

Supplementary material: A tropospheric ozone source attribution system for CESM 1.2.2

Tim Butler¹, Aurelia Lupascu¹, Jane Coates¹, and Shuai Zhu²

¹Institute for Advanced Sustainability Studies, Potsdam, Germany

²now at China Unicom System Integration Limited Corporation

Correspondence to: Tim Butler tim.butler@iass-potsdam.de

1 Reactions of tagged species

In this supplement we present all reactions of the tagged tracers added to the chemical mechanism as described in the main paper, along with the corresponding reactions from the base chemical mechanism. NO_x-tagged reactions are shown in Table S1, and VOC-tagged reactions are shown in Table S2.

Table S1. Full list of reactions modified for NO_x tagging. Original reactions from the base mechanism are shown in the left column, and their tagged counterparts in the right column. Here, only one user-specified tag identity “TAG” is applied. Additional reactions producing tagged tracers with the ‘STR’ and “XTR” identities (as described in the main paper) are also shown.

Original reaction			NO _x -tagged reaction		
O ₂ + <i>hν</i>	→	2 O	O ₂ + <i>hν</i>	→	2 O_X_STR + O ₂
O ₃ + <i>hν</i>	→	O1D + O ₂	O3_X_TAG + <i>hν</i>	→	O1D_X_TAG
O ₃ + <i>hν</i>	→	O + O ₂	O3_X_TAG + <i>hν</i>	→	O_X_TAG
N ₂ O + <i>hν</i>	→	O1D + N ₂	N ₂ O + <i>hν</i>	→	O1D_X_STR + N ₂ O
NO ₂ + <i>hν</i>	→	NO + O	NO ₂ _TAG + <i>hν</i>	→	NO_TAG
			NO ₂ _X_TAG + <i>hν</i>	→	O_X_TAG
N ₂ O ₅ + <i>hν</i>	→	NO ₂ + NO ₃	NO ₃ NO ₂ _TAG + <i>hν</i>	→	NO ₂ _TAG
			NO ₂ NO ₃ _TAG + <i>hν</i>	→	NO ₃ _TAG
			NO ₃ NO ₂ _X_TAG + <i>hν</i>	→	NO ₂ _X_TAG
			NO ₂ NO ₃ _X_TAG + <i>hν</i>	→	NO ₃ _X_TAG
HNO ₃ + <i>hν</i>	→	NO ₂ + OH	HNO ₃ _TAG + <i>hν</i>	→	NO ₂ _TAG
			HNO ₃ _X_TAG + <i>hν</i>	→	NO ₂ _X_TAG
NO ₃ + <i>hν</i>	→	.89 NO ₂ + .11 NO + .89 O ₃	NO ₃ _TAG + <i>hν</i>	→	.89 NO ₂ _TAG + .11 NO_TAG
			NO ₃ _X_TAG + <i>hν</i>	→	.89 NO ₂ _X_TAG + .89 O ₃ _X_TAG
HO ₂ NO ₂ + <i>hν</i>	→	.33 OH + .33 NO ₃ + .66 NO ₂	HO ₂ NO ₂ _TAG + <i>hν</i>	→	.33 NO ₃ _TAG + .66 NO ₂ _TAG
		+ .66 HO ₂	HO ₂ NO ₂ _X_TAG + <i>hν</i>	→	.33 NO ₃ _X_TAG + .66 NO ₂ _X_TAG
PAN + <i>hν</i>	→	.6 CH ₃ CO ₃ + .6 NO ₂ + .4 CH ₃ O ₂	PAN_TAG + <i>hν</i>	→	.6 NO ₂ _TAG + .4 NO ₃ _TAG
		+ .4 NO ₃ + .4 CO ₂	PAN_X_TAG + <i>hν</i>	→	.6 NO ₂ _X_TAG + .4 NO ₃ _X_TAG
MPAN + <i>hν</i>	→	MCO ₃ + NO ₂	MPAN_TAG + <i>hν</i>	→	NO ₂ _TAG
			MPAN_X_TAG + <i>hν</i>	→	NO ₂ _X_TAG
ONITR + <i>hν</i>	→	HO ₂ + CO + NO ₂	ONITR_TAG + <i>hν</i>	→	NO ₂ _TAG
		+ CH ₂ O	ONITR_X_TAG + <i>hν</i>	→	NO ₂ _X_TAG
O + O ₂ + M	→	O ₃ + M	O_X_TAG + O ₂ + M	→	O ₃ _X_TAG + O ₂ + M
O + O ₃	→	2 O ₂	O_X_TAG + O ₃	→	O ₃
			O + O ₃ _X_TAG	→	O
O1D + N ₂	→	O + N ₂	O1D_X_TAG + N ₂	→	O_X_TAG + N ₂
O1D + O ₂	→	O + O ₂	O1D_X_TAG + O ₂	→	O_X_TAG + O ₂
O1D + H ₂ O	→	2 OH	O1D_X_TAG + H ₂ O	→	H ₂ O
H ₂ + O1D	→	HO ₂ + OH	H ₂ + O1D_X_TAG	→	H ₂
O + OH	→	HO ₂ + O ₂	O_X_TAG + OH	→	OH

Original reaction			NO _x -tagged reaction		
HO2 + O	→	OH + O2	HO2 + O_X_TAG	→	HO2
OH + O3	→	HO2 + O2	OH + O3_X_TAG	→	OH
HO2 + O3	→	OH + 2 O2	HO2 + O3_X_TAG	→	HO2
OH + OH	→	H2O + O	OH + OH	→	O_X_XTR + 2 OH
N2O + O1D	→	2 NO	N2O + O1D_X_TAG	→	N2O
			N2O + O1D	→	2 NO_STR + N2O + O1D
NO + HO2	→	NO2 + OH	NO_TAG + HO2	→	NO2_TAG + NO2_X_TAG + HO2
NO + O3	→	NO2 + O2	NO_TAG + O3	→	NO2_TAG + O3
			NO + O3_X_TAG	→	NO + NO2_X_TAG
NO2 + O	→	NO + O2	NO2_TAG + O	→	NO_TAG + O
			NO2 + O_X_TAG	→	NO2
			NO2_X_TAG + O	→	O
NO2 + O3	→	NO3 + O2	NO2_TAG + O3	→	NO3_TAG + O3
			NO2_X_TAG + O3	→	NO3_X_TAG + O3
			NO2 + O3_X_TAG	→	NO2
NO3 + HO2	→	OH + NO2	NO3_TAG + HO2	→	HO2 + NO2_TAG
			NO3_X_TAG + HO2	→	HO2 + NO2_X_TAG
NO2 + NO3 + M	→	N2O5 + M	NO2_TAG + NO3 + M	→	NO3NO2_TAG + NO3 + M
			NO2 + NO3_TAG + M	→	NO2NO3_TAG + NO2 + M
			NO2_X_TAG + NO3 + M	→	NO3NO2_X_TAG + NO3 + M
			NO2 + NO3_X_TAG + M	→	NO2NO3_X_TAG + NO2 + M
N2O5 + M	→	NO2 + NO3 + M	NO3NO2_TAG + M	→	NO2_TAG + M
			NO2NO3_TAG + M	→	NO3_TAG + M
			NO3NO2_X_TAG + M	→	NO2_X_TAG + M
			NO2NO3_X_TAG + M	→	NO3_X_TAG + M
NO2 + OH + M	→	HNO3 + M	NO2_TAG + OH + M	→	HNO3_TAG + OH + M
			NO2_X_TAG + OH + M	→	HNO3_X_TAG + OH + M
HNO3 + OH	→	NO3 + H2O	HNO3_TAG + OH	→	NO3_TAG + OH
			HNO3_X_TAG + OH	→	NO3_X_TAG + OH
NO3 + NO	→	2 NO2	NO3_TAG + NO	→	NO2_TAG + NO
			NO3 + NO_TAG	→	NO2_TAG + NO3
			NO3_X_TAG + NO	→	2 NO2_X_TAG + NO
NO2 + HO2 + M	→	HO2NO2 + M	NO2_TAG + HO2 + M	→	HO2NO2_TAG + HO2 + M
			NO2_X_TAG + HO2 + M	→	HO2NO2_X_TAG + HO2 + M

Original reaction			NO _x -tagged reaction		
HO2NO2 + OH	→	H2O + NO2 + O2	HO2NO2_TAG + OH	→	NO2_TAG + OH
			HO2NO2_X_TAG + OH	→	NO2_X_TAG + OH
HO2NO2 + M	→	HO2 + NO2 + M	HO2NO2_TAG + M	→	NO2_TAG + M
			HO2NO2_X_TAG + M	→	NO2_X_TAG + M
CH4 + O1D	→	.75 CH3O2 + .75 OH + .25 CH2O + .4 HO2 + .05 H2	CH4 + O1D_X_TAG	→	CH4
CH3O2 + NO	→	CH2O + NO2 + HO2	CH3O2 + NO_TAG	→	CH3O2 + NO2_TAG + NO2_X_TAG
CH2O + NO3	→	CO + HO2 + HNO3	CH2O + NO3_TAG	→	CH2O + HNO3_TAG
			CH2O + NO3_X_TAG	→	CH2O + HNO3_X_TAG
HOCH2OO + NO	→	HCOOH + NO2 + HO2	HOCH2OO + NO_TAG	→	HOCH2OO + NO2_TAG + NO2_X_TAG
C2H4 + O3	→	CH2O + .12 HO2 + .5 CO + .12 OH + .5 HCOOH	C2H4 + O3_X_TAG	→	C2H4
EO2 + NO	→	EO + NO2	EO2 + NO_TAG	→	EO2 + NO2_TAG + NO2_X_TAG
C2H5O2 + NO	→	CH3CHO + HO2 + NO2	C2H5O2 + NO_TAG	→	C2H5O2 + NO2_TAG + NO2_X_TAG
CH3CHO + NO3	→	CH3CO3 + HNO3	CH3CHO + NO3_TAG	→	CH3CHO + HNO3_TAG
			CH3CHO + NO3_X_TAG	→	CH3CHO + HNO3_X_TAG
CH3CO3 + NO	→	CH3O2 + CO2 + NO2	CH3CO3 + NO_TAG	→	CH3CO3 + NO2_TAG + NO2_X_TAG
CH3CO3 + NO2 + M	→	PAN + M	CH3CO3 + NO2_TAG + M	→	PAN_TAG + CH3CO3 + M
			CH3CO3 + NO2_X_TAG + M	→	PAN_X_TAG + CH3CO3 + M
CH3CO3 + HO2	→	.75 CH3COOOH + .25 CH3COOH + .25 O3	CH3CO3 + HO2	→	.25 O3_X_XTR + CH3CO3 + HO2
PAN + OH	→	CH2O + NO3 + CO2	PAN_TAG + OH	→	NO3_TAG + OH
			PAN_X_TAG + OH	→	NO3_X_TAG + OH
PAN + M	→	CH3CO3 + NO2 + M	PAN_TAG + M	→	NO2_TAG + M
			PAN_X_TAG + M	→	NO2_X_TAG + M
C3H6 + O3	→	.54 CH2O + .19 HO2 + .33 OH + .08 CH4 + .56 CO + .5 CH3CHO + .31 CH3O2 + .25 CH3COOH	C3H6 + O3_X_TAG	→	C3H6
C3H6 + NO3	→	ONIT	C3H6 + NO3_TAG	→	ONIT_TAG + C3H6
			C3H6 + NO3_X_TAG	→	ONIT_X_TAG + C3H6
PO2 + NO	→	CH3CHO + CH2O + HO2 + NO2	PO2 + NO_TAG	→	PO2 + NO2_TAG + NO2_X_TAG
C3H7O2 + NO	→	.82 CH3COCH3 + NO2 + HO2 + .27 CH3CHO	C3H7O2 + NO_TAG	→	C3H7O2 + NO2_TAG + NO2_X_TAG
RO2 + NO	→	CH3CO3 + CH2O + NO2	RO2 + NO_TAG	→	RO2 + NO2_TAG + NO2_X_TAG

Original reaction		NO _x -tagged reaction	
ONIT + OH	→ NO ₂ + CH ₃ COCHO	ONIT_TAG + OH	→ NO ₂ _TAG + OH
		ONIT_X_TAG + OH	→ NO ₂ _X_TAG + OH
CH ₃ COCHO + NO ₃	→ HNO ₃ + CO + CH ₃ CO ₃	CH ₃ COCHO + NO ₃ _TAG	→ HNO ₃ _TAG + CH ₃ COCHO
		CH ₃ COCHO + NO ₃ _X_TAG	→ HNO ₃ _X_TAG + CH ₃ COCHO
ENE ₂ + NO	→ CH ₃ CHO + .5 CH ₂ O + .5 CH ₃ COCH ₃ + HO ₂ + NO ₂	ENE ₂ + NO_TAG	→ ENE ₂ + NO ₂ _TAG + NO ₂ _X_TAG
MEK ₂ + NO	→ CH ₃ CO ₃ + CH ₃ CHO + NO ₂	MEK ₂ + NO_TAG	→ MEK ₂ + NO ₂ _TAG + NO ₂ _X_TAG
MPAN + OH + M	→ .5 HYAC + .5 NO ₃ + .5 CH ₂ O + .5 HO ₂ + .5 CO ₂ + M	MPAN_TAG + OH + M	→ .5 NO ₃ _TAG + OH + M
		MPAN_X_TAG + OH + M	→ .5 NO ₃ _X_TAG + OH + M
ALK ₂ + NO	→ .4 CH ₃ CHO + .1 CH ₂ O + .25 CH ₃ COCH ₃ + .9 HO ₂ + .75 MEK + .9 NO ₂ + .1 ONIT	ALK ₂ + NO_TAG	→ ALK ₂ + .9 NO ₂ _TAG + .9 NO ₂ _X_TAG + .1 ONIT_TAG + .1 ONIT_X_TAG
ISOP + O ₃	→ .4 MACR + .2 MVK + .07 C ₃ H ₆ + .27 OH + .06 HO ₂ + .6 CH ₂ O + .3 CO + .1 O ₃ + .2 MCO ₃ + .2 CH ₃ COOH	ISOP + O ₃ _X_TAG	→ ISOP + .1 O ₃ _X_TAG
ISOPO ₂ + NO	→ .08 ONITR + .92 NO ₂ + HO ₂ + .55 CH ₂ O + .23 MACR + .32 MVK + .37 HYDRALD	ISOPO ₂ + NO_TAG	→ ISOPO ₂ + .92 NO ₂ _TAG + .92 NO ₂ _X_TAG + .08 ONITR_TAG + .08 ONITR_X_TAG
ISOPO ₂ + NO ₃	→ HO ₂ + NO ₂ + .6 CH ₂ O + .25 MACR + .35 MVK + .4 HYDRALD	ISOPO ₂ + NO ₃ _TAG	→ ISOPO ₂ + NO ₂ _TAG
		ISOPO ₂ + NO ₃ _X_TAG	→ ISOPO ₂ + NO ₂ _X_TAG
ISOP + NO ₃	→ ISOPNO ₃	ISOP + NO ₃ _TAG	→ ISOPNO ₃ _TAG + ISOP
		ISOP + NO ₃ _X_TAG	→ ISOPNO ₃ _X_TAG + ISOP
ISOPNO ₃ + NO	→ 1.206 NO ₂ + .794 HO ₂ + .072 CH ₂ O + .167 MACR + .039 MVK + .794 ONITR	ISOPNO ₃ _TAG + NO	→ .794 ONITR_TAG + .206 NO ₂ _TAG + NO
		ISOPNO ₃ + NO_TAG	→ NO ₂ _TAG + NO ₂ _X_TAG + ISOPNO ₃
		ISOPNO ₃ _X_TAG + NO	→ .794 ONITR_X_TAG + .206 NO ₂ _X_TAG + NO
ISOPNO ₃ + NO ₃	→ 1.206 NO ₂ + .072 CH ₂ O + .167 MACR + .039 MVK + .794 ONITR + .794 HO ₂	ISOPNO ₃ _TAG + NO ₃	→ .794 ONITR_TAG + .206 NO ₂ _TAG + NO ₃
		ISOPNO ₃ + NO ₃ _TAG	→ NO ₂ _TAG + ISOPNO ₃
		ISOPNO ₃ _X_TAG + NO ₃	→ .794 ONITR_X_TAG + .206 NO ₂ _X_TAG + NO ₃
		ISOPNO ₃ + NO ₃ _X_TAG	→ 1.00 NO ₂ _X_TAG + ISOPNO ₃
ISOPNO ₃ + HO ₂	→ .206 NO ₂ + .794 HO ₂ + .008 CH ₂ O + .167 MACR + .039 MVK + .794 ONITR	ISOPNO ₃ _TAG + HO ₂	→ .206 NO ₂ _TAG + .794 ONITR_TAG + HO ₂
		ISOPNO ₃ _X_TAG + HO ₂	→ .206 NO ₂ _X_TAG + .794 ONITR_X_TAG + HO ₂
MVK + O ₃	→ .8 CH ₂ O + .95 CH ₃ COCHO + .08 OH + .2 O ₃ + .06 HO ₂ + .05 CO	MVK + O ₃ _X_TAG	→ MVK + .2 O ₃ _X_TAG

Original reaction		NO _x -tagged reaction	
MACR + O3	→	MACR + O3_X_TAG	→ MACR + .2 O3_X_TAG
	+ .04 CH3CHO + .8 CH3COCHO + .275 HO2 + .2 CO + .2 O3 + .7 CH2O + .215 OH		
MACRO2 + NO	→	MACRO2 + NO_TAG	→ NO2_TAG + NO2_X_TAG + MACRO2
	+ .25 CH3COCHO + .53 CH3CO3 + .53 GLYALD + .22 HYAC + .22 CO		
MACRO2 + NO	→ 0.8 ONITR	MACRO2 + NO_TAG	→ 0.8 ONITR_TAG + 0.8 ONITR_X_TAG + MACRO2
MACRO2 + NO3	→	MACRO2 + NO3_TAG	→ NO2_TAG + MACRO2
	+ .25 CH3COCHO + .22 CO + .53 GLYALD + .22 HYAC + .53 CH3CO3		
MCO3 + NO	→	MCO3 + NO_TAG	→ NO2_TAG + NO2_X_TAG + MCO3
	+ CH2O + CH3CO3 + CO2		
MCO3 + NO3	→	MCO3 + NO3_TAG	→ NO2_TAG + MCO3
	+ CH2O + CH3CO3 + CO2		
MCO3 + HO2	→	MCO3 + HO2	→ .25 O3_X_XTR + MCO3 + HO2
	+ .25 O3 + .25 CH3COOH + .75 CH3COOOH + .75 O2		
MCO3 + NO2 + M	→	MCO3 + NO2_TAG + M	→ MPAN_TAG + M + MCO3
	MPAN + M		
MPAN + M	→	MCO3 + NO2_X_TAG + M	→ MPAN_X_TAG + M + MCO3
	MCO3 + NO2 + M		
ONITR + OH	→	MPAN_TAG + M	→ NO2_TAG + M
	HYDRALD + .4 NO2 + HO2		
ONITR + NO3	→	ONITR_TAG + OH	→ OH + .4 NO2_TAG
	HYDRALD + NO2 + HO2		
ONITR + NO3	→	ONITR_X_TAG + OH	→ OH + .4 NO2_X_TAG
	HYDRALD + NO2 + HO2		
ONITR + NO3	→	ONITR_TAG + NO3	→ .5 NO2_TAG + NO3
	HYDRALD + NO2 + HO2		
ONITR + NO3	→	ONITR + NO3_TAG	→ .5 NO2_TAG + ONITR
	HYDRALD + NO2 + HO2		
ONITR + NO3	→	ONITR_X_TAG + NO3	→ .5 NO2_X_TAG + NO3
	HYDRALD + NO2 + HO2		
ONITR + NO3	→	ONITR + NO3_X_TAG	→ .5 NO2_X_TAG + ONITR
	HYDRALD + NO2 + HO2		
XO2 + NO	→	XO2 + NO_TAG	→ NO2_TAG + NO2_X_TAG + XO2
	+ NO2 + HO2 + .5 CO + .25 GLYOXAL + .25 HYAC + .25 CH3COCHO + .25 GLYALD		
XO2 + NO3	→	XO2 + NO3_TAG	→ NO2_TAG + XO2
	+ NO2 + HO2 + 0.5 CO + .25 HYAC + 0.25 GLYOXAL + .25 CH3COCHO + .25 GLYALD		
XO2 + NO3	→	XO2 + NO3_X_TAG	→ NO2_X_TAG + XO2
	+ NO2 + HO2 + 0.5 CO + .25 HYAC + 0.25 GLYOXAL + .25 CH3COCHO + .25 GLYALD		
XOH + NO2	→	XOH + NO2_TAG	→ XOH + .7 NO2_TAG
	+ .7 NO2 + .7 BIGALD + .7 HO2		
XOH + NO2	→	XOH + NO2_X_TAG	→ XOH + .7 NO2_X_TAG
	+ .7 NO2 + .7 BIGALD + .7 HO2		

Original reaction		NO _x -tagged reaction	
TOLO2 + NO	→ .45 GLYOXAL + .45 CH3COCHO +.9 BIGALD + .9 NO2 + .9 HO2	TOLO2 + NO_TAG	→ TOLO2 + .9 NO2_TAG + .9 NO2_X_TAG
C10H16 + O3	→ .7 OH + MVK + MACR + HO2	C10H16 + O3_X_TAG	→ C10H16
C10H16 + NO3	→ TERPO2 + NO2	C10H16 + NO3_TAG	→ C10H16 + NO2_TAG
		C10H16 + NO3_X_TAG	→ C10H16 + NO2_X_TAG
TERPO2 + NO	→ .1 CH3COCH3 + HO2 + MVK + MACR + NO2	TERPO2 + NO_TAG	→ TERPO2 + NO2_TAG + NO2_X_TAG
N2O5	→ 2 HNO3	NO3NO2_TAG	→ HNO3_TAG
		NO2NO3_TAG	→ HNO3_TAG
		NO3NO2_X_TAG	→ HNO3_X_TAG
		NO2NO3_X_TAG	→ HNO3_X_TAG
NO3	→ HNO3	NO3_TAG	→ HNO3_TAG
		NO3_X_TAG	→ HNO3_X_TAG
NO2	→ 0.5 OH + 0.5 NO + 0.5 HNO3	NO2_TAG	→ 0.5 NO_TAG + 0.5 HNO3_TAG
		NO2_X_TAG	→ 0.5 HNO3_X_TAG
DMS + NO3	→ SO2 + HNO3	DMS + NO3_TAG	→ DMS + HNO3_TAG
		DMS + NO3_X_TAG	→ DMS + HNO3_X_TAG

Table S2. Full list of reactions modified for VOC tagging. Original reactions from the base mechanism are shown in the left column, and their tagged counterparts in the right column. Here, only one user-specified tag identity “TAG” is applied. Additional reactions producing tagged tracers with the ‘STR’ and “XTR” identities (as described in the main paper) are also shown.

Original reaction			VOC-tagged reaction		
$O_2 + h\nu$	\rightarrow	$2 O$	$O_2 + h\nu$	\rightarrow	$2 O_X_STR + O_2$
$O_3 + h\nu$	\rightarrow	$O_1D + O_2$	$O_3_X_TAG + h\nu$	\rightarrow	$O_1D_X_TAG$
$O_3 + h\nu$	\rightarrow	$O + O_2$	$O_3_X_TAG + h\nu$	\rightarrow	O_X_TAG
$N_2O + h\nu$	\rightarrow	$O_1D + N_2$	$N_2O + h\nu$	\rightarrow	$O_1D_X_STR + N_2O$
$NO_2 + h\nu$	\rightarrow	$NO + O$	$NO_2_X_TAG + h\nu$	\rightarrow	O_X_TAG
$N_2O_5 + h\nu$	\rightarrow	$NO_2 + NO_3$	$NO_3NO_2_X_TAG + h\nu$	\rightarrow	$NO_2_X_TAG$
			$NO_2NO_3_X_TAG + h\nu$	\rightarrow	$NO_3_X_TAG$
$HNO_3 + h\nu$	\rightarrow	$NO_2 + OH$	$HNO_3_X_TAG + h\nu$	\rightarrow	$NO_2_X_TAG$
$NO_3 + h\nu$	\rightarrow	$.89 NO_2 + .11 NO + .89 O_3$	$NO_3_X_TAG + h\nu$	\rightarrow	$.89 NO_2_X_TAG + .89 O_3_X_TAG$
$HO_2NO_2 + h\nu$	\rightarrow	$.33 OH + .33 NO_3 + .66 NO_2$	$HO_2NO_2_X_TAG + h\nu$	\rightarrow	$.33 NO_3_X_TAG + .66 NO_2_X_TAG$
		$+ .66 HO_2$	$NO_2HO_2_X_TAG + h\nu$	\rightarrow	$.66 HO_2_X_TAG$
$CH_3OOH + h\nu$	\rightarrow	$CH_2O + HO_2 + OH$	$CH_3OOH_TAG + h\nu$	\rightarrow	$CH_2O_TAG + HO_2_X_TAG$
$CH_2O + h\nu$	\rightarrow	$CO + 2 HO_2$	$CH_2O_TAG + h\nu$	\rightarrow	$CO_TAG + 2 HO_2_X_TAG$
$CH_2O + h\nu$	\rightarrow	$CO + H_2$	$CH_2O_TAG + h\nu$	\rightarrow	$CO_TAG + H_2_TAG$
$CH_3CHO + h\nu$	\rightarrow	$CH_3O_2 + CO + HO_2$	$CH_3CHO_TAG + h\nu$	\rightarrow	$CH_3O_2_TAG + CO_TAG + HO_2_X_TAG$
$POOH + h\nu$	\rightarrow	$CH_3CHO + CH_2O + HO_2$	$POOH_TAG + h\nu$	\rightarrow	$CH_2O_TAG + CH_3CHO_TAG + HO_2_X_TAG$
		$+ OH$			
$CH_3COOOH + h\nu$	\rightarrow	$CH_3O_2 + OH + CO_2$	$CH_3COOOH_TAG + h\nu$	\rightarrow	$CH_3O_2_TAG$
$PAN + h\nu$	\rightarrow	$.6 CH_3CO_3 + .6 NO_2 + .4 CH_3O_2$	$PAN_TAG + h\nu$	\rightarrow	$.6 CH_3CO_3_TAG + .4 CH_3O_2_TAG$
		$+ .4 NO_3 + .4 CO_2$	$PAN_X_TAG + h\nu$	\rightarrow	$.6 NO_2_X_TAG + .4 NO_3_X_TAG$
$MPAN + h\nu$	\rightarrow	$MCO_3 + NO_2$	$MPAN_TAG + h\nu$	\rightarrow	MCO_3_TAG
			$MPAN_X_TAG + h\nu$	\rightarrow	$NO_2_X_TAG$
$MACR + h\nu$	\rightarrow	$.67 HO_2 + .33 MCO_3 + .67 CH_2O$	$MACR_TAG + h\nu$	\rightarrow	$.67 CH_2O_TAG + .67 CH_3CO_3_TAG + .67 CO_TAG$
		$+ .67 CH_3CO_3 + .33 OH + .67 CO$			$+ .33 MCO_3_TAG + .67 HO_2_X_TAG$
$MVK + h\nu$	\rightarrow	$.7 C_3H_6 + .7 CO + .3 CH_3O_2$	$MVK_TAG + h\nu$	\rightarrow	$.7 C_3H_6_TAG + .3 CH_3CO_3_TAG + .3 CH_3O_2_TAG$
		$+ .3 CH_3CO_3$			$+ .7 CO_TAG$
$C_2H_5OOH + h\nu$	\rightarrow	$CH_3CHO + HO_2 + OH$	$C_2H_5OOH_TAG + h\nu$	\rightarrow	$CH_3CHO_TAG + HO_2_X_TAG$
$C_3H_7OOH + h\nu$	\rightarrow	$.82 CH_3COCH_3 + OH + HO_2$	$C_3H_7OOH_TAG + h\nu$	\rightarrow	$.82 CH_3COCH_3_TAG + HO_2_X_TAG$
$ROOH + h\nu$	\rightarrow	$CH_3CO_3 + CH_2O + OH$	$ROOH_TAG + h\nu$	\rightarrow	$CH_2O_TAG + CH_3CO_3_TAG$
$CH_3COCH_3 + h\nu$	\rightarrow	$CH_3CO_3 + CH_3O_2$	$CH_3COCH_3_TAG + h\nu$	\rightarrow	$CH_3CO_3_TAG + CH_3O_2_TAG$

