

# Gas-Phase Chemistry

## Default Chemical Mechanism used in CESM 2.0 and CESM 2.1

All CAM-chem [compsets](#) default to the MOZART-TS1 chemical mechanism, which includes comprehensive chemistry relevant to the troposphere and stratosphere. All WACCM compsets default to TSMLT1 chemical mechanism, which includes all chemistry relevant to the troposphere, stratosphere, mesosphere, and lower thermosphere. The TS1 and TSMLT1 chemical mechanisms are described in [Emmons et al. \(2020\)](#). These mechanisms include the Modal Aerosol Model (MAM4) and a VBS-SOA scheme described in [Tilmes et al. \(2019\)](#). More details of the stratospheric chemistry are provided in [Gent et al. \(2019\)](#).

## Chemical mechanisms in CESM2.2

**MOZART-TS1.1:** The default CAM-chem MOZART-TS1 chemistry has been updated in CESM2 to include NO<sub>x</sub>-dependence in the VBS-SOA scheme, as described in [Jo et al. \(2020\)](#).

### **MOZART-TS2: Improved isoprene and terpene oxidation (Rebecca Schwantes, NCAR)**

The isoprene chemical mechanism was updated to include the most recent advances in our theoretical/experimental understanding of isoprene OH, NO<sub>3</sub>, and O<sub>3</sub> oxidation (e.g., [Wennberg et al. 2018](#)). The terpene (monoterpenes and sesquiterpenes) chemistry was expanded to include 5 surrogate species (APIN, BPIN, LIMON, MYRC, and BCARY) rather than 2 (MTERP and BCARY) with terpenes grouped according to their chemical structure and oxidation products. These terpene chemistry updates are based on the most recent theoretical/experimental understanding of terpene OH, NO<sub>3</sub>, and O<sub>3</sub> oxidation. A description and evaluation of the MOZART-TS2 chemical mechanism is provided in [Schwantes et al. \(2020\)](#). CESM2.2 includes a compset ("FCts2nudged") for the MOZART-TS2 chemical mechanism

## Current gas-phase chemical mechanism development:

**MOZART-TS3: Speciated alkane oxidation (Rebecca Schwantes, NCAR):** The alkane chemical mechanism is expanded from one surrogate species (BIGALK) to 5 surrogate species (NBUTANE, ISOBUTANE, NPENTANE, IPENTANE, and C6ALKANES).

**MOZART-TS4:** An updated version of MOZART-2 chemistry to be suitable for climate simulations and a cheaper option for use with MOSAIC-MAM (forming nitrate aerosols). (Louisa Emmons, NCAR)

**Tagged NO<sub>x</sub> scheme (Louisa Emmons, NCAR):** A tagged NO<sub>x</sub> scheme is under development, which will be useful for tracking NO<sub>x</sub> emissions in CAM-chem. This scheme will allow the user to tag NO<sub>x</sub> emissions from certain sectors or regions. The tagged NO<sub>x</sub> will be chemically processed in the same manner as untagged NO<sub>x</sub> and the O<sub>3</sub> production from the tagged NO<sub>x</sub> will be tracked.

If you are working on updating certain aspects of the gas-phase chemistry in CAM-Chem, please complete the form on [Users and Projects](#) page. We will add your project to this list, and ensure your updates are contributed back to the main code.