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The GEOS-Chem Unified Tropospheric-Stratospheric Chemistry Extension (UCX) (Interim Distribution)

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1 Document Purpose

This technical note explains how to acquire and install the GEOS-Chem Unified Chemistry Extension (UCX), which implements stratospheric chemistry in the formerly primarily tropospheric chemistry-transport model GEOS-Chem. A scientific description and model evaluation can be found in the following paper:

Sebastian D. Eastham, Debra K. Weisenstein, Steven R.H. Barrett, Development and evaluation of the unified tropospheric-stratospheric chemistry extension (UCX) for the global chemistry-transport model GEOS-Chem. *Atmospheric Environment* (In Press). ISSN 1352-2310, doi: http://dx.doi.org/10.1016/j.atmosenv.2014.02.001

This is intended to be an interim distribution for researchers who want access to GEOS-Chem UCX right away. It will no longer be necessary once UCX is incorporated into the main GEOS-Chem branch, which is planned for early 2014.

2 Contact

Contact Sebastian Eastham (seastham@mit.edu) with questions.

3 Installation Instructions

The file UCXv1_5.tgz contains code and an example run directory for the UCX. Installation instructions are identical to the base GEOS-Chem (http://acmg.seas.harvard.edu/geos/), although the UCX requires a small additional set of input files for long-lived species. These input files are collected in the directory "InitCFC", included in the UCX download. The local path of this directory must be specified in the input.geos file. UCX currently expects 1°×1° aircraft emissions grids. While these are available at http://lae.mit.edu, we suggest that you disable aviation emissions in the interim UCX unless aviation emissions are important to your study (in which case you will need the large 1°×1° aircraft emissions files).

It is highly recommended that the KPP chemistry solver is used when running GEOS-Chem UCX. Accordingly, the option "CHEM=UCX" must be specified at compile time.

4 Disclaimer

This is a beta version only. Some functions, such as running the model in troposphere-only mode or applying random cloud overlap, have either not been tested or are not yet fully implemented. Additionally, there are likely to be uncaptured conflicts (e.g. disabling methane emissions without disabling the UCX), which will cause model failures or unrealistic results. We suggest running in the pre-configured full troposphere/stratosphere mode without merged vertical layers.

5 New Options

The input.geos file contains the following new run options:

5.1 Emissions Menu

Emit CH4 (emiss. inv.)?	Enable methane emissions based on a methane emissions inventory
Emit CH4 (sfc. BC.)?	Enable a fixed surface mixing ratio for methane (recommended)
Emit OCS (sfc. BC.)?	Fix surface mixing ratios of OCS

Emit CFCs (sfc. BC.)?	Fix surface mixing ratios of CFCs, HCFCs and halons to match WMO projections under the Montreal Protocol
Emit Cl spcs (sfc. BC.)?	Fix surface mixing ratios of other chlorinated carbon species (eg CCl_4) and inorganic chlorine to WMO projections under the Montreal Protocol
Emit Br spcs (sfc. BC.)?	As above, for bromine species. Not recommended if other bromine emissions are enabled
Emit N2O (sfc. BC.)	Fix surface mixing ratios of N_2O
Set initial strat. H2O?	Calculates stratospheric H_2O mixing ratios based on meteorology data for the first timestep, overriding any restart file values
Set initial CH4?	Extracts CH_4 from the default GEOS-Chem climatology for the first timestep, overriding any restart file values
Set initial OCS?	Set initial OCS distribution based on zonal means from a 2D model
Set initial CFCs?	As above for CFCs, HCFCs and halons
Set initial Cl species?	As above for other chlorinated carbon and inorganic chlorine species
Set GCCM Bry in strat?	Initialize stratospheric bromine to match the old climatology (recommended)
Set initial Br species?	Set initial Br distribution based on zonal means from a 2D model
Set strat. Br species?	As above but only within the stratosphere
Set strat. NOx/HNO3?	As above for stratospheric NO_x and HNO_3
Set initial N2O?	Set initial N_2O distribution based on zonal means from a 2D model
Set initial strat. SO4?	As above for stratospheric sulfates
Reference emissions year	Future year for which emissions should be scaled (set to 0 for current year)
Directory for 2D data	This should be the absolute path to the InitCFC input data folder

5.2 Aerosol Menu

Settle strat. Aerosols	Apply gravitational settling to stratospheric solid particulate aerosols (SPA, trapezoidal scheme) and stratospheric liquid aerosols (SLA, corrected Stokes' law)
Online PSC AEROSOLS	Calculate stratospheric aerosol formation
Allow homogeneous NAT?	Allow NAT to form homogeneously from freezing of HNO_3
NAT supercooling req. (K)	Degrees K of supercooling required for homogeneous NAT nucleation
Ice supersaturation req.	Supersaturation factor required for ice nucleation (recommend 1.2 for coarse grids, 1.5 for fine grids)
Perform PSC het. chem.?	Allow heterogeneous chemistry on stratospheric aerosols
Calc. strat. aero. OD?	Include online stratospheric aerosols in extinction calculations for photolysis

5.3 Chemistry Menu

Use lin. high alt. chem?	Apply linearized high-altitude chemistry **in the mesosphere**
Use Linoz for O3?	As above for **mesospheric** ozone
Use UCX?	Activate UCX
Active strat. H2O?	Allow stratospheric H_2O tracer to influence specific/relative humidity
Online O3 for Fast-JX?	Use calculated ozone profiles rather than climatology when calculation ozone interaction with UV