

Supplementary Table S2. Atmospheric species in the Archean photochemical code with lower boundary condition type and values. Lower boundary conditions are given in cm/s for deposition velocity (Vdep), a dimensionless mixing ratio by volume for fixed concentration (f_0), and molecules/cm²/s for flux (flux). Species names ending in “AER” are types of aerosols.

Species	Lower Boundary Type	Vdep/ f_0 /flux
Long-Lived Species		
O	constant deposition velocity	1
O ₂	constant mixing ratio	$1 \cdot 10^{-08}$
H ₂ O	constant deposition velocity	0
H	constant deposition velocity	1
OH	constant deposition velocity	1
HO ₂	constant deposition velocity	1
H ₂ O ₂	constant deposition velocity	$2 \cdot 10^{-01}$
H ₂	constant deposition velocity*	$2.4 \cdot 10^{-04}$
CO	constant deposition velocity	$1.2 \cdot 10^{-04}$
HCO	constant deposition velocity	1
H ₂ CO	constant deposition velocity	$2 \cdot 10^{-01}$
CH ₄	constant mixing ratio	variable [†]
CH ₃	constant deposition velocity	1
C ₂ H ₆	constant deposition velocity	0
NO	constant deposition velocity	$3 \cdot 10^{-04}$
NO ₂	constant deposition velocity	$3 \cdot 10^{-03}$
HNO	constant deposition velocity	1
O ₃	constant deposition velocity	$7 \cdot 10^{-02}$
HNO ₃	constant deposition velocity	$2 \cdot 10^{-01}$
N	constant deposition velocity	0
H ₂ S	constant deposition velocity*	$2 \cdot 10^{-02}$
HS	constant deposition velocity	0
S	constant deposition velocity	0
SO	constant deposition velocity	0
SO ₂	constant deposition velocity*	1
SO ₃	constant deposition velocity	0
H ₂ SO ₄	constant deposition velocity	1
HSO	constant deposition velocity	1
S ₂	constant deposition velocity	0
C ₂	constant deposition velocity	0
CH	constant deposition velocity	0
C ₂ H	constant deposition velocity	0
CH ₂ ³	constant deposition velocity	0
C ₂ H ₅	constant deposition velocity	0
C ₂ H ₂	constant deposition velocity	0
C ₂ H ₄	constant deposition velocity	0
C ₃ H ₈	constant deposition velocity	0
C ₃ H ₇	constant deposition velocity	0
C ₃ H ₅	constant deposition velocity	0
C ₂ H ₃	constant deposition velocity	0
C ₃ H ₆	constant deposition velocity	0

C ₃ H ₂	constant deposition velocity	0
C ₃ H ₃	constant deposition velocity	0
CH ₂ CCH ₂	constant deposition velocity	0
CH ₂ CO	constant deposition velocity	0
CH ₃ CO	constant deposition velocity	0
CH ₃ CHO	constant deposition velocity	0
CH ₃ O	constant deposition velocity	0
CH ₃ O ₂	constant deposition velocity	0
C ₂ H ₄ OH	constant deposition velocity	0
C ₂ H ₂ OH	constant deposition velocity	0
C ₂ H ₅ CHO	constant deposition velocity	0
CH ₃ C ₂ H	constant deposition velocity	0
CS ₂	constant deposition velocity	0
HCS	constant deposition velocity	0
OCS	constant deposition velocity	0
CS	constant deposition velocity	0
SO ₄ AER	constant deposition velocity	1·10 ⁻⁰²
S ₈ AER	constant deposition velocity	1·10 ⁻⁰²
HCAER	constant deposition velocity	1·10 ⁻⁰²
HCAER2	constant deposition velocity	1·10 ⁻⁰²
Short-Lived Species		
HNO ₂	constant deposition velocity	0
O ¹ D	constant deposition velocity	0
CH ₂ ¹	constant deposition velocity	0
C	constant deposition velocity	0
SO ₂ ¹	constant deposition velocity	0
SO ₂ ³	constant deposition velocity	0
HSO ₃	constant deposition velocity	0
OCS ₂	constant deposition velocity	0
CS ₂ [*]	constant deposition velocity	0
S ₃	constant deposition velocity	0
S ₄	constant deposition velocity	0
Inert Species		
CO ₂	constant mixing ratio	variable [†]
N ₂	constant mixing ratio	remainder [‡]

* - In addition to a constant deposition velocity, we also use a volcanic flux for these gases. Specifically, we used volcanic fluxes of $3.5 \cdot 10^9$ molecules/cm²/s of H₂, $1 \cdot 10^{10}$ molecules/cm²/s of SO₂, and $3.5 \cdot 10^8$ molecules/cm²/s of H₂S.

† - See text for information on these mixing ratios.

‡ - N₂ fills the remainder of the atmosphere.