CMIP6 Model Documentation

Institute:	HAMMOZ-CONSORTIUM
Model:	MPI-ESM-1-2-HAM
Topic:	atmosChem
Doc. Generated:	2020-04-08
Doc. Seeded From:	Spreadsheet
Specialization Version:	1.0.0
Further Info:	https://es-doc.org/cmip6
Note:	* indicates a required property

Documentation Contents

1 Key Properties

Key properties of the atmospheric chemistry

1.1.1 Top level properties

Key properties of the atmospheric chemistry

1.1.1.1 Name *

Name of atmoschem model code

HAM2.3

1.1.1.2 Keywords *

Keywords associated with atmoschem model code

Sulfur chemistry

1.1.1.3 Overview *

Overview of atmoschem model.

The sulfur chemistry module treats three sulfur species prognostically: sulfur dioxide (SO2), dimethyl sulfide (DMS) and sulfate (the latter not only in the gas phase but also as an aerosol). Three-dimensional climatological fields for oxidants are used i.e. ozone (O3), OH, H2O2, NO2 and NO3. Climatological monthly mean mixing ratios these oxidants from an eight-years (2003-2010) mean Monitoring Atmospheric Composition and Climate (MACC) reanalysis are used. In the gas phase, DMS and SO2 are oxidised by OH and DMS reacts with NO3. In the aqueous phase the oxidation of SO2 by H2O2 and O3 is considered. Sulfuric acid gas produced from gasphase chemistry can either condense on existing aerosol particles or nucleate to form new particles. Sulfate produced from aqueous phase chemistry is distributed to pre-existing soluble accumulation mode and coarse mode aerosol particles. For details see Tegen et al. (2018).

1.1.1.4 Chemistry Scheme Scope *

Atmospheric domains covered by the atmospheric chemistry model

- ☒ Troposphere
- ☐ Stratosphere
- ☐ Mesosphere
- ☐ Mesosphere
- ☐ Whole atmosphere
- ☐ Other - please specify:

1.1.1.5 Basic Approximations *

Basic approximations made in the atmospheric chemistry model

Only sulfur chemistry is considered

1.1.1.6 Prognostic Variables Form *

Form of prognostic variables in the atmospheric chemistry component.

☒ 3D mass/mixing ratio for gas

☐ Other - please specify:

1.1.1.7 Number Of Tracers *

Number of advected tracers in the atmospheric chemistry model

3

1.1.1.8 Family Approach *

Atmospheric chemistry calculations (not advection) generalized into families of species?

☐ True ☒ False

1.1.1.9 Coupling With Chemical Reactivity *

Atmospheric chemistry transport scheme turbulence is couple with chemical reactivity?

☐ True ☒ False

1.2.1 Software Properties

Software properties of aerosol code

1.2.1.1 Repository

Location of code for this component.

Https://redmine.hammoz.ethz.ch/projects/hammoz

1.2.1.2 Code Version

Code version identifier.

2.3

1.2.1.3 Code Languages

Code language(s).

FORTRAN

1.3.1 Timestep Framework

Timestepping in the atmospheric chemistry model

1.3.1.1 Method *

Mathematical method deployed to solve the evolution of a given variable

- ☐ Operator splitting
- ☒ Integrated
- ☐ Other - please specify:

1.3.1.2 Split Operator Advection Timestep

Timestep for chemical species advection (in seconds)

Enter INTEGER value:

1.3.1.3 Split Operator Physical Timestep

Timestep for physics (in seconds).

Enter INTEGER value:

1.3.1.4 Split Operator Chemistry Timestep

Timestep for chemistry (in seconds).

Enter INTEGER value:

1.3.1.5 Split Operator Alternate Order

?

Select either TRUE or FALSE:

☐ True ☐ False

1.3.1.6 Integrated Timestep *

Timestep for the atmospheric chemistry model (in seconds)

450

1.3.1.7 Integrated Scheme Type *

Specify the type of timestep scheme

- ☒ Explicit
- ☐ Implicit
- ☐ Semi-implicit
- ☐ Semi-analytic

- ☐ Impact solver
- ☐ Back Euler
- ☐ Newton Raphson
- ☐ Rosenbrock
- ☐ Other - please specify:

1.3.2 Split Operator Order

1.3.2.1 Turbulence

Call order for turbulence scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

1

1.3.2.2 Convection

Call order for convection scheme This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

1

1.3.2.3 Precipitation

Call order for precipitation scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

1

1.3.2.4 Emissions

Call order for emissions scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

1

1.3.2.5 Deposition

Call order for deposition scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

