How to use GTMM.

The mercury soil model GTMM was coupled to GEOS-Chem in a way that the same code can be run within GEOS-Chem (online) or by itself (offline).

1   Running GTMM by itself.

1.1 Data files

GTMM requires a large number of data files to run by itself. They consist of:

- Meteorology files from GEOS-4

- Mercury deposition files from GEOS-Chem

- Vegetation types

- LAI

These data files can be downloaded from the Harvard ftp site at: ftp://ftp.as.harvard.edu/pub/geos_chem/data/GEOS_4x5/mercury_201007/GTMM_data

1.2 Input files

GTMM requires one to three input files depending if it is a starting run or a continuation of a previous run.

1.2.1 Input.gtmm: to define simulation.

In the run directory, you must have one input file named input.gtmm (fixed name). This file looks like (line numbers are not part of the file and are added for easier reference):

01: Years for NPP equilibrium   : 50

02: Years for Hg pools equilibrium : 10000

03: Number for preindustrial years : 10000

04: Is it a continuation run?   : F

05: File with Hg pools value for restart: '/home/ccarouge/GTM/output/ifort/v2/HgPools.0'

Line	Description
01	Number of years to reach NPP equilibrium. 50 years is enough. For continuation runs, the equilibrium was reached before so put 0 year here.
02	Total number of years for the run (mercury pools years + carbon years if any)
03	Number of preindustrial years for mercury. Must be inferior or equal to line 02
04	Put T for a continuation run, else F
05	If running a continuation run gives the full path and name of the restart file for the Hg pools.

1.2.2 Restart files: for continuation runs.

For a continuation run, in addition to input.gtmm, you need two restart files for the carbon pools and the Hg pools. The restart files are created at the end of the previous run in the output directory of your run. Note that continuation runs are only implemented to reach the equilibrium for the mercury. The equilibrium for the carbon is reached very quickly (typically 50 years) and so one run is sufficient. Both restart files are written in brut unformatted Fortran. Please refer to subroutines in dorestart_mod.f90 to know how to read these files.

The restart file for the carbon pools must be named *restart* and placed in the output directory of your GTMM run.

The restart file for the Hg pools is fully named (full path and file name) in input.gtmm.

1.2.3 Running script: for automatic renaming of restart files.

1.2.4

Input.gtmm and the restart files are the only input files necessary for running GTMM, but we distribute in addition the script "runGTMM" and the template "input.gtmm_template" that allow

a fully automatic handling of the restart files for the mercury pools. At the end of each run, GTMM writes the mercury restart file in the output directory under the name "HgPools". If you want to keep all restart files, you then need to rename these files and give the new name to input.gtmm. The file "runGTMM" determines automatically if the submitted run is the first run or a continuation run. If it is the first run, it will automatically run 50 years to reach carbon equilibrium. If it is a continuation run, it will run 0 years for the carbon. In addition, at the end of each run, the "HgPools" file is renamed to "HgPools.#" where # is a number following the last existing "HgPools" file. Of course, you must make sure that the simulations run one after the other and not concurrently.

E.g.:

- If there is no HgPools.* file in the output directory, runGTMM considers it is a first run. So it sets up input.gtmm to run 50 years for the carbon. At the end, the file "restart" is created and the file "HgPools" is renamed to HgPools.0.

- If we launch runGTMM again with the same output directory. The HgPools.0 file is recognized, so it is a continuation run. Input.gtmm is setup to run 0 year for the carbon, the restart file for Hg is set to HgPools.0. At the end of the run, the HgPools file is renamed to HgPools.1. Etc.

With this script, the user has only to decide on the number of total years to run and the number of preindustrial years (lines 02 and 03 in input.gtmm_template). The number of years to reach the carbon equilibrium can be changed in runGTMM.

1.3 Before compiling

The data directory and the output directory have to be defined in the GTMM code (not read from input files) before compiling. For this look into GTMM/defineConstants.f90 for filepath and outputpath variables. Change the paths to the ones of your liking, and be careful to change the length of the character strings, f_len, f_len_output.

1.4 Compilation

To compile go into your GEOS-Chem code directory, then into the GTMM subdirectory. From here simply type:

make -j4 gtmm

Note that the make command uses the same options as the compilation of GEOS-Chem. As such, make will use ifort as default for the compilation, unless you add the option "COMPILER=*xxx*", where *xxx* is the name of your compiler (or the COMPILER option is defined as an environment variable on your system). You can also give the debugging option, DEBUG=yes, or check for out of bounds error, BOUNDS=yes. See all available options with "make help".

A successful compilation will create the executable file "gtmm" in the GTMM/ directory. You will have to copy it to your run directory.

2   Running GEOS-Chem mercury simulation coupled to GTMM

This file only focuses on how to setup GTMM. If you need help to setup GEOS-Chem please refer to the manual and/or the GEOS-Chem wiki: http://acmg.seas.harvard.edu/geos/doc/man/, http://wiki.seas.harvard.edu/geos-chem/index.php/Main_Page.

Note that before running GTMM within GEOS-Chem, you need to run GTMM offline to get a soil equilibrium for carbon and mercury.

Also, when running GTMM within GEOS-Chem, do not use any "MM" or "mm" in your filenames or directory names. Otherwise these are likely to be changed to the month number or the minutes in the simulation. This would result in an error while trying to find a file or a directory.

2.1 Before compilation

As for running GTMM offline, you need to define the data and the output directories in

GTMM/defineConstants.f90. Look for filepath and outputpath variables in this file. Your output directory (outputpath) must contain the "restart" file and the last "HgPools" file produced during the equilibrium run of GTMM offline (see paragraph 1 for details).

2.2 Compilation

GTMM is relatively long to compile and such is not compiled by default with GEOS-Chem. To get GTMM to compile successfully with GEOS-Chem you need to do two things:

1. In Headers/define.h: uncomment the GTMM_Hg C-preprocessor switch:

!----- Simulation type -----

#define GTMM_Hg

2. Give a specific target when compiling:

make -j4 hg

You can also add any of the options used to compile GEOS-Chem (type "make help" for a full list).

This will create the GEOS-Chem executable in bin/ subdirectory as usual.

2.3 Running options

In input.geos, the mercury menu has two lines for GTMM:

Use GTMM soil model?   : T

GTMM Hg restart file   : GTM.totHg.YYYYMMDDhh

Put the first one to T (true) to use GTMM within GEOS-Chem, to F otherwise. Having this option to T when using a GEOS-Chem executable compiled without GTMM might result in error.

GTMM needs a specific restart file that contains the total Hg depositions for the previous month since GTMM has a monthly time step. When downloading the input directory (see GEOS-Chem manual), you will be provided with a GTMM restart file. It is recommended to spin-up your simulation when using this restart file. Also, as said at the start of paragraph 2, do not name your restart file "GTMM.YYYMMDDhh", all "MM" combinations would be

replaced by the month number. You can use "GTM.YYYMMDDhh" for example.