

# CMIP6 Model Documentation

<b>Institute:</b>	MESSY-CONSORTIUM
<b>Model:</b>	EMAC-2-53-AERCHEM
<b>Topic:</b>	Atmospheric Chemistry
<b>Doc. Generated:</b>	2018-04-12
<b>Doc. Seeded From:</b>	N/A
<b>Specialization Version:</b>	0.3.1
<b>Further Info:</b>	<a href="https://es-doc.org/cmip6">https://es-doc.org/cmip6</a>
<b>Note:</b>	* indicates a required property

# Documentation Contents

<b>1</b>	<b>Key Properties</b>	<b>1</b>
1.1	Key Properties . . . . .	1
1.2	Software Properties . . . . .	2
1.3	Timestep Framework . . . . .	2
1.4	Split Operator Order . . . . .	4
1.5	Tuning Applied . . . . .	5
<b>2</b>	<b>Grid</b>	<b>7</b>
2.1	Grid . . . . .	7
2.2	Resolution . . . . .	7
<b>3</b>	<b>Transport</b>	<b>9</b>
3.1	Transport . . . . .	9
<b>4</b>	<b>Emissions Concentrations</b>	<b>10</b>
4.1	Emissions Concentrations . . . . .	10
4.2	Surface Emissions . . . . .	10
4.3	Atmospheric Emissions . . . . .	11
4.4	Concentrations . . . . .	12
<b>5</b>	<b>Gas Phase Chemistry</b>	<b>14</b>
5.1	Gas Phase Chemistry . . . . .	14
<b>6</b>	<b>Stratospheric Heterogeneous Chemistry</b>	<b>17</b>
6.1	Stratospheric Heterogeneous Chemistry . . . . .	17
<b>7</b>	<b>Tropospheric Heterogeneous Chemistry</b>	<b>19</b>
7.1	Tropospheric Heterogeneous Chemistry . . . . .	19
<b>8</b>	<b>Photo Chemistry</b>	<b>21</b>
8.1	Photo Chemistry . . . . .	21
8.2	Photolysis . . . . .	21

# 1 Key Properties

*Key properties of the atmospheric chemistry*

## 1.1 Key Properties

*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:**

- ☐ Troposphere
- ☐ 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 Method \*

*Mathematical method deployed to solve the evolution of a given variable*

Select SINGLE option:

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

### 1.3.3 Split Operator Advection Timestep

*Timestep for chemical species advection (in seconds)*

Enter INTEGER value:

### 1.3.4 Split Operator Physical Timestep

*Timestep for physics (in seconds).*

Enter INTEGER value:

### 1.3.5 Split Operator Chemistry Timestep

*Timestep for chemistry (in seconds).*

Enter INTEGER value:

### 1.3.6 Split Operator Alternate Order

?

Select either TRUE or FALSE:

- ☐ True      ☐ False

### 1.3.7 Integrated Timestep \*

*Timestep for the atmospheric chemistry model (in seconds)*

Enter INTEGER value:

### 1.3.8 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:

## 1.4 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.*

**Enter INTEGER value:**

#### 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 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.*

Enter INTEGER value:

### 2.2.5 Number Of Vertical Levels

*Number of vertical levels resolved on computational grid.*

**Enter INTEGER value:**

### 2.2.6 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 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 \*

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

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*

### 4.1 Emissions Concentrations

*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 **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:**

- ☐ HO<sub>x</sub>
- ☐ NO<sub>y</sub>
- ☐ O<sub>x</sub>
- ☐ Cly
- ☐ HSO<sub>x</sub>
- ☐ Bry
- ☐ VOCs
- ☐ Isoprene
- ☐ H<sub>2</sub>O
- ☐ Other - please specify:

#### 5.1.4 Number Of Bimolecular Reactions \*

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

**Enter INTEGER value:**



#### 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 photo-chemical 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

#### 5.1.11 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:

☐

True

☐

False

### 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

*Atmospheric chemistry startospheric heterogeneous chemistry*

#### 6.1.1 Name

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

Enter TEXT:

#### 6.1.2 Overview

*Overview of atmospheric chemistry startospheric heterogeneous chemistry in atmoschem model.*

Enter TEXT:

#### 6.1.3 Gas Phase Species

*Gas phase species included in the stratospheric heterogeneous chemistry scheme.*

Select 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.*

Enter INTEGER value:

### 6.1.6 Sedimentation \*

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

Select either TRUE or FALSE:

☐ True      ☐ False

### 6.1.7 Coagulation \*

*Is coagulation 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 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.*

**Enter INTEGER value:**

### 7.1.6 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

### 7.1.7 Coagulation \*

*Is coagulation 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 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:**