1

1.3.2.6 Gas Phase Chemistry

Call order for gas phase chemistry scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

1

1.3.2.7 Tropospheric Heterogeneous Phase Chemistry

Call order for tropospheric heterogeneous phase chemistry scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

1

1.3.2.8 Stratospheric Heterogeneous Phase Chemistry

Call order for stratospheric heterogeneous phase chemistry scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

Enter INTEGER value:

1.3.2.9 Photo Chemistry

Call order for photo chemistry scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

Enter INTEGER value:

1.3.2.10 Aerosols

Call order for aerosols scheme. This should be an integer greater than zero, and may be the same value as for another process if they are calculated at the same time.

1

1.4.1 Tuning Applied

Tuning methodology for atmospheric chemistry component

1.4.1.1 Description *

General overview description of tuning: explain and motivate the main targets and metrics retained. andDocument the relative weight given to climate performance metrics versus process oriented metrics, andand on the possible conflicts with parameterization level tuning. In particular describe any struggle andwith a parameter value that required pushing it to its limits to solve a particular model deficiency.

No parameter tuning applied.

1.4.1.2 Global Mean Metrics Used

List set of metrics of the global mean state used in tuning model/component

Enter COMMA SEPARATED list:

1.4.1.3 Regional Metrics Used

List of regional metrics of mean state used in tuning model/component

Enter COMMA SEPARATED list:

1.4.1.4 Trend Metrics Used

List observed trend metrics used in tuning model/component

Enter COMMA SEPARATED list:

2 Grid

Atmospheric chemistry grid

2.1.1 Top level properties

Atmospheric chemistry grid

2.1.1.1 Name

Name of grid in atmoschem model.

Enter TEXT:

2.1.1.2 Overview

Overview of grid in atmoschem model.

Enter TEXT:

2.1.1.3 Matches Atmosphere Grid *

Does the atmospheric chemistry grid match the atmosphere grid?

☒ True ☐ False

2.2.1 Resolution

Resolution in the atmospheric chemistry grid

2.2.1.1 Name *

This is a string usually used by the modelling group to describe the resolution of this grid, e.g. ORCA025, N512L180, T512L70 etc.

T63L47

2.2.1.2 Canonical Horizontal Resolution

Expression quoted for gross comparisons of resolution, eg. 50km or 0.1 degrees etc.

Enter TEXT:

2.2.1.3 Number Of Horizontal Gridpoints

Total number of horizontal (XY) points (or degrees of freedom) on computational grid.

18432

2.2.1.4 Number Of Vertical Levels

Number of vertical levels resolved on computational grid.

47

2.2.1.5 Is Adaptive Grid

Default is False. Set true if grid resolution changes during execution.

Select either TRUE or FALSE:

☐ True ☐ False

3 Transport

Atmospheric chemistry transport

3.1.1 Top level properties

Atmospheric chemistry transport

3.1.1.1 Name

Commonly used name for the transport in atmoschem model.

Enter TEXT:

3.1.1.2 Overview

Overview of atmospheric chemistry transport in atmoschem model.

Aerosol transport is handled by the atmospheric model ECHAM6.3

3.1.1.3 Use Atmospheric Transport *

Is transport handled by the atmosphere, rather than within atmospheric cehmistry?

☒ True ☐ False

3.1.1.4 Transport Details

If transport is handled within the atmospheric chemistry scheme, describe it.

Enter TEXT:

4 Emissions Concentrations

Atmospheric chemistry emissions

4.1.1 Top level properties

Atmospheric chemistry emissions

4.1.1.1 Name

Commonly used name for the emissions concentrations in atmoschem model.

Enter TEXT:

4.1.1.2 Overview

Overview of atmospheric chemistry emissions in atmoschem model.

Sulfur dioxide (SO2) emissions are from the CMIP6 forcing datasets (CEDS, Open Biomass Burning). Dimethyl sulfide (DMS) emissions are from the CMIP6 Open Biomass Burning forcing dataset. Oceanic DMS emissions are computed online based on near surface wind speeds. Terrestrial biogenic DMS emissions are prescribed. Tropospheric SO2 emissions from volcanoes are prescribed from an AeroCom dataset.

4.2.1 Surface Emissions

4.2.1.1 Sources

Sources of the chemical species emitted at the surface that are taken into account in the emissions scheme

- ☒ Vegetation
- ☐ Soil
- ☒ Sea surface
- ☒ Anthropogenic
- ☐ Biomass burning
- ☐ Other - please specify:

4.2.1.2 Method

Methods used to define chemical species emitted directly into model layers above the surface (several methods allowed because the different species may not use the same method).

- ☒ Climatology
- ☐ Spatially uniform mixing ratio
- ☐ Spatially uniform concentration
- ☒ Interactive

☐ Other - please specify:

4.2.1.3 Prescribed Climatology Emitted Species

List of chemical species emitted at the surface and prescribed via a climatology, and the nature of the climatology (E.g. CO (monthly), C2H6 (constant))

SO2 (monthly), DMS (monthly)

4.2.1.4 Prescribed Spatially Uniform Emitted Species

List of chemical species emitted at the surface and prescribed as spatially uniform

Enter COMMA SEPARATED list:

4.2.1.5 Interactive Emitted Species

List of chemical species emitted at the surface and specified via an interactive method

DMS

4.2.1.6 Other Emitted Species

List of chemical species emitted at the surface and specified via any other method

Enter COMMA SEPARATED list:

4.3.1 Atmospheric Emissions

TO DO

4.3.1.1 Sources

Sources of chemical species emitted in the atmosphere that are taken into account in the emissions scheme.

☒ Aircraft

☒ Biomass burning

☐ Lightning

☒ Volcanos

☐ Other - please specify:

4.3.1.2 Method

Methods used to define the chemical species emitted in the atmosphere (several methods allowed because the different species may not use the same method).

☒ Climatology

☐ Spatially uniform mixing ratio

☐ Spatially uniform concentration

☐ Interactive

☐ Other - please specify:

4.3.1.3 Prescribed Climatology Emitted Species

List of chemical species emitted in the atmosphere and prescribed via a climatology (E.g. CO (monthly), C2H6 (constant))

SO2 (monthly), DMS (monthly)

4.3.1.4 Prescribed Spatially Uniform Emitted Species

List of chemical species emitted in the atmosphere and prescribed as spatially uniform

Enter COMMA SEPARATED list:

4.3.1.5 Interactive Emitted Species

List of chemical species emitted in the atmosphere and specified via an interactive method

Enter COMMA SEPARATED list:

4.3.1.6 Other Emitted Species

List of chemical species emitted in the atmosphere and specified via an "other method"

Enter COMMA SEPARATED list:

4.4.1 Concentrations

TO DO

4.4.1.1 Prescribed Lower Boundary

List of species prescribed at the lower boundary.

Enter COMMA SEPARATED list:

4.4.1.2 Prescribed Upper Boundary

List of species prescribed at the upper boundary.

Enter COMMA SEPARATED list:

5 Gas Phase Chemistry

Atmospheric gas phase chemistry transport

5.1.1 Top level properties

Atmospheric gas phase chemistry transport

5.1.1.1 Name

Commonly used name for the gas phase chemistry in atmoschem model.

Enter TEXT:

5.1.1.2 Overview

Overview of atmospheric gas phase chemistry transport in atmoschem model.

DMS is oxidized by reaction with OH during the day and NO3 at night. SO2 is oxidised by OH.

5.1.1.3 Species

Species included in the gas phase chemistry scheme.

Select MULTIPLE options:

- ☐ HOx
- ☐ NOy
- ☐ Ox
- ☐ Cly
- ☐ HSOx
- ☐ Bry
- ☐ VOCs
- ☐ Isoprene
- ☐ H2O
- ☐ Other - please specify:

5.1.1.4 Number Of Bimolecular Reactions *

The number of bi-molecular reactions in the gas phase chemistry scheme.

3

5.1.1.5 Number Of Termolecular Reactions *

The number of ter-molecular reactions in the gas phase chemistry scheme.

0

5.1.1.6 Number Of Tropospheric Heterogenous Reactions *

The number of reactions in the tropospheric heterogeneous chemistry scheme.

2

5.1.1.7 Number Of Stratospheric Heterogenous Reactions *

The number of reactions in the stratospheric heterogeneous chemistry scheme.

0

5.1.1.8 Number Of Advected Species *

The number of advected species in the gas phase chemistry scheme.

3

5.1.1.9 Number Of Steady State Species *

The number of gas phase species for which the concentration is updated in the chemical solver assuming photochemical steady state

0

5.1.1.10 Interactive Dry Deposition *

Is dry deposition interactive (as opposed to prescribed)? Dry deposition describes the dry processes by which gaseous species deposit themselves on solid surfaces thus decreasing their concentration in the air.

☒ True ☐ False

5.1.1.11 Wet Deposition *

Is wet deposition included? Wet deposition describes the moist processes by which gaseous species deposit themselves on solid surfaces thus decreasing their concentration in the air.

☒ True ☐ False

5.1.1.12 Wet Oxidation *

Is wet oxidation included? Oxidation describes the loss of electrons or an increase in oxidation state by a molecule

Select either TRUE or FALSE:

☐ True ☐ False

6 Stratospheric Heterogeneous Chemistry

Atmospheric chemistry startospheric heterogeneous chemistry

6.1.1 Top level properties

Atmospheric chemistry startospheric heterogeneous chemistry

6.1.1.1 Name

Commonly used name for the stratospheric heterogeneous chemistry in atmoschem model.

Enter TEXT:

6.1.1.2 Overview

Overview of atmospheric chemistry startospheric heterogeneous chemistry in atmoschem model.

Enter TEXT:

6.1.1.3 Gas Phase Species

Gas phase species included in the stratospheric heterogeneous chemistry scheme.

Select MULTIPLE options:

- ☐ Cly
- ☐ Bry
- ☐ NOy

6.1.1.4 Aerosol Species

Aerosol species included in the stratospheric heterogeneous chemistry scheme.

Select MULTIPLE options:

- ☐ Sulphate
- ☐ Polar stratospheric ice
- ☐ NAT (Nitric acid trihydrate)
- ☐ NAD (Nitric acid dihydrate)
- ☐ STS (supercooled ternary solution aerosol particule))

6.1.1.5 Number Of Steady State Species *

The number of steady state species in the stratospheric heterogeneous chemistry scheme.

Enter INTEGER value:

6.1.1.6 Sedimentation *

Is sedimentation is included in the stratospheric heterogeneous chemistry scheme or not?

Select either TRUE or FALSE:

☐ True ☐ False

6.1.1.7 Coagulation *

Is coagulation is included in the stratospheric heterogeneous chemistry scheme or not?

Select either TRUE or FALSE:

☐ True ☐ False

7 Tropospheric Heterogeneous Chemistry

Atmospheric chemistry tropospheric heterogeneous chemistry

7.1.1 Top level properties

Atmospheric chemistry tropospheric heterogeneous chemistry

7.1.1.1 Name

Commonly used name for the tropospheric heterogeneous chemistry in atmoschem model.

Enter TEXT:

7.1.1.2 Overview

Overview of atmospheric chemistry tropospheric heterogeneous chemistry in atmoschem model.

In the aqueous phase the oxidation of SO2 by H2O2 and O3 is considered.

7.1.1.3 Gas Phase Species

List of gas phase species included in the tropospheric heterogeneous chemistry scheme.

SO2, H2O2, O3

7.1.1.4 Aerosol Species

Aerosol species included in the tropospheric heterogeneous chemistry scheme.

- ☒ Sulphate
- ☐ Nitrate
- ☐ Sea salt
- ☐ Dust
- ☐ Ice
- ☐ Organic
- ☐ Black carbon/soot
- ☐ Polar stratospheric ice
- ☐ Secondary organic aerosols
- ☐ Particulate organic matter

7.1.1.5 Number Of Steady State Species *

The number of steady state species in the tropospheric heterogeneous chemistry scheme.

2

7.1.1.6 Interactive Dry Deposition *

Is dry deposition interactive (as opposed to prescribed)? Dry deposition describes the dry processes by which gaseous species deposit themselves on solid surfaces thus decreasing their concentration in the air.

☒ True ☐ False

7.1.1.7 Coagulation *

Is coagulation is included in the tropospheric heterogeneous chemistry scheme or not?

Select either TRUE or FALSE:

☐ True ☐ False

8 Photo Chemistry

Atmospheric chemistry photo chemistry

8.1.1 Top level properties

Atmospheric chemistry photo chemistry

8.1.1.1 Name

Commonly used name for the photo chemistry in atmoschem model.

Enter TEXT:

8.1.1.2 Overview

Overview of atmospheric chemistry photo chemistry in atmoschem model.

Enter TEXT:

8.1.1.3 Number Of Reactions *

The number of reactions in the photo-chemistry scheme.

Enter INTEGER value:

8.2.1 Photolysis

Photolysis scheme

8.2.1.1 Method *

Photolysis scheme

Select SINGLE option:

- ☐ Offline (clear sky)
- ☐ Offline (with clouds)
- ☐ Online

8.2.1.2 Environmental Conditions

Describe any environmental conditions taken into account by the photolysis scheme (e.g. whether pressure- and temperature-sensitive cross-sections and quantum yields in the photolysis calculations are modified to reflect the modelled conditions.)

Enter TEXT: