. New process submodules may also be added to address emerging aerosol-related air quality issues.

2.0 STRUCTURE OF THE NEW AEROSOL MODULE

The new aerosol module structure is built on the major considerations of process level modularity, separation of data from executable code, and code flexibility and generality.

2.1 Process level modularity

Each kinetic, thermodynamic, or other process that affects the values of the aerosol-related quantities is structured as a submodule of the aerosol module. Submodules are independent of each other. Each submodule can be added, removed, modified, and/or replaced without affecting or being affected by other submodules.

Each kinetic process submodule calculates contributions of the process to the kinetic differential equations that describe the time evolution of aerosol species mass, number (0-th moment), and 2nd moment concentrations. The calculations of the contributing terms are based on the current values of the aerosol-related quantities. The contributing terms generated by all kinetic process submodules are added together. The resulting differential equations are solved analytically using a generalized differential equation solver, which uses the same mathematical formulation embedded in the current AERO2 code. The solutions of the differential equations are used to update the concentration fields of the aerosol-related quantities.

Each thermodynamic process modifies the concentration fields of the aerosol-related quantities by solving the equilibrium equations based on chemical thermodynamics. Similar to the calculations in the kinetic process submodules, the starting points of thermodynamic calculations are the current values of the aerosol-related quantities. The equilibria that are solved include both heterogeneous equilibria between the gas and aerosol phases and homogeneous equilibria in the aerosol phase.

* *Corresponding author address:* Weimin Jiang, National Research Council Canada, Room 233, M2, 1200 Montreal Road, Ottawa, Ontario, Canada K1A 0R6

In addition to kinetic and thermodynamic processes, other processes, such as mode merging (Byun and Ching 1999), can also be structured as submodules of the aerosol module.

2.2 Separation of data and executable code

Within the new aerosol module structure, data and executable code are separated. Here, data include direct and derived aerosol quantity names and values, relevant emission and meteorological variable values, physical and chemical properties, as well as parameters and constants. Data constitute the objects to be operated upon by the executable code.

The separation of data and executable code are done at two different levels.

1. At the aerosol module level, data are defined, classified, and stored in Fortran data modules. Depending on its functionality, each aerosol process submodule uses different data modules. The process submodules refer to and operate on the data objects by their variable and array names. The variable and array names reflect the nature of the chemical and physical quantities that the data objects represent. This is in contrast to current CMAQ aerosol modules that extensively use aerosol species- and size-dependent variable and array names.

2. At the aerosol process submodule level, data are defined, classified, and assigned initial values in the data declaration section prior to the executable code. Similar to the data in the data modules, the variables and/or arrays representing the data are named according to the nature of the data. The executable code is independent of species and size names.

Separation of data and executable code ensures thin interfaces between the aerosol process submodules and driver subroutines, and between the kinetic submodules and the differential equation solver. It facilitates the data transfer among various parts of the aerosol module. It also enables the development of flexible and generalized code, which is discussed in Section 2.3.

2.3 Code flexibility and generality

Based on the aforementioned separation of data and executable code, elements of a data object can be added, removed, and/or changed without changing the executable code. For example, when the name of H_2SO_4 is changed from "SULF" to "Sulfuric acid" or when "AROSOA" is added as a new secondary organic aerosol (SOA) species modeled by the same SOA algorithm, changes are only made to data, and the executable code is kept as is. This ensures the flexibility and generality of the code.

3.0 CURRENT STATUS OF THE MODULE

The AERO2 module has been completely restructured using the newly developed aerosol module structure. Original AERO2 code has been substantially rewritten or modified to implement the new structure. Some errors and potential problems in the original code were corrected. The new aerosol module has been tested independently using a test platform that we developed. Detailed testing and debugging of the complete CMAQ built with the new aerosol module is underway, and new progress will be reported as soon as the testing and debugging is completed.

Table 1 lists the components, including aerosol submodules, of the new aerosol module. For each aerosol process, there are currently one or two operational submodules and one non-operational submodule available, which can be selected by the user when the model is built. The operational submodules are classified into kinetic, thermodynamic, and other submodules based on the processes that they deal with.

Figure 1 shows the relationships among the components listed in Table1. For the aerosol processes, all available operational and non-operational submodules for the same process are given in the same block. Only one submodule in each block is selected when a CMAQ model is built. The submodules can also be easily replaced by other independently developed submodules as long as their interfaces with the calling subroutines are kept the same. Fortran data modules used by each component of the aerosol module are represented by circled numbers in Figure 1.

Table 1 Components of the new aerosol module

Components		Name	Task/content
Fortran data modules		aero_data precursr_data aeroemis_data air_data const_data	aerosol quantity-related data gas phase aerosol precursor data aerosol emission data air property data constants, parameters, and data type definitions
Drivers & solvers		aero_driver aeroproc aerostep ode_solver	aero module driver aero process driver kinetic process driver kinetic differential equation solver
Operational submodules	kinetic	PMemis cond_nucl nucleation_KLP98 nucleation_HK98 SOA_Pandis SOA_Odum coagulation	Primary particle emissions inorganic condensation and driver for nucleation nucleation - KLP98 method nucleation - HK98 method Secondary organic aerosols - Pandis method Secondary organic aerosols - Odum method coagulation
	thermodynamic	inoreql_eql3	inorganic equilibria
	other	mode_merging	mode merging
Non-operational submodules		PMemis_noop cond_nucl_noop nucleation_noop SOA_noop coagulation_noop inoreql_eql3_noop mode_merging_noop	Primary particle emissions: no operation inorganic condensation and driver for nucleation: no-operation nucleation: no-operation Secondary organic aerosols: no operation coagulation: no operation inorganic equilibria: no-operation mode merging: no operation
Others		sizevar	size-related variables

4.0 FUTURE WORK

After successful completion of the testing and debugging of the new CMAQ built with the new aerosol module, various aerosol process submodules will be modified or replaced to reflect updated science. Subject to resource availability, the new process submodules will be obtained either by implementing new science code that we have developed, analyzing and using the new science code in the newly released AERO3 module, or by collaborating with other organizations. In the near future, the focus will be on the SOA formation and primary particle processing.

5.0 ACKNOWLEDGEMENT

The AERO2 module developed by the Environment Protection Agency of the United States is used as the basis for this model development effort. The Pollution Data Branch and the Pacific & Yukon Region of Environment Canada provided emission and meteorological data that have been used in the process of testing the new aerosol module. Éric Giroux of our group at the National Research Council of Canada provided substantial technical help to the project.

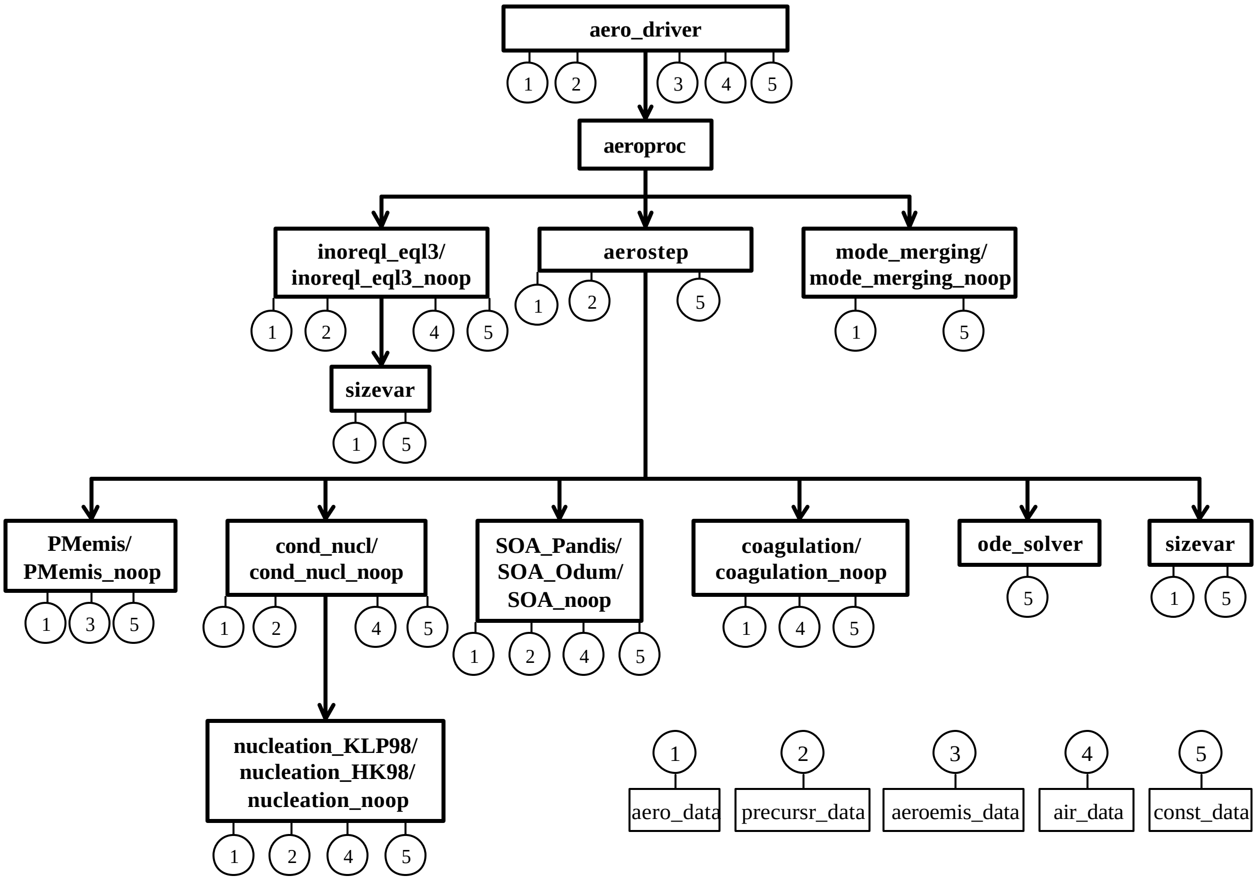

Figure 1 Relationship among the components of the new aerosol module.

Contributions mentioned above are very much appreciated.

The project is funded by the interdepartmental Program of Energy Research and Development in Canada and by the National Research Council of Canada.

6.0 REFERENCES

Byun D.W. and Ching J.K.S. (1999). Science algorithms of the EPA Models-3 Community Air Quality (CMAQ) modeling system. EPA-600/R-99/030, United States Environmental Protection Agency, Washington, DC 20460, USA.

Jiang W. and Roth H. (2002). A detailed review and analysis of science, algorithms, and code in the aerosol components of Models-3/CMAQ. I. Kinetic and thermodynamic processes in the AERO2 module. Draft report, Institute for Chemical Process and Environmental Technology, National Research Council Canada, Ottawa, Ontario, Canada.