CMIP6 Model Documentation

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1 Key Properties

Key properties of the atmospheric chemistry

1	.1.	1 T	'op	level	pro	perties

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 SEPARATED 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			
П	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			
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			
$Code\ language(s).$			

1.3.1 Timestep Framework Timestepping in the atmospheric che

Timesteppi	ng in the atmospheric chemistry model
1.3.1.1 Me	ethod *
Mathematica	l method deployed to solve the evolution of a given variable
Select S	INGLE option:
□ o:	perator splitting
☐ In	tegrated
O-	ther - please specify:
1.3.1.2 Sp	lit Operator Advection Timestep
Timestep for	$chemical\ species\ advection\ (in\ seconds)$
Enter II	NTEGER value:
1.3.1.3 Sp	lit Operator Physical Timestep
Timestep for	physics (in seconds).
Enter II	NTEGER value:
1.3.1.4 Sp	lit Operator Chemistry Timestep
Timestep for	chemistry (in seconds).
Enter II	NTEGER value:
101 7 0	
1.3.1.5 Sp	lit Operator Alternate Order
Select e	ither TRUE or FALSE:
☐ Tru	e False
1.3.1.6 Int	tegrated Timestep *

 $Timestep\ for\ the\ atmospheric\ chemistry\ model\ (in\ seconds)$

Enter INTEGER value:

5

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

1.3.2 Split Operator Order

Other - please specify:

Rosenbrock

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.

Enter INTEGER value:

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 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 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

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:

______ 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.

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 is False. Set true if grid 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

 $Commonly\ used\ name\ for\ the\ transport\ in\ atmoschem\ model.$

Enter TEXT:

3.1.1.2 Overview

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

Enter TEXT:

3.1.1.3 Use Atmospheric Transport *

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

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.

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

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

Select MULTIPLE options:			
	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))
Enter COMMA SEPARATED list:
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
Enter COMMA SEPARATED list:
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.
Select MULTIPLE options:
☐ 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).

Select 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 SEPARATED 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 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.

4.4.1.2 Prescribed Upper Boundary

 $List\ of\ species\ prescribed\ at\ the\ upper\ boundary.$

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 *

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

5.1.1.5 Number Of Termole	cular Reactions *
The number of ter-molecular reaction	ns in the gas phase chemistry scheme.
Enter INTEGER value:	
5.1.1.6 Number Of Troposp	heric Heterogenous Reactions *
The number of reactions in the tropo	spheric heterogeneous chemistry scheme.
Enter INTEGER value:	
5.1.1.7 Number Of Stratosp	oheric Heterogenous Reactions *
The number of reactions in the strate	ospheric heterogeneous chemistry scheme.
Enter INTEGER value:	
5.1.1.8 Number Of Advecte	ed Species *
The number of advected species in the	e gas phase chemistry scheme.
Enter INTEGER value:	
5.1.1.9 Number Of Steady S	State Species *
The number of gas phase species for chemical steady state	which the concentration is updated in the chemical solver assuming photo
Enter INTEGER value:	
5.1.1.10 Interactive Dry De	position *
	posed to prescribed)? Dry deposition describes the dry processes by which a solid surfaces thus decreasing their concentration in the air.
Select either TRUE or FALS	SE:
☐ 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 \ molecular \ oxidation \ state \ by \ a \ molecular \ oxidation \$
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)	
П	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 *
${\it Is sedimentation is included in the stratospheric heterogeneous chemistry scheme or not?}$
Select either TRUE or FALSE:
☐ True ☐ False
6.1.1.7 Coagulation *
${\it Is coagulation is included in the stratospheric heterogeneous chemistry scheme or not?}$
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 SEPARATED list:

7.1.1.4 Aerosol Species

Aerosol species included in the tropospheric heterogeneous chemistry scheme.

Selec	t 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 Sp	pecies	ж
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 $The \ number \ of \ steady \ state \ species \ in \ the \ tropospheric \ heterogeneous \ chemistry \ scheme.$

Enter INTEGER value:

☐ True ☐ False

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.
Select either TRUE or FALSE:
☐ True ☐ False
7.1.1.7 Coagulation *
Is coagulation is included in the tropospheric heterogeneous chemistry scheme or not?
Select either TRUE or 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: