# CMIP6 Model Documentation

Institute: NASA-GISS
Model: GISS-E2-1-H

**Topic**: Atmospheric Chemistry

**Doc. Generated**: 2018-10-04

**Doc. Seeded From**: N/A

Specialization Version: 1.0.0

Further Info: https://es-doc.org/cmip6

**Note**: \* indicates a required property

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# 1 Key Properties

Key properties of the atmospheric chemistry

1.1	$\mathbf{Kev}$	Prop	erties

Key properties of the atmospheric chemistry

# 1.1.1 Name \*

Name of atmoschem model code

Enter TEXT:

### 1.1.2 Keywords \*

Keywords associated with atmoschem model code

Enter COMMA SEPERATED list:

### 1.1.3 Overview \*

Overview of atmoschem model.

Enter TEXT:

# 1.1.4 Chemistry Scheme Scope \*

Atmospheric domains covered by the atmospheric chemistry model

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

# 1.1.5 Basic Approximations \*

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

Enter TEXT:

# 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:
1.1.7 Number Of Tracers *  Number of advected tracers in the atmospheric chemistry model
Enter INTEGER value:
1.1.8 Family Approach *
Atmospheric chemistry calculations (not advection) generalized into families of species:
Select either TRUE or FALSE:
☐ True ☐ False
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 Software Properties
Software properties of aerosol code
1.2.1 Repository
Location of code for this component.
Enter TEXT:
1.2.2 Code Version
Code version identifier.
Enter TEXT:
1.2.3 Code Languages
$Code\ language(s).$
Enter COMMA SEPERATED list:
1.3 Timestep Framework
Timestepping in the atmospheric chemistry model
1.3.1 Overview
Overview of timestepping in the atmospheric chemistry model in atmoschem model.

Enter TEXT:

1.3.2	
	natical method deployed to solve the evolution of a given variable
	Operator splitting Integrated Other - please specify:
	Split Operator Advection Timestep  sep for chemical species advection (in seconds)  ter INTEGER value:
	Split Operator Physical Timestep  sep for physics (in seconds).  ter INTEGER value:
	Split Operator Chemistry Timestep ep for chemistry (in seconds). ter INTEGER value:
<b>1.3.6</b> ?	Split Operator Alternate Order
Sel	ect either TRUE or FALSE:
	True False
	Integrated Timestep * ep for the atmospheric chemistry model (in seconds) ter INTEGER value:
	Integrated Scheme Type *  the type of timestep scheme  ect SINGLE option:  Explicit

Implicit
Semi-implicit
Semi-analytic
Impact solver
Back Euler
Newton Raphson
Rosenbrock
Other - please specify:

# 1.4 Split Operator Order

#### 1.4.1 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:

#### 1.4.2 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:

## 1.4.3 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:

## 1.4.4 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.

#### 1.4.5 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:

#### 1.4.6 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:

### 1.4.7 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:

### 1.4.8 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:

#### 1.4.9 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:

#### 1.4.10 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:

# 1.5 Tuning Applied

Tuning methodology for atmospheric chemistry component

#### 1.5.1 Overview

 $Overview\ of\ tuning\ methodology\ for\ atmospheric\ chemistry\ component\ in\ atmoschem\ model.$ 

Enter TEXT:

### 1.5.2 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:

#### 1.5.3 Global Mean Metrics Used

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

Enter COMMA SEPERATED list:

# 1.5.4 Regional Metrics Used

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

Enter COMMA SEPERATED list:

#### 1.5.5 Trend Metrics Used

List observed trend metrics used in tuning model/component

Enter COMMA SEPERATED list:

# 2 Grid

Atmospheric chemistry grid

# 2.1 Grid

Atmospheric chemistry grid

#### 2.1.1 Name

Name of grid in atmoschem model.

Enter TEXT:

#### 2.1.2 Overview

Overview of grid in atmoschem model.

