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

For the Chemistry Climate Model Initiative:

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## Introduction

The specifications and forcing data for the historical hindcast simulation (REF-D1) was released to groups in September 2020 and requested fields from participating modelling groups are currently being submitted to the CCMI-2022 data archive hosted by the Centre for Environment Data Analysis (CEDA). These hindcast simulations will provide an important resource for model assessment, and provide new insights into the ability of models to reproduce observed trends in ozone over the recent past and the role of internal variability.

To further support the high profile scientific topics that have been identified for the 2022 Ozone Assessment, namely updated projections of ozone recovery and the request from Parties to the Montreal Protocol for information on the effects of geoengineering, two projection simulations have been developed and assigned a high priority. The baseline projection (REF-D2) for updated projections of ozone recovery roughly follows the same specifications as for the SSP2-4.5 scenario of CMIP6. The geoengineering scenario (SEN-D2-geo) will be based on the REF-D2 simulation, but using a revised dataset of specified stratospheric aerosols and a specified repeating annual cycle of SSTs and sea-ice over 2025 - 2100. For modelling groups with sufficient resources, an additional two scenarios have been defined following SSP3-7.0 and SSP1-2.6, though to focus available resources on the baseline and geoengineering scenarios these two additional scenarios have been assigned a lower priority.

As with the REF-D1 hindcast, recognizing the need for a statistically robust multi-model ensemble, we strongly encourage participating modelling groups commit to producing a minimum of three ensemble members for each experiment and to participating in both of the specified high priority simulations.

## Branching the geoengineering simulation

As detailed further below, the geoengineering scenario will branch from the REF-D2 simulation at January 1, 2025. Modelling groups will need to ensure they have the capability to restart model simulations at January 1, 2025 using specified SSTs/sea-ice and an alternate dataset of stratospheric aerosols.

**Timeline to submit simulations**
The deadline for papers to be citable in the 2022 Ozone Assessment will likely be sometime in May 2022, though the writing of the chapters will have been completed several months before then. **Given the timeline for the writing of the Assessment, we kindly ask participating modelling groups to prioritize these scenario simulations as much as possible and work to have data submitted to the CCMI-2022 archive at CEDA no later than August of 2021.**

**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-D2 Baseline projection simulation for 1960 - 2100

The baseline projection of ozone recovery will be based on a small ensemble of simulations for the 1960 – 2100 period, with a sufficient spin-up prior to 1960 (~ 10 years) that the stratosphere is properly initialized. The baseline projection will follow the SSP 2-4.5 scenario of CMIP6 and will largely follow the same specifications as used for CMIP6. One significant difference is the time evolution of the near-surface concentration of Ozone Depleting Substances, which are to be taken from the baseline scenario of WMO (2018) given in Table 6-4 of the 2018 Assessment. As many of the forcing datasets used for the REF-D2 scenario are the ones developed by the input4MIPs activity for CMIP6, note that a general discussion of the 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 2100 following SSP2-4.5 (Meinshausen et al., 2020). While a modified version of the methane forcing was developed for the 2015 – 2019 period of the REF-D1 historical simulation, this data should not be used for the projection simulations.
Note that input4MIPs provides four different versions of the concentration forcing files with different temporal and latitudinal resolution. 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 timeseries of global average near-surface mixing ratios with annual time resolution for 1949 - 2101, with values valid at the beginning of each calendar year, can be found here.
The WMO-2018 scenario was based on observed near-surface concentrations until 2017 and, as was the case for methane, modified concentrations for a number of the ODSs were specified for the REF-D1 simulation based on more recent observations. For the REF-D2 simulations the original concentration timeseries from WMO-2018 should be used.

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 follow SSP2-4.5 until 2100. 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 scenario of CMIP6 (Gidden et al., 2019), which provides 12 monthly fields for 2015, 2020, then every 10 years after and will need to be interpolated in time to provide data 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. 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/.

At the end of the historical period, groups should use version 1-1 of the SSP2-4.5 'openburning' emissions files provided at 0.5° x 0.5° for 2015, 2020 and every 10 years after. The available emissions need to be interpolated in time to provide data for intermediate years.
Note that unlike other CMIP6 historical emission files, the historical biomass burning emissions files have emissions until the end of 2015. For the scenario simulations groups should not use 2015 from the historical biomass burning emission files, instead take emissions for 2015 from the SSP2-4.5 dataset. Also note that the open burning emissions for the years 1997 – 2015 are based on year-specific data and, as a result, have considerably larger year-to-year variability than other years. Modelling groups may decide to apply some degree of temporal smoothing before using the open burning emissions.