Original reaction			VOC-tagged reaction		
CH ₃ COCHO + <i>hν</i>	→	CH ₃ CO ₃ + CO + HO ₂	CH ₃ COCHO_TAG + <i>hν</i>	→	CH ₃ CO ₃ _TAG + CO_TAG + HO ₂ _X_TAG
XOOH + <i>hν</i>	→	OH	XOOH_TAG + <i>hν</i>	→	
ONITR + <i>hν</i>	→	HO ₂ + CO + NO ₂	ONITR_TAG + <i>hν</i>	→	CH ₂ O_TAG + CO_TAG + HO ₂ _X_TAG
		+ CH ₂ O	ONITR_X_TAG + <i>hν</i>	→	NO ₂ _X_TAG
ISOPOOH + <i>hν</i>	→	.402 MVK + .288 MACR + .69 CH ₂ O	ISOPOOH_TAG + <i>hν</i>	→	.69 CH ₂ O_TAG + .288 MACR_TAG + .402 MVK_TAG
		+ HO ₂			+ HO ₂ _X_TAG
HYAC + <i>hν</i>	→	CH ₃ CO ₃ + HO ₂ + CH ₂ O	HYAC_TAG + <i>hν</i>	→	CH ₂ O_TAG + CH ₃ CO ₃ _TAG + HO ₂ _X_TAG
GLYALD + <i>hν</i>	→	2 HO ₂ + CO + CH ₂ O	GLYALD_TAG + <i>hν</i>	→	CH ₂ O_TAG + CO_TAG + 2 HO ₂ _X_TAG
MEK + <i>hν</i>	→	CH ₃ CO ₃ + C ₂ H ₅ O ₂	MEK_TAG + <i>hν</i>	→	C ₂ H ₅ O ₂ _TAG + CH ₃ CO ₃ _TAG
BIGALD + <i>hν</i>	→	.45 CO + .13 GLYOXAL + .56 HO ₂	BIGALD_TAG + <i>hν</i>	→	.13 CH ₃ CO ₃ _TAG + .18 CH ₃ COCHO_TAG + .45 CO_TAG
		+ .13 CH ₃ CO ₃ + .18 CH ₃ COCHO			+ .13 GLYOXAL_TAG + .56 HO ₂ _X_TAG
GLYOXAL + <i>hν</i>	→	2 CO + 2 HO ₂	GLYOXAL_TAG + <i>hν</i>	→	2 CO_TAG + 2 HO ₂ _X_TAG
ALKOOH + <i>hν</i>	→	.4 CH ₃ CHO + .1 CH ₂ O + .25 CH ₃ COCH ₃	ALKOOH_TAG + <i>hν</i>	→	.1 CH ₂ O_TAG + .4 CH ₃ CHO_TAG + .25 CH ₃ COCH ₃ _TAG
		+ .9 HO ₂ + .8 MEK + OH			+ .8 MEK_TAG + .9 HO ₂ _X_TAG
MEKOOH + <i>hν</i>	→	OH + CH ₃ CO ₃ + CH ₃ CHO	MEKOOH_TAG + <i>hν</i>	→	CH ₃ CHO_TAG + CH ₃ CO ₃ _TAG
TOLOOH + <i>hν</i>	→	OH + .45 GLYOXAL + .45 CH ₃ COCHO	TOLOOH_TAG + <i>hν</i>	→	.9 BIGALD_TAG + .45 CH ₃ COCHO_TAG + .45 GLYOXAL_TAG
		+ .9 BIGALD			
TERPOOH + <i>hν</i>	→	OH + .1 CH ₃ COCH ₃ + HO ₂	TERPOOH_TAG + <i>hν</i>	→	.1 CH ₃ COCH ₃ _TAG + MACR_TAG + MVK_TAG
		+ MVK + MACR			+ HO ₂ _X_TAG
O + O ₂ + M	→	O ₃ + M	O_X_TAG + O ₂ + M	→	O ₃ _X_TAG + O ₂ + M
O + O ₃	→	2 O ₂	O_X_TAG + O ₃	→	O ₃
			O + O ₃ _X_TAG	→	O
O ₁ D + N ₂	→	O + N ₂	O ₁ D_X_TAG + N ₂	→	O_X_TAG + N ₂
O ₁ D + O ₂	→	O + O ₂	O ₁ D_X_TAG + O ₂	→	O_X_TAG + O ₂
O ₁ D + H ₂ O	→	2 OH	O ₁ D_X_TAG + H ₂ O	→	H ₂ O
H ₂ + O ₁ D	→	HO ₂ + OH	H ₂ _TAG + O ₁ D	→	O ₁ D + HO ₂ _X_TAG
			H ₂ + O ₁ D_X_TAG	→	H ₂
H ₂ + OH	→	H ₂ O + HO ₂	H ₂ _TAG + OH	→	OH + HO ₂ _X_TAG
O + OH	→	HO ₂ + O ₂	O_X_TAG + OH	→	OH + HO ₂ _X_TAG
HO ₂ + O	→	OH + O ₂	HO ₂ + O_X_TAG	→	HO ₂
			HO ₂ _X_TAG + O	→	O
OH + O ₃	→	HO ₂ + O ₂	OH + O ₃ _X_TAG	→	OH + HO ₂ _X_TAG
HO ₂ + O ₃	→	OH + 2 O ₂	HO ₂ + O ₃ _X_TAG	→	HO ₂
			HO ₂ _X_TAG + O ₃	→	O ₃

Original reaction			VOC-tagged reaction		
HO2 + HO2	→	H2O2 + O2	HO2_X_TAG + HO2	→	HO2
H2O2 + OH	→	H2O + HO2	H2O2 + OH	→	HO2_X_XTR + H2O2 + OH
OH + HO2	→	H2O + O2	OH + HO2_X_TAG	→	OH
OH + OH	→	H2O + O	OH + OH	→	O_X_XTR + 2 OH
N2O + O1D	→	2 NO	N2O + O1D_X_TAG	→	N2O
NO + HO2	→	NO2 + OH	NO + HO2_X_TAG	→	NO2_X_TAG + NO
NO + O3	→	NO2 + O2	NO + O3_X_TAG	→	NO + NO2_X_TAG
NO2 + O	→	NO + O2	NO2 + O_X_TAG	→	NO2
			NO2_X_TAG + O	→	O
NO2 + O3	→	NO3 + O2	NO2_X_TAG + O3	→	NO3_X_TAG + O3
			NO2 + O3_X_TAG	→	NO2
NO3 + HO2	→	OH + NO2	NO3_X_TAG + HO2	→	HO2 + NO2_X_TAG
			NO3 + HO2_X_TAG	→	NO3
NO2 + NO3 + M	→	N2O5 + M	NO2_X_TAG + NO3 + M	→	NO3NO2_X_TAG + NO3 + M
			NO2 + NO3_X_TAG + M	→	NO2NO3_X_TAG + NO2 + M
N2O5 + M	→	NO2 + NO3 + M	NO3NO2_X_TAG + M	→	NO2_X_TAG + M
			NO2NO3_X_TAG + M	→	NO3_X_TAG + M
NO2 + OH + M	→	HNO3 + M	NO2_X_TAG + OH + M	→	HNO3_X_TAG + OH + M
HNO3 + OH	→	NO3 + H2O	HNO3_X_TAG + OH	→	NO3_X_TAG + OH
NO3 + NO	→	2 NO2	NO3_X_TAG + NO	→	2 NO2_X_TAG + NO
NO2 + HO2 + M	→	HO2NO2 + M	NO2_X_TAG + HO2 + M	→	HO2NO2_X_TAG + HO2 + M
			NO2 + HO2_X_TAG + M	→	NO2HO2_X_TAG + M + NO2
HO2NO2 + OH	→	H2O + NO2 + O2	HO2NO2_X_TAG + OH	→	NO2_X_TAG + OH
			NO2HO2_X_TAG + OH	→	OH
HO2NO2 + M	→	HO2 + NO2 + M	HO2NO2_X_TAG + M	→	NO2_X_TAG + M
			NO2HO2_X_TAG + M	→	HO2_X_TAG + M
CH4 + OH	→	CH3O2 + H2O	CH4_TAG + OH	→	OH + CH3O2_TAG
CH4 + O1D	→	.75 CH3O2 + .75 OH + .25 CH2O + .4 HO2 + .05 H2	CH4_TAG + O1D	→	O1D + .25 CH2O_TAG + .75 CH3O2_TAG + .05 H2_TAG + .4 HO2_X_TAG
			CH4 + O1D_X_TAG	→	CH4
CH3O2 + NO	→	CH2O + NO2 + HO2	CH3O2_TAG + NO	→	NO + CH2O_TAG + NO2_X_TAG + HO2_X_TAG
CH3O2 + M	→	M + .7 CH2O + .3 CH3OH + .4 HO2	CH3O2_TAG + M	→	M + .7 CH2O_TAG + .3 CH3OH_TAG + .4 HO2_X_TAG