Enter TEXT:

# 2.1.3 Matches Atmosphere Grid \*

Does the atmospheric chemistry grid match the atmosphere grid?

Select either TRUE or FALSE:

\_\_\_\_\_\_ True \_\_\_\_\_ False

#### 2.2 Resolution

Resolution in the atmospheric chemistry grid

### 2.2.1 Overview

Overview of resolution in the atmospheric chemistry grid in atmoschem model.

Enter TEXT:

### 2.2.2 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:

# 2.2.3 Canonical Horizontal Resolution

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

Enter TEXT:

### 2.2.4 Number Of Horizontal Gridpoints

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

# 2.2.5 Number Of Vertical Levels

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

2.2.6	Is Ad	aptive Gri	$\mathbf{d}$			
Default a	is False.	Set true if gr	rid resolution o	changes	during	execution.
Sele	ct eithe	er TRUE or	FALSE:			
	True		False			

# 3 Transport

 $Atmospheric\ chemistry\ transport$ 

# 3.1 Transport

 $Atmospheric\ chemistry\ transport$ 

### 3.1.1 Name

Commonly used name for the transport in atmoschem model.

Enter TEXT:

#### 3.1.2 Overview

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

Enter TEXT:

# 3.1.3 Use Atmospheric Transport \*

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

Select either TRUE or FALSE:

\_\_\_\_\_\_ True \_\_\_\_\_\_ False

# 3.1.4 Transport Details

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

Enter TEXT:

# 4 Emissions Concentrations

Atmospheric chemistry emissions

4 -4	т		
4.1	Himissions	Concentration	•

 $Atmospheric\ chemistry\ emissions$ 

### 4.1.1 Name

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

Enter TEXT:

#### 4.1.2 Overview

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

Enter TEXT:

# 4.2 Surface Emissions

#### 4.2.1 Overview

Overview of in atmoschem model.

Enter TEXT:

# 4.2.2 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:	

#### **4.2.3** 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:
4.2.4 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 SEPERATED list:
4.2.5 Prescribed Spatially Uniform Emitted Species
List of chemical species emitted at the surface and prescribed as spatially uniform
Enter COMMA SEPERATED list:
4.2.6 Interactive Emitted Species
List of chemical species emitted at the surface and specified via an interactive method
Enter COMMA SEPERATED list:
4.2.7 Other Emitted Species
List of chemical species emitted at the surface and specified via any other method
Enter COMMA SEPERATED list:
4.3 Atmospheric Emissions
TO DO
4.3.1 Overview
Overview of to do in atmoschem model.
Enter TEXT:
4.3.2 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:

#### **4.3.3** 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	t MULTIPLE options:
	Climatology
	Spatially uniform mixing ratio
	Spatially uniform concentration
	Interactive
	Other - please specify:

# 4.3.4 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:

# 4.3.5 Prescribed Spatially Uniform Emitted Species

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

Enter COMMA SEPERATED list:

### 4.3.6 Interactive Emitted Species

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

Enter COMMA SEPERATED list:

#### 4.3.7 Other Emitted Species

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

Enter COMMA SEPERATED list:

## 4.4 Concentrations

TO DO

#### 4.4.1 Overview

Overview of to do in atmoschem model.

Enter TEXT:

# 4.4.2 Prescribed Lower Boundary

List of species prescribed at the lower boundary.

Enter COMMA SEPERATED list:

# 4.4.3 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 Gas Phase Chemistry

 $Atmospheric\ gas\ phase\ chemistry\ transport$ 

### 5.1.1 Name

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

Enter TEXT:

#### 5.1.2 Overview

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

Enter TEXT:

### 5.1.3 Species

Species included in the gas phase chemistry scheme.

