CMIP6 Model Documentation

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1 Key Properties

Key properties of the atmospheric chemistry

1.	1.	1	Top	level	pro	$\mathbf{perties}$
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Key properties of the atmospheric chemistry

1.1.1.1 Name *

Name of atmoschem model code

Enter TEXT:

1.1.1.2 Keywords *

Keywords associated with atmoschem model code

Enter COMMA SEPERATED list:

1.1.1.3 Overview *

Overview of atmoschem model.

Enter TEXT:

1.1.1.4 Chemistry Scheme Scope *

Atmospheric domains covered by the atmospheric chemistry model

Select MULTIPLE options:			
	Troposphere		
	Stratosphere		
	Mesosphere		
	Mesosphere		
	Whole atmosphere		
	Other - please specify:		

1.1.1.5 Basic Approximations *

 $Basic\ approximations\ made\ in\ the\ atmospheric\ chemistry\ model$

Enter TEXT:

1.1.1.6 Prognostic Variables Form *

Form of prognostic variables in the atmospheric chemistry component.

Select MULTIPLE options:

☐ 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
Enter INTEGER value:
1.1.1.8 Family Approach *
Atmospheric chemistry calculations (not advection) generalized into families of species?
Select either TRUE or FALSE:
☐ True ☐ False
1.1.1.9 Coupling With Chemical Reactivity *
Atmospheric chemistry transport scheme turbulence is couple with chemical reactivity?
Select either TRUE or FALSE:
☐ True ☐ False
1.2.1 Software Properties
Software properties of aerosol code
1011D %
1.2.1.1 Repository
Location of code for this component.
Enter TEXT:
1.2.1.2 Code Version
Code version identifier.
Enter TEXT:
1.2.1.3 Code Languages
$Code\ language(s).$
Enter COMMA SEPERATED list:

$1.3.1 \ {\bf Timestep \ Framework}$

 $Time stepping \ in \ the \ atmospheric \ chemistry \ model$

1.3.1.1 Method *
Mathematical method deployed to solve the evolution of a given variable
Select SINGLE option:
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)
Enter INTEGER value:
1.3.1.7 Integrated Scheme Type * Specify the type of timestep scheme
Select SINGLE option:
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.

Enter INTEGER value:

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.

Enter INTEGER value:

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.

Enter INTEGER value:

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.

1.3.2.5 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.

Enter INTEGER value:

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.

Enter INTEGER value:

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.

Enter INTEGER value:

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.

Enter INTEGER value:

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. and Document the relative weight given to climate performance metrics versus process oriented metrics, and on the possible conflicts with parameterization level tuning. In particular describe any struggle and with a parameter value that required pushing it to its limits to solve a particular model deficiency.

Enter TEXT:

1.4.1.2 Global Mean Metrics Used

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

Enter COMMA SEPERATED list:

1.4.1.3 Regional Metrics Used

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

Enter COMMA SEPERATED list:

1.4.1.4 Trend Metrics Used

List observed trend metrics used in tuning model/component

Enter COMMA SEPERATED 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?

Select either TRUE or FALSE: $\begin{tabular}{llll} \hline & True & \begin{tabular}{llll} \hline & False \\ \hline \end{tabular}$

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.

Enter TEXT:

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.

2.2.1.4 Number Of Vertical Levels

 $Number\ of\ vertical\ levels\ resolved\ on\ computational\ grid.$

2.2.1.5 Is Adaptive Grid			
Default 1	is False. Set tru	ie if g	rid resolution changes during execution.
Sele	ct either TRU	J E 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.

 ${f Enter\ TEXT}:$

3.1.1.2 Overview

 $Overview\ of\ atmospheric\ chemistry\ transport\ in\ atmoschem\ model.$

Enter TEXT:

3.1.1.3 Use Atmospheric Transport *

 ${\it Is\ transport\ handled\ by\ the\ atmosphere,\ rather\ than\ within\ atmospheric\ cehmistry?}$

Select either TRUE or FALSE:

_____ 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

 $Commonly\ used\ name\ for\ the\ emissions\ concentrations\ in\ atmoschem\ model.$

 ${f Enter\ TEXT}:$

4.1.1.2 Overview

 $Overview\ of\ atmospheric\ chemistry\ emissions\ in\ atmoschem\ model.$

Enter TEXT:

