1 Introduction

The Size Composition Resolved Aerosol Model (SCRAM) can simulate coagulation, condensation/evaporation and nucleation processes of externally mixed particles.

SCRAM is a free software. You can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation.

2 Hardware and Software Requirement

SCRAM is written in the programming language FORTRAN with the support of some foreign functions written in C++. It can run on PC or a cluster with both the gfortran and the GUN gcc Compiler and under a Linux system. Before the compilation, make sure the construction tool: SCONS has already been installed. If not you can obtain it through the following instruction of the site below:

http://www.scons.org/wiki/SconsTutorial1

The random access memory (RAM) requirement for the 0D simulation is very small. For example: it only takes 4MB RAM for the fully dynamic external simulation case presents in the fourth section of the manuscript. And it finished the 12 hours simulation in about 2 minutes on a standard pc with a processor clocked at 3.20 GHz and requires about 1MB of disk space.

The NetCDF library is also required, you can download from the following site:

http://www.unidata.ucar.edu/downloads/netcdf/index.jsp

After all the required software and library are ready, the compilation can be done by typing a simple command: scons, within a terminal under the program main path.

3 SCRAM Folder Directory

The SCRAM package contains 5 sub-folders:

1. SRC: where all source code files are stored. The main program file (ProgramSCRAM.f90) along with 12 module files are stored directly under the "SRC" folder. Besides, there are 4 sub-folders under SRC directory, each of them contains utility function files necessary for SCRAM execution.

   -rdb: contains 7 subroutines for size redistribution.

   -isorropia: a well known module for the computation of inorganic thermodynamic equilibrium between gas and aerosol.

   -H2O: a up-to-date module for the computation of organic thermodynamic equilibrium between gas and aerosol.

   -AtmoData: a tool for data processing in atmospheric sciences.

2. INIT: stores both configuration file and the aerosol composition discretization file.

3. INC: contains 5 *.inc files which define some system parameter variables.

4. RESULT: where all simulation results are stored. Including (number, mass and volume) concentration dates of each species and group both before and after the simulation. A file named "report" summarizes the overall performance of the simulation.

5. COEFF_REPARTITION: contains a standalone C++ program to compute the repartition coefficient database for the coagulation process. Two coefficient repartition data files correspond to the realistic simulation cases in the fourth section in the manuscript are already provided under the main path:

   -coef_s1_f1_b7.nc for internal mixing case

   -coef_s5_f3_b7.nc for external mixing case

The detailed function description of each code files come be fund at the beginning of each code files.

4 Model Operation

The program should be executed with a configuration file which contains all the initial condition and parametrization information. Two examples files correspond to the realistic simulation cases in the fourth section in the manuscript are provide under the sub-folder: INIT

-cfg_megapole_01072009_i.cfg for internal mixing case

-cfg_megapole_01072009.cfg for external mixing case

For example, you can repeat the all dynamic external mixing simulation within the article with following command: ./ProgramSCRAM INIT/cfg_megapole_01072009.cfg

5 Handling Output Files

Results of the simulation are well recorded in SCRAM. The following table explains the content of different output file which can be fund under the RESULT sub-folder.

Table 1: Initial and result files (located in "RESULT" folder)

Section	File name	Content
Initial files	number_init.txt	Average diameter, number concentration (m^{-3}) in each cell and total concentration of each size bin. Similar for mass file.
	concentration_number _init.txt	Average diameter, number concentration (m^{-3}) of each size bin. Similar for mass and volume files.
	mass_init_sX.txt	Average diameter, mass concentration (m^{-3}) of aerosol with fraction and size distribution of specie X. Similar for number and volume files.
	mass_init_gX.txt	Average diameter, mass concentration (m^{-3}) of aerosol with fraction and size distribution of group X. Similar for number files.
Result files	mass_result.txt	Average diameter, mass concentration (m^{-3}) in each cell and total concentration of each size bin. The same for number and volume files.
	mass_water.txt	Average diameter, mass (aerosol+water) concentration (m^{-3}) in each cell and total concentration of each size bin.
	mass_result_sbin.txt	Average diameter, mass concentration (m^{-3}) of each size bin. The same for number and volume files.
	mass_result_sX.txt	Average diameter, mass concentration (m^{-3}) of aerosol with fraction and size distribution of specie X. The same for number and volume files.
	mass_result_gX.txt	Average diameter, mass concentration (m^{-3}) of aerosol with fraction and size distribution of group X. The same for number files.

Contact

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