Select MULTIPLE options:			
	HOx		
	NOy		
	Ox		
	Cly		
	HSOx		
	Bry		
	VOCs		
	Isoprene		
	H2O		
	Other - please specify:		

# 5.1.4 Number Of Bimolecular Reactions \*

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

5.1.5 Number Of Termolecular Reactions *  The number of ter-molecular reactions in the gas phase chemistry scheme.  Enter INTEGER value:
5.1.6 Number Of Tropospheric Heterogenous Reactions *
The number of reactions in the tropospheric heterogeneous chemistry scheme.
Enter INTEGER value:
5.1.7 Number Of Stratospheric Heterogenous Reactions *  The number of reactions in the stratospheric heterogeneous chemistry scheme.  Enter INTEGER value:
5.1.8 Number Of Advected Species *
The number of advected species in the gas phase chemistry scheme.
Enter INTEGER value:
5.1.9 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
Enter INTEGER value:
5.1.10 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

Is wnselve

.11 V	Wet Deposi	tion	*			
			deposition describes the moist processes by which gaseous reasing their concentration in the air.	species	deposit	then
Select	either TRUE	or F	ALSE:			
☐ Tr	rue	] F	alse			

5.1.12 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 Stratospheric Heterogeneous Chemistry

$Atmos_{i}$	pheric chemistry startospheric heterogeneous chemistry
6.1.1	Name
Commo	nly used name for the stratospheric heterogeneous chemistry in atmoschem model.
Ent	er TEXT:
6.1.2	Overview
Overvie	$w\ of\ atmospheric\ chemistry\ startospheric\ heterogeneous\ chemistry\ in\ atmoschem\ model.$
Ent	er TEXT:
6.1.3	Gas Phase Species
Gas pho	ise species included in the stratospheric heterogeneous chemistry scheme.
Sele	ect MULTIPLE options:
	Cly
	Bry
	NOy

# 6.1.4 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))		

# 6.1.5 Number Of Steady State Species \*

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

6.1.6	Sedimentation *
Is sedim	entation is included in the stratospheric heterogeneous chemistry scheme or not?
Sele	ect either TRUE or FALSE:
	True
6.1.7	Coagulation *
Is coagu	lation is included in the stratospheric heterogeneous chemistry scheme or not?
Sele	ect either TRUE or FALSE:
	True

# 7 Tropospheric Heterogeneous Chemistry

Atmospheric chemistry tropospheric heterogeneous chemistry

# 7.1 Tropospheric Heterogeneous Chemistry

Atmospheric chemistry tropospheric heterogeneous chemistry

#### 7.1.1 Name

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

Enter TEXT:

#### 7.1.2 Overview

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

Enter TEXT:

#### 7.1.3 Gas Phase Species

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

Enter COMMA SEPERATED list:

# 7.1.4 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		

# 7.1.5 Number Of Steady State Species \*

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

7.1.6	Interactive Dry Deposition *
	deposition interactive (as opposed to prescribed)? Dry deposition describes the dry processes by which species deposit themselves on solid surfaces thus decreasing their concentration in the air.
Sele	ect either TRUE or FALSE:
	True
7.1.7	Coagulation *
Is coagu	lation is included in the tropospheric heterogeneous chemistry scheme or not?
Sele	ect either TRUE or FALSE:
	True

# 8 Photo Chemistry

Atmospheric chemistry photo chemistry

# 8.1 Photo Chemistry

Atmospheric chemistry photo chemistry

#### 8.1.1 Name

Commonly used name for the photo chemistry in atmoschem model.

Enter TEXT:

#### 8.1.2 Overview

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

Enter TEXT:

#### 8.1.3 Number Of Reactions \*

The number of reactions in the photo-chemistry scheme.

Enter INTEGER value:

# 8.2 Photolysis

Photolysis scheme

#### 8.2.1 Overview

Overview of photolysis scheme in atmoschem model.

Enter TEXT:

#### 8.2.2 Method \*

 $Photolysis\ scheme$ 

# Select SINGLE option:

Offline (clear sky)
Offline (with clouds)
Online

#### 8.2.3 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: