Proposed Chemistry-Climate Model Initiative Simulations in support of the 2022 WMO/UNEP Scientific Assessment of Ozone Depletion

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Introduction

We consider it a very high priority to provide updated guidance on the future evolution of stratospheric ozone to the Parties to the Montreal Protocol and we believe this guidance is highly valued by the Parties. To support the 2022 Assessment, we plan to ask for simulations in two steps. The first request, the one detailed here, is for a hindcast simulation covering 1960 – 2018 that will be used to assess the models against observations (REF-D1). A second request for future scenarios including a baseline (REF-D2, following one of the SSPs defined for CMIP6) with an additional, but very limited, number of scenarios addressing important scientific issues that have been identified by the Parties to the protocol will follow.

A concern that has strongly shaped the form of the request is the need for a more statistically robust multi-model ensemble. There are two aspects to this: a more homogeneous participation of models across experiments and the generation of a small ensemble by each model for each experiment. We strongly encourage participating modelling groups commit to producing a minimum of three ensemble members for each experiment and to participating fully across all of the specified simulations. Given the increased demands on modelling groups that these requirements will entail, we have worked to limit the number of scenarios and streamlined the data request.

Model Assessment for WMO-2022

The second phase of the Chemistry-Climate Model Validation Activity (CCMVal-2) (Eyring et al., 2007) produced an extensive assessment of the dynamical and chemical aspects of many CCMs against a wide range of available observations that took the form of a 400-page report (SPARC CCMVal, 2010) and provided an important base of information for the 2010 WMO/UNEP Scientific Assessment of Ozone Depletion. Chemistry climate models have evolved considerably since CCMVal-2 and there was some criticism during the preparation of the 2018 Ozone Assessment (WMO, 2018) that it was not possible to assess the validity of the CCMs being used for the projections. While more recent comparisons of models against observations have been performed (the analysis of ozone trends in the CCMI-1 simulations in the LOTUS report, for example), we feel there is tremendous value in having a more holistic and process-based analysis of CCMs to more fully understand the strengths and weaknesses of our current generation of models. In addition, during the 10 years since the last community-wide assessment was undertaken many new datasets have been produced (ERA-Interim, ERA5, MERRA, GOZCARDS, etc.) and assessed (SPARC-DI, LOTUS, S-RIP etc.). Given this background, to support the 2022 Scientific Assessment of Ozone Depletion we plan to conduct an assessment of the current generation of CCMs by revisiting and extending the suite of diagnostics that were performed for CCMVal-2 using data from the REF-D1 hindcast.

Timeline to submit simulations

Given the timelines of previous Ozone Assessments, the 2022 Assessment will likely be drafted over the course of 2021. Given the situation, we would ask as many modelling groups as possible to submit data from their REF-D1 simulations by January 2021. If your modelling group is planning on submitting REF-D1 simulations, please contact one of the CCMI co-chairs to let us know of your participation and the likely time window when results might be expected.

Further details

A dedicated webpage with links to the experiment description, the data request and ancillary data can be found on the CCMI website at: https://blogs.reading.ac.uk/ccmi/ccmi-2022/. Updates as the work progresses will also be found at this location.

REF-D1 Hindcast simulation for 1960 - 2018

The model assessment will be based on a small ensemble of hindcast simulations performed using specified SSTs and sea-ice cover for the 1960 – 2018 period, with a sufficient spin-up prior to 1960 (~ 10 years) that the stratosphere is properly initialized. As the primary focus of the REF-D1 simulation will be to assess models against observations, the forcing data is based as much as possible on observations, largely using databases developed for CMIP6 and available through the input4MIPs activity. A discussion of the different input4MIPs forcing datasets can be found at http://goo.gl/r8up31 and a list of links to the individual input4MIPs datasets can be found in the Resources section at the end of this document.

Long-lived Greenhouse Gases:

Mixing ratios of the long-lived greenhouse gases such as CO_2, CH_4 and N_2O are to be specified following the CMIP6 historical database (Meinshausen et al., 2017) up to 2014 and extended to the end of 2018 following SSP2-4.5 (Meinshausen et al., 2020).

Note that methane in all of the SSPs has an unrealistically large increase over 2016 – 2017: see the comparison against observed annual average concentrations here. To avoid introducing this increase into the models the original SSP2-4.5 methane files have been scaled to better reproduce the observed increase. The four different versions of the CH_4 forcing files produced for input4MIPs, with different time and latitudinal resolution, have been scaled using a set of monthly-varying, global correction factors to produce new files for 2015 to 2019. Updated versions of the following files are recommended for the REF-D1 simulation: annual average global and hemispheric means (here), monthly global and hemispheric means (here), monthly with 15° latitude resolution (here) and monthly with 0.5° latitude resolution (here) are available. We leave it to the individual modelling groups to decide which version they wish to use.

Ozone Depleting Substances:
The near-surface mixing ratios of Ozone Depleting Substances controlled under the Montreal Protocol (CFC-11, CFC-12, CFC-113, CFC-114, CFC-115, CCl_4, CH_3CCl_3, HCFC-22, HCFC-141b, HCFC-142b, Halon-1211, Halon-1202, Halon-1301, Halon-2402, CH_3Br, and CH_3Cl) are to follow the WMO(2018) baseline scenario given in Table 6-4 of the report. The WMO-2018 scenario was based on observed near-surface concentrations until 2017. For the REF-D1 simulation the timeseries for CFC-11, CFC-12, CCl_4, HCFC-22 and CH_3Cl have been revised for 2018 and 2019 based on more recent NOAA/ESRL Global Monitoring Laboratory data, while the original values from WMO-2018 are used for the remaining species. The timeseries of global average near-surface mixing ratios with annual time resolution, with values valid at the beginning of each calendar year, can be found here.
For models that do not represent all of the specified brominated and chlorinated species, the halogen content of species that are considered should be adjusted such that model inputs for total chlorine and total bromine match the time series of total chlorine and bromine. The chlorine and bromine content from missing species should be added to existing model tracers with similar lifetimes to preserve total chlorine or bromine.

Very Short-Lived Source Gases:
As was the case for previous community simulations, we ask modelling groups to account for the additional bromine introduced to the stratosphere by Very Short-Lived Source Gases (VSL-SGs) by explicitly including two of the important VSL-SG species $CHBr_3$ and CH_2Br_2. By imposing a near-surface volume mixing ratio of 1.2 pptv each (6.0 pptv of Br) and having these two source gases decompose to inorganic bromine species directly, models should achieve the required 4.5 to 5.0 pptv of bromine from VSL-SGs in the stratosphere. For modelling groups that do not wish to include these VSL-SGs and model tropospheric loss, the model CH_3Br tracer can be increased by a constant 5 pptv.
Note that these experiments do not explicitly consider chlorine-containing VSL-SGs. If groups do include a representation of VSL-SGs containing chlorine we ask them to limit the concentration imposed as a lower boundary condition to a small, constant value. If groups specify a flux boundary condition, we ask groups to zero out the anthropogenic component.

Natural biogenic emissions and lightning emissions of NOx:
These emissions are sensitive to meteorological variability and climate change and it is therefore preferable that models diagnose these emissions online using their own suite of interactive parameterizations. Climatological emissions may provide an acceptable solution for those models with an upper tropospheric / stratospheric emphasis. Lightning emissions are more difficult to specify in an externally consistent manner, but are important to upper tropospheric variability and the tropospheric oxidant balance.

Anthropogenic precursor emissions:
The complete set of anthropogenic emissions is to be taken from the CMIP6 input4MIPs databases for the historical period to 2014 and following RCP2-4.5 until 2018. Emissions from sectors other than open biomass burning (aircraft; non-combustion agricultural emissions; energy; industry; surface transportation; residential, commercial and other; solvents; waste disposal; international shipping) are to be taken from the 0.5° x 0.5° monthly files produced from the Community Emissions Data System (CEDS) as detailed in Hoesly et al. (2018) for the historical period. For 2015 and subsequent years, emissions are to be taken from version 1-1 of

SSP2-4.5, which provides emissions as 12 monthly fields for 2015 and 2020 and will need to be interpolated in time to provide emissions for intermediate years.

Open biomass burning emissions:

For open biomass burning, emissions are to be taken from the historical dataset constructed for CMIP6 and detailed in van Marle et al. (2017). The data are monthly files at 0.25° x 0.25° resolution and version 1.2 (BB4CMIP6-1-2) are to be used. Unlike other CMIP6 historical emission files, the historical biomass burning emissions files have emissions until the end of 2015. Take special note that the open biomass burning emissions of NOx ($NO + NO_2$) are expressed as kg-NO/m^2/s while the other anthropogenic NOx emissions are in units of kg-NO_2/m^2/s. More information on the CMIP6 historical open biomass burning emissions can be found at http://globalfiredata.org/pages/ar6-historic/.