Original reaction			VOC-tagged reaction		
CH3O2 + HO2	→	CH3OOH + O2	CH3O2_TAG + HO2	→	HO2 + CH3OOH_TAG
			CH3O2 + HO2_X_TAG	→	CH3O2
CH3OOH + OH	→	.7 CH3O2 + .3 OH + .3 CH2O + H2O	CH3OOH_TAG + OH	→	OH + .3 CH2O_TAG + .7 CH3O2_TAG
CH2O + NO3	→	CO + HO2 + HNO3	CH2O_TAG + NO3	→	NO3 + CO_TAG + HO2_X_TAG
			CH2O + NO3_X_TAG	→	CH2O + HNO3_X_TAG
CH2O + OH	→	CO + H2O + HO2	CH2O_TAG + OH	→	OH + CO_TAG + HO2_X_TAG
CO + OH + M	→	CO2 + HO2 + M	CO_TAG + OH + M	→	OH + M + HO2_X_TAG
CO + OH	→	CO2 + HO2	CO_TAG + OH	→	OH + HO2_X_TAG
CH3OH + OH	→	HO2 + CH2O	CH3OH_TAG + OH	→	OH + CH2O_TAG + HO2_X_TAG
HCOOH + OH	→	HO2 + CO2 + H2O	HCOOH_TAG + OH	→	OH + HO2_X_TAG
CH2O + HO2	→	HOCH2OO	CH2O_TAG + HO2	→	HO2 + HOCH2OO_TAG
			CH2O + HO2_X_TAG	→	CH2O
HOCH2OO	→	CH2O + HO2	HOCH2OO_TAG	→	CH2O_TAG + HO2_X_TAG
HOCH2OO + NO	→	HCOOH + NO2 + HO2	HOCH2OO_TAG + NO	→	NO + HCOOH_TAG + NO2_X_TAG + HO2_X_TAG
HOCH2OO + HO2	→	HCOOH	HOCH2OO_TAG + HO2	→	HO2 + HCOOH_TAG
			HOCH2OO + HO2_X_TAG	→	HOCH2OO
C2H2 + OH + M	→	.65 GLYOXAL + .65 OH + .35 HCOOH + .35 HO2 + .35 CO + M	C2H2_TAG + OH + M	→	OH + M + .35 CO_TAG + .65 GLYOXAL_TAG + .35 HCOOH_TAG + .35 HO2_X_TAG
C2H4 + OH + M	→	.75 EO2 + .5 CH2O + .25 HO2 + M	C2H4_TAG + OH + M	→	OH + M + .5 CH2O_TAG + .75 EO2_TAG + .25 HO2_X_TAG
C2H4 + O3	→	CH2O + .12 HO2 + .5 CO + .12 OH + .5 HCOOH	C2H4_TAG + O3	→	O3 + CH2O_TAG + .5 CO_TAG + .5 HCOOH_TAG + .12 HO2_X_TAG
			C2H4 + O3_X_TAG	→	C2H4
EO2 + NO	→	EO + NO2	EO2_TAG + NO	→	NO + EO_TAG + NO2_X_TAG
EO + O2	→	GLYALD + HO2	EO_TAG + O2	→	O2 + GLYALD_TAG + HO2_X_TAG
EO	→	2 CH2O + HO2	EO_TAG	→	2 CH2O_TAG + HO2_X_TAG
C2H6 + OH	→	C2H5O2 + H2O	C2H6_TAG + OH	→	OH + C2H5O2_TAG
C2H5O2 + NO	→	CH3CHO + HO2 + NO2	C2H5O2_TAG + NO	→	NO + CH3CHO_TAG + NO2_X_TAG + HO2_X_TAG
C2H5O2 + HO2	→	C2H5OOH + O2	C2H5O2_TAG + HO2	→	HO2 + C2H5OOH_TAG
			C2H5O2 + HO2_X_TAG	→	C2H5O2
C2H5O2 + M	→	M + .8 CH3CHO + .2 C2H5OH	C2H5O2_TAG + M	→	M + .2 C2H5OH_TAG + .8 CH3CHO_TAG

Original reaction			VOC-tagged reaction		
		+ .6 HO2			+ .6 HO2_X_TAG
C2H5OOH + OH	→	.5 C2H5O2 + .5 CH3CHO + .5 OH	C2H5OOH_TAG + OH	→	OH + .5 C2H5O2_TAG + .5 CH3CHO_TAG
CH3CHO + OH	→	CH3CO3 + H2O	CH3CHO_TAG + OH	→	OH + CH3CO3_TAG
CH3CHO + NO3	→	CH3CO3 + HNO3	CH3CHO_TAG + NO3	→	NO3 + CH3CO3_TAG
			CH3CHO + NO3_X_TAG	→	CH3CHO + HNO3_X_TAG
CH3CO3 + NO	→	CH3O2 + CO2 + NO2	CH3CO3_TAG + NO	→	NO + CH3O2_TAG + NO2_X_TAG
CH3CO3 + NO2 + M	→	PAN + M	CH3CO3_TAG + NO2 + M	→	NO2 + M + PAN_TAG
			CH3CO3 + NO2_X_TAG + M	→	PAN_X_TAG + CH3CO3 + M
CH3CO3 + HO2	→	.75 CH3COOOH + .25 CH3COOH + .25 O3	CH3CO3_TAG + HO2	→	HO2 + .25 CH3COOH_TAG + .75 CH3COOOH_TAG + .25 O3_X_TAG
			CH3CO3 + HO2_X_TAG	→	CH3CO3
CH3CO3 + M	→	M + .9 CH3O2 + .3 CH2O + .5 HO2 + .9 CO2 + .1 CH3COOH	CH3CO3_TAG + M	→	M + .3 CH2O_TAG + .1 CH3COOH_TAG + .9 CH3O2_TAG + .5 HO2_X_TAG
CH3COOOH + OH	→	.5 CH3CO3 + .5 CH2O + .5 CO2 + H2O	CH3COOOH_TAG + OH	→	OH + .5 CH2O_TAG + .5 CH3CO3_TAG
PAN + OH	→	CH2O + NO3 + CO2	PAN_TAG + OH	→	OH + CH2O_TAG
			PAN_X_TAG + OH	→	NO3_X_TAG + OH
PAN + M	→	CH3CO3 + NO2 + M	PAN_TAG + M	→	M + CH3CO3_TAG
			PAN_X_TAG + M	→	NO2_X_TAG + M
GLYALD + OH	→	HO2 + .2 GLYOXAL + .8 CH2O + .8 CO2	GLYALD_TAG + OH	→	OH + .8 CH2