**Sea surface temperatures (SSTs) and sea ice concentrations (SICs)**:
To avoid potential discontinuities, SSTs and sea ice concentrations should be consistently specified throughout the entire 1960 – 2100 period. Depending on the capabilities of each modelling group, SSTs and sea-ice can be specified in a number of different ways:

i) Groups with a chemistry climate model fully coupled to a 3-D ocean model should perform coupled ocean-atmosphere simulations. Because of the long time constants inherent in the ocean, these simulations should be started at 1850 from an equilibrium pre-industrial control climate following the standard protocol for historical coupled model simulations with prescribed $CO_2$ concentrations.
ii) Chemistry climate modelling groups requiring specified SSTs and sea ice but with a closely related coupled atmosphere-ocean GCM within their institution, should use specified SSTs/sea ice taken from coupled model simulations performed by the related AOGCM. Ideally the AOGCM simulations used to calculate the SSTs and sea ice fields will have been performed following the CMIP6 historical and SSP2-4.5 forcings. If not available, the SSTs and sea ice should be taken from a simulation performed with radiative forcing close to that of the CMIP6 SSP2-4.5 scenario, the CMIP5 RCP4.5 for example. Note that if using specified SSTs and sea ice, different REF-D2 ensemble members should be performed with sets of SSTs/sea ice derived from different ensemble members of the AOGCM.
iii) Groups that do not have access to a coupled atmosphere-ocean GCM within their institution should use SSTs/sea ice from one of the combined historical/SSP2-4.5 simulations available in the CMIP6 archive. If using specified SSTs and sea-ice, different REF-D2 ensemble members should be performed with sets of SSTs/ sea ice taken from different ensemble members of the chosen CMIP6 model.

If specifying monthly average SSTs and sea ice, 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).

**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. For models that do not internally generate a QBO, a dataset of monthly average tropical winds has been created by extending the historical record derived from observations (Naujokat, 1986) from March 2019 to December 2100. Models that do not internally generate a QBO should relax (or nudge) zonal winds in the QBO domain towards this

record. An ascii data file of monthly tropical zonal winds to 2100 can be found here, while a set of figures documenting the construction of the dataset and the final timeseries can be found here. More complete information, including the input data files and programs used to construct the QBO timeseries, are packaged in a compressed tar file (.tgz) that can be found on the CCMI website.

Modelling groups that are able to internally generate a QBO in the configuration being used for the REF-D2 experiment may choose to nudge to the specified QBO timeseries or allow their QBO to run freely as they see fit.

**Extra-terrestrial solar flux and solar cycle**:

For the REF-D1 hindcast the SOLARIS-HEPPA group extended the CMIP6 historical solar spectral irradiance (SSI) dataset to the end of 2019 based on a longer observational record then available. For the future scenario simulations we recommend using the original CMIP6 dataset (Matthes et al. 2017), version 3.2, as it will correctly transition between the observation-based historical portion of the record and the projections of solar activity to 2100. Datasets with daily and monthly-average total and spectrally-resolved solar irradiance data are available. The daily 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 at https://solarisheppa.geomar.de/cmip6.

**Stratospheric aerosol surface area density (SAD)**:

A version of the CMIP6 SAD dataset extended to the end of 2018 was created for the REF-D1 simulation. The extended version of the CMIP6 SAD dataset is identical to the original CMIP6 dataset except for some minor differences following the Pinatubo eruption. For the scenario simulations, we recommend using the extended SAD dataset created for the REF-D1 simulation, but follow the CMIP6 recipe to extend the record to 2100. The time-evolving SAD would be used to the end of 2014, then over a 10-year period the SAD would transition from a repeating annual cycle of 2014 data to a repeating annual cycle of monthly average SAD constructed from the 1850 – 2014 average.

The format of the extended SAD dataset is identical to the CMIP6 dataset, on a constant height vertical coordinate with 0.5 km resolution from 5.0 to 39.5 km altitude and 5° latitude resolution, and 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.

## SEN-D2-geo projection simulation for 2025 - 2100

The purpose of the CCMI-2022 geoengineering experiment is to explore the impact of an enhanced stratospheric aerosol burden due to geoengineering on stratospheric chemistry and transport, while assuming that the tropospheric climate (SSTs) is maintained at 2025 conditions. This is achieved by prescribing the same transient stratospheric aerosol distribution for all models, a distribution that is continuously increasing with increasing greenhouse gas forcing. Since different models will produce a different climate response using the same prescribed aerosol distribution, this experiment requires keeping sea surface temperatures at 2025 (defined as the 2020 – 2030 average from the REF-D2 baseline scenario) conditions for each model. Groups will need to ensure they have the ability to branch from their REF-D2 simulation at January 1, 2025.

The SEN-D2-geo scenario will run for 2025 – 2100 and will use identical forcings as were used in the REF-D2 scenario, with two exceptions. The specified stratospheric aerosol surface area density (SAD) fields of the original REF-D2 simulation will be replaced with a transient stratospheric aerosol SAD that has been calculated by CESM2(WACCM6) using a feedback control algorithm to ensure that SSTs in CESM2(WACCM6) remained at 2025 values. Work is currently underway to produce the specified stratospheric aerosol fields in a format identical to the specified SAD fields already used in the REF-D1 and REF-D2 simulations. Details of the geoengineering SAD dataset will be available soon.

In addition, individual modelling groups will use a repeating annual cycle of sea surface temperatures and sea ice for 2025 – 2100 constructed as the 2020 – 2030 average of the SSTs/sea-ice used in the corresponding ensemble member for their REF-D2 simulation. If groups performed the REF-D2 simulation with a coupled atmosphere-ocean model, specified SSTs and sea-ice calculated from the REF-D2 simulation as just described must be used for the SEN-D2-geo simulation. Please also ensure that other aspects of the model setup (e.g. resolution, number of model levels) remains identical for both the REF-D2 and SEN-D2-geo simulations.

## Alternate radiative forcing scenario simulations for 1960 - 2100

The REF-D2 and SEN-D2-geo simulations are assigned high priority as they directly address headline scientific issues identified for the 2022 Ozone Assessment. For groups that have the necessary capacity, additional scenarios have also been defined with a lower priority. One scenario follows the CMIP6 SSP3-7.0 scenario. The SSP3-7.0 scenario is one with low climate mitigation and high emissions of tropospheric ozone and aerosol precursors. The SSP3-7.0 scenario was also the central scenario for AerChemMIP simulations and would provide an important link between AerChemMIP and the CCMI-2022 simulations.

The other scenario is SSP1-2.6 which represents a high climate mitigation scenario to explore the effects of a low future climate forcing. The SSP1-2.6 scenario will also produce a tropospheric climate similar to that produced in the SEN-D2-geo simulation with geoengineering, thus providing an interesting comparison of two possible paths to a similar level of climate warming.

**Forcings for SSP3-7.0 and SSP1-2.6**:

Both SSP3-7.0 and SSP1-2.6 should follow the CMIP6 specifications for these two scenarios with the same exceptions as was were noted for the REF-D2 scenario compared to SSP2-4.5; the near-surface concentrations of ozone depleting substance should follow the WMO (2018) baseline scenario and a QBO, either internally generated or through relaxation to the provided tropical wind profile, should be included.

**Requested Model Output**
The model output requested for the scenario simulations are identical to that requested for the REF-D1 historical hindcast. An excel version of the data request can be found here. Please note that the instantaneous fields in the A10dayPt table are only requested for one REF-D1 ensemble member, so are not requested from any of the scenario simulations.
Output from the simulations 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 the required MIP tables in JSON format for CMOR3 are available at https://github.com/cedadev/ccmi-2022.

**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 $O(^1D) + H_2O \rightarrow 2OH$; $k_B$ is the rate constant for $OH + O_3 \rightarrow HO_2 + O_2$; $k_C$ is the rate constant for $HO_2 + O_3 \rightarrow OH + 2O_2$.

## 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
Open burning 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

**Quasi-Biennial Oscillation**

For groups relaxing tropical winds to include a QBO in the scenario simulations, a timeseries of zonal average winds at monthly time resolution constructed to cover 1950 – 2100 can be found at:
https://drive.google.com/file/d/1pv_tT1EaFhcoBGIDjV-R_qBje7ADTyKX/view?usp=sharing

**Solar Forcing**

The scenario simulations should use the original SOLARIS-HEPPA solar forcing dataset created for CMIP6, version 3.2. Groups may use either the daily or monthly data as they prefer. The data can be found on the input4MIPs site through:
https://esgf-node.llnl.gov/search/input4mips/?institution_id=SOLARIS-HEPPA

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