For 2016 and subsequent years, open biomass burning emissions are to be calculated from the GFED4s database (https://globalfiredata.org/pages/data/#emissions), which will provide a consistent extension of the open biomass burning emissions as the CMIP6 historical emissions use GFED4s for years 1997 – 2015. Note that the GFED4s data is in a significantly different format to that of the CMIP6 emission dataset and, if groups prefer, they may construct a repeating annual cycle of open biomass burning emission from the CMIP6 historical dataset using data from 2010 – 2014. Avoid including 2015 in the average as this was an extreme burning year in south-east Asia.

Sea surface temperatures (SSTs) and sea ice concentrations (SICs):

The historical simulation uses specified SSTs and SICs, prescribed as monthly mean boundary conditions following the global HadISST1 sea ice concentration and sea surface temperature data set provided by the UK Met Office Hadley Centre (Rayner et al., 2003). The data set can be downloaded from https://www.metoffice.gov.uk/hadobs/hadisst/index.html. To prepare the data for use in forcing a model, and in particular to correct for the loss of variance due to time-interpolation of monthly mean data, it is recommended that each group apply the AMIP II variance correction method (see https://pcmdi.llnl.gov/mips/amip/details/index.html for details) to the HadISST1 data.

Quasi-Biennial Oscillation (QBO):

The QBO, an internal mode of variability in the tropical stratosphere, dominates the interannual variability in the tropics and has important effects in the extratropics. In addition to the influence of the QBO on dynamical quantities, there are additional important effects on chemical constituents including ozone. While it is possible to internally generate a QBO in models, it is generally not possible to guarantee that the model-generated QBO is in phase with the observed historical variability. To ensure the model QBO remains synchronized with the historical variability, whether a model is capable of internally generating a QBO or not we ask modelling groups to relax zonal winds (nudge) in the QBO domain towards the observed historical variations from radiosonde observations. A dataset is provided for this purpose that is based on updated radiosonde measurements following the method of Naujokat (1986) and extended to the upper stratosphere. The dataset, an update to the one provided for CCMI-1 and covering years 1953 – 2019, can be found here.

Extra-terrestrial solar flux and solar cycle:

The dataset of time-varying extraterrestrial solar flux produced for CMIP6 contains important revisions to the solar spectrum through the ultra-violet wavelengths compared to what has been used for CCMI-1 (Matthes et al. 2017). We strongly recommend modelling groups adopt the

CMIP6 time-varying solar spectral irradiance (SSI) for the calculation of chemistry. For the REF-D1 simulation the SOLARIS-HEPPA group has produced an extended daily, spectrally-resolved solar irradiance that is consistent with the historical forcing dataset produced for CMIP6, but with data to the end of 2019. The dataset also includes atmospheric ionization rates due to mid-energy electrons, solar protons and cosmic rays and, for models that are capable of simulating the indirect effects of particle precipitation through an upper boundary condition on NOy, there is a package available to calculate the necessary quantities to specify NOy as an upper boundary condition. More information on the SOLARIS-HEPPA solar forcing dataset can be found https://solarisheppa.geomar.de/solarisheppa/ccmi2022.

Stratospheric aerosol surface area density (SAD):
An extended version of the CMIP6 stratospheric aerosol SAD has been prepared using version 2.0 of the Global Space-based Stratospheric Aerosol Climatology (Kovilakam et al., 2020). This dataset extends to the end of 2018 the version 3-0-0 zonal mean monthly mean stratospheric aerosol SAD produced for the CMIP6 historical period. The format of the data is identical to the CMIP6 data, on a constant height vertical coordinate with 0.5 km resolution from 5.0 to 39.5 km altitude and 5° latitude resolution. The updated dataset can be found at:
ftp://iacftp.ethz.ch/pub_read/luo/CMIP6_SAD_radForcing_v4.0.0_1850-2018/
Note that aerosol values that appear in the troposphere are not considered reliable and should not be used. These values are included to allow for a seamless merging of the specified aerosols in the stratosphere with the model representation of tropospheric aerosols and should be ignored for model levels below the diagnosed local tropopause. The file also includes additional aerosol quantities such as mean radius, volume density and H_2SO_4 mass derived from the assumed single mode lognormal aerosol size distribution if required by models. Fields of extinction, single scattering albedo and asymmetry calculated for the specific wavelength bands of individual model radiation schemes are also available at the same web address.

Requested Model Output
An excel version of the data request can be found here. Output from this simulation will be collected in netCDF version 4 format files that are compliant with the Climate and Forecast (CF) standard. Note that the specifics of the requested variables have been harmonized as much as possible with those requested for CMIP6, including aspects such as variable names and the set of constant pressure surfaces for zonal average fields. In particular, take note that because of the CMIP6 harmonization the units for Eliassen-Palm flux (epfy and epfz) are not the same as previously used and are now scaled by the air density.
The use of CMOR for conversion to netCDF is strongly encouraged and we will be providing CMOR tables for all requested output through the CCMI website. Model output are to be submitted to a central archive at the Centre for Environmental Data Analysis (CEDA) in the United Kingdom. More details on the directory structure and the construction of file names will be provided.

Diagnostic Tracers
We ask modelling groups to include two diagnostic tracers in their simulation. The first is the standard 'Age of Stratospheric Air' tracer (meanage), defined as the mean time that a stratospheric air mass has been out of contact with the well-mixed troposphere. Different approaches can be used to estimate the mean age, though we recommend a tracer that is continually reset to zero in the troposphere and allowed to increase in value everywhere at a rate equal to the passage of time in the model.

The second diagnostic tracer is the 'Stratospheric Ozone' tracer (o3strat), that is set equal to the model ozone for all grid points above the local tropopause, decays with the odd oxygen chemical loss rate in the troposphere and deposits at the surface with the deposition velocity of ozone. We strongly recommend that groups use a common method to calculate the chemical loss of o3strat by specifying a first-order loss process with a chemical loss frequency given by

$$f_{o3strat}\ (s^{-1}) = \frac{k_A[O(^1D)][H_2O] + \ k_B[OH][O_3] + k_C[HO_2][O_3]}{[O_3]}.$$

The loss frequency is calculated at each model grid point using the local reaction rates (k_A, k_B and k_C) and local species concentrations, denoted by the square brackets. Here k_A is the reaction rate constant for $O(^1D) + H_2O$ -> 2OH; k_B is the rate constant for $OH + O_3$ -> $HO_2 + O_2$; k_C is the rate constant for $HO_2 + O_3$ -> $OH + 2O_2$.

Resources:

Near-surface mixing ratios of Long-Lived GHGs

Version 1-2-0 of the CMIP6 historical data can be found in the input4MIPs database at: https://esgf-node.llnl.gov/search/input4mips/?source_id=UoM-CMIP-1-2-0.
Version 1-2-1 of the CMIP6 SSP2-4.5 data for 2015 – 2018 can be found at: https://esgf-node.llnl.gov/search/input4mips/?source_id=UoM-MESSAGE-GLOBIOM-ssp245-1-2-1.

Anthropogenic precursor emissions

Anthropogenic emissions for years up to 2014 and for all sectors except open biomass burning (em-anthro) should use version 2017-05-18 of the CMIP6 forcing dataset, available through input4MIPs at
https://esgf-node.llnl.gov/search/input4mips/?source_id=CEDS-2017-05-18
Aircraft emissions (em-AIR-anthro) for the historical period should use version 2017-08-30: https://esgf-node.llnl.gov/search/input4mips/?source_id=CEDS-2017-08-30
Total VOC emissions are given in the em-anthro set of files, while a set of supplemental files provide speciated emissions. The supplemental files can be found at:
https://esgf-node.llnl.gov/search/input4mips/?source_id=CEDS-2017-05-18-supplemental-data
Details on how the splitting was derived can be found on the CEDS website at:
http://www.globalchange.umd.edu/data/ceds/README-CEDS-VOC-speciation_2017-05-18.txt
Note that the set of supplemental data files include emissions from solid biofuels (em-SOLID-BIOFUEL) and these should not be used as these emissions are already included in the em-anthro emissions.
Anthropogenic emissions for subsequent years are to be taken from SSP2-4.5, version 1-1, which can be found at:
https://esgf-node.llnl.gov/search/input4mips/?source_id=IAMC-MESSAGE-GLOBIOM-ssp245-1-1

Open biomass burning emissions

Version 1.2 of the CMIP6 open biomass burning emissions dataset (BB4CMIP6-1-2), with data to the end of 2015, is to be used and can be found at:

https://esgf-node.llnl.gov/search/input4mips/?institution_id=VUA
See the main text for options to specify open biomass burning emissions for 2016 onwards.

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