

Minutes of GEOS-CHEM meeting discussion

June 3, 2003

Emission data sets, model “options”

The general approach to implementing new emission data sets (and more generally new input data sets) in GEOS-CHEM is to in response to state-of-the-science improvements developed by users for their research purposes. These improvements should be implemented in the standard model as soon as they are considered mature (e.g., paper submitted). This implementation is the responsibility of the developer to initiate and the code manager to accommodate.

There may not always be a consensus within the GEOS-CHEM community on whether a change to an emission data set represents an objective improvement to the model, and we should then support two options within the standard model until the smoke clears. This should be done as necessary to ensure that all users are comfortable with using the standard model. However, we don't want the number of options to multiply because of the implications for maintenance and traceability of the standard code. As the smoke clears and one particular option gains the consensus of the GEOS-CHEM community we will disable the others.

There was some discussion about whether improvements in emissions arrived at on the basis of top-down constraints (as from inverse model analyses) should be implemented in the standard model. A problem with doing this is that the top-down approach offers no direct insight on processes. Ideally, top-down constraints should be used to improve the representation of processes in the bottom-up inventories, and the improved bottom-up inventories would then be implemented in the standard model. However, top-down constraints implemented on an ad hoc basis are sometimes necessary to enable matching of observations (example – terrestrial sink of CO₂). Again, this is a matter to be discussed on a case-by-case basis. Top-down scaling factors for emissions may be implemented as options in the standard code, following the same principles as above.

We went on to discuss some specific data sets to be implemented. Kasibhatla has a mature VIRS inventory for carbon burned that all agreed should be implemented in the standard model as an option, considering the uncertainty in the current Logan biomass burning inventory but also acknowledging apparent weaknesses in the VIRS product. Emission inventories currently being implemented by users at Harvard include regional estimates for East Asia from Streets, EC/OC from Bond/Streets, and MEGAN BVOC from Guenther. They are not yet mature but will be in a matter of months.

Benchmark/ Traceability/Evaluation

We discussed the shortcomings of the current 1-month benchmark run. We agreed that a 1-year coupled ozone-sulfate run with 4x5 resolution (18 months including initialization) should be conducted after any major changes to the code, and results compared against Logan's climatology of observations (we need a similar climatology for aerosols – Adams suggested AERONET AOT, which is a good idea but should first be addressed at a research stage). We should start doing this with v5.4, for which a 1-year run with monthly archive of concentrations is available from Rokjin. Inna (working with Jennifer) is presently automating

the comparison process. She will do the comparison with Rokjin and the results will be posted on the GEOS-CHEM web site.

Any major changes to the code affecting transport must also be benchmarked using chemical tracers of transport. We presently conduct a Rn/Pb/Be benchmark. This was not considered sufficient. In particular we should add a tracer of interhemispheric exchange and get interhemispheric exchange times; a 3-year ⁸⁵Kr simulation will be used for that purpose (Kr is already a tracer in the code). Other tracers of transport, including artificial tracers, were proposed as part of the benchmark process, but Jacob expressed concern over the resulting workload. It was agreed that we would look to the GMI benchmarking process to identify any additional tracers of transport to be added to the GEOS-CHEM benchmark.

An important tool for examining benchmarks and tracing the evolution of the code is Jaeglé's web-based plotting routines for GEOS-CHEM output at UW. Jaeglé agreed to maintain and expand her GEOS-CHEM web site. Should be posted there:

- results (monthly means) from major benchmarks
- results (monthly means) from published papers

Consistency between on-line and off-line transport using GMAO fields was also a concern. Pawson proposed to implement the chemical tracers on-line at GMAO and conduct simulations for comparison with the off-line GEOS-CHEM products. This was considered an excellent idea for the transition from GEOS-3 to GEOS-4. Some other specific issues going from GEOS-3 to GEOS-4 are mentioned at the end of this document.

Meteorological data / NCCS

We need to find a better way for users to access the GMAO meteorological data (i.e., other than asking Yantosca). The ideal solution would be to have a "CTM data set" generated at GMAO and posted either at GMAO or on the DAAQ. Pawson will examine this possibility.

The issue was raised of interfacing GEOS-CHEM with other meteorological datasets. Again, this has to emerge from users' interests and needs. Mickley and Wu are presently working to interface GEOS-CHEM with GISS meteorological data.

One source of frustration with the GMAO data is the lack of a consistent long-term meteorological data set. A GEOS-4 reanalysis starting in 1991 is presently on its way but may take some time to complete. We will need to push GMAO to produce a longer reanalysis (to 1980). We decided to wait until results from the current reanalysis.

We all agreed that NCCS would be of considerable value as a common computing platform for GEOS-CHEM users. Porting of the code to NCCS using MPI parallelization is ongoing. Once this is successful we will have to work with NCCS to achieve the best mode of user access.

Management plan

Jacob presented a "management charter" for GEOS-CHEM in his overview presentation. It was endorsed by the user community. A summary of the charter is present here:

Model scientist (Jacob) is responsible in consultation with users for

- code integrity
- development prioritization
- relationships in user community, issues of general benefit
- admission of new users

Model programmer (Yantosca) is responsible for

- maintenance of standard version
- code updates
- user support
- interface with GMAO

Users are responsible for

- maintaining communication with other users (web site)
- updating regularly to latest version of model
- giving credit to developers in publications
- not distributing code

Developers are responsible for

- providing codes and data sets (when mature) for implementation in standard version
- working with model programmer in this implementation
- updating to new standard version (no growing parallel versions of code!)

The model is owned by the ensemble of its users. Harvard (Jacob/Yantosca) provides central management support for GEOS-CHEM now and for the foreseeable future. All users and developers agreed to abide by their responsibilities. Indeed the integrity and success of the model rely on this.

The current approach of frequent model version updates will be maintained. Jacob/Yantosca now list on the web the version updates presently in the queue. Input from users is important to prioritize the updates.

Communication/Web interface

Good communication between GEOS-CHEM users is essential. An effective way should be through the user groups' research web sites. It was agreed that users should maintain a current research web site describing specifically their uses of GEOS-CHEM. These web sites will be linked from the central GEOS-CHEM web site.

Coding Issues

Some parts of the code are a mess and need to be rewritten, in particular the emissions. This is in the queue. We also need to redesign the input files so that there is a clear list of input flags

Appendix: To go from GEOS3 to GEOS4 (contributed by Mat Evans)

1) Workout what input fields need to be converted to the new grid. If the vertical resolution is different we need (and there will be more)

- a restart file
- a tropopause file
- aerosol fields
- the 2d fields for the stratosphere O₃, NO_y, OH production

2) Take a look at the input meteorology how does it compare with the current met fields. It would be good to look at the differences with GEOS 1 / GEOS STRAT / GEOS 3 and fv-das over a year

- a) Water vapor.
- b) Cloud cover
- c) Temperatures - air and surface d) Convection
- e) Boundary layer depths
- f) Precipitation on the ground

3) Run with just the emissions for a year to gauge soil NO_x, isoprene and lightning NO_x emissions and to check that there are no differences for anthro, biomass, biofuel, aircraft etc . Scale the soil, lightning and isoprene emissions to the appropriate amounts if needed

4) List of output diagnostics needed for the one-month benchmark run emissions

- anthropogenic [ND36]
(don't expect a change)
- biofuel [ND34]
(don't expect a change)
- biomass [ND28]
(don't expect a change)
- aircraft [ND32]
(don't expect a change)
- lightning [ND32]
(should have been scaled in previous stage)
- soil nox [ND32]
(should have been scaled in previous stage)
- biogenics [ND46]
(should have been scaled in previous stage)

fluxes

- stratospheric flux of O₃ and NO_y [ND27]
(expect changes in trop / strat circulation
and thus strat trop exchange see below)

dry deposition [ND44]

- wet deposition [ND17+ND18+ND37+ND39]
expect differing cloud field
photolysis rates [ND22]
expect differences due to cloud fields

O₃ production and loss [ND20]

- we will need to run the tagged O₃ simulation later

24h mean concentrations of tracers and OH