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

Select MULTIPLE options:			
	Vegetation		
	Soil		
	Sea surface		
	Anthropogenic		
	Biomass burning		
	Other - please specify:		

4.2.1.2 Method

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

Selec	et MULTIPLE options:
	Climatology
	Spatially uniform mixing ratio
	Spatially uniform concentration
П	Interactive

	Other - please specify:
	Prescribed Climatology Emitted Species
	nemical species emitted at the surface and prescribed via a climatology, and the nature of the climatology $(monthly),\ C2H6\ (constant))$
Ente	r COMMA SEPERATED list:
4.2.1.4	Prescribed Spatially Uniform Emitted Species
List of ch	nemical species emitted at the surface and prescribed as spatially uniform
Ente	r COMMA SEPERATED list:
4.2.1.5	Interactive Emitted Species
List of ch	nemical species emitted at the surface and specified via an interactive method
Ente	r COMMA SEPERATED list:
4.2.1.6	Other Emitted Species
List of ch	nemical species emitted at the surface and specified via any other method
Ente	r COMMA SEPERATED list:
4.3.1	Atmospheric Emissions
TO DO	-
4.3.1.1	Sources
Sources of	of chemical species emitted in the atmosphere that are taken into account in the emissions scheme.
Selec	et MULTIPLE options:
	Aircraft
	Biomass burning
	Lightning
	Volcanos
	Other - please specify:
	Method used to define the chemical species emitted in the atmosphere (several methods allowed because the dif
	used to define the chemical species emitted in the atmosphere (several methods allowed because the aij exies may not use the same method).
Selec	et MULTIPLE options:
	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))

Enter COMMA SEPERATED list:

4.3.1.4 Prescribed Spatially Uniform Emitted Species

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

Enter COMMA SEPERATED list:

4.3.1.5 Interactive Emitted Species

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

Enter COMMA SEPERATED list:

4.3.1.6 Other Emitted Species

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

Enter COMMA SEPERATED list:

4.4.1 Concentrations

TO DO

4.4.1.1 Prescribed Lower Boundary

List of species prescribed at the lower boundary.

Enter COMMA SEPERATED list:

4.4.1.2 Prescribed Upper Boundary

List of species prescribed at the upper boundary.

Enter COMMA SEPERATED 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

 $Overview\ of\ atmospheric\ gas\ phase\ chemistry\ transport\ in\ atmoschem\ model.$

Enter TEXT:

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 *

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

5.1.1.5 Number Of Termolecular Reactions * The number of ter-molecular reactions in the gas phase chemistry scheme.
Enter INTEGER value:
5.1.1.6 Number Of Tropospheric Heterogenous Reactions *
The number of reactions in the tropospheric heterogeneous chemistry scheme.
Enter INTEGER value:
5.1.1.7 Number Of Stratospheric Heterogenous Reactions *
The number of reactions in the stratospheric heterogeneous chemistry scheme.
Enter INTEGER value:
5.1.1.8 Number Of Advected Species *
The number of advected species in the gas phase chemistry scheme.
Enter INTEGER value:
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 photo chemical steady state
Enter INTEGER value:
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.
Select either TRUE or FALSE:
☐ 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.

Select either TRUE or FALSE:

☐ False

☐ True

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

Select MULTIPLE options:

Gas phase species included in the stratospheric heterogeneous chemistry scheme.

	Cly	
	Bry	
	NOy	
	Aerosol Species vecies 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.

6.1.1.6 Sedimentation * Is sedimentation is included in the stratospheric heterogeneous chemistry scheme or not?		
☐ 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

 $Overview\ of\ atmospheric\ chemistry\ tropospheric\ heterogeneous\ chemistry\ in\ atmoschem\ model.$

Enter TEXT:

7.1.1.3 Gas Phase Species

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

Enter COMMA SEPERATED list:

7.1.1.4 Aerosol Species

Aerosol species included in the tropospheric heterogeneous chemistry scheme.

Select MULTIPLE options:		
	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.

7.1.1.6	Interactive	\mathbf{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.

	ect either TRU	UE or FALSE: False
	7 Coagulatio	on * ed in the tropospheric heterogeneous chemistry scheme or not?
Sele	ect either TR	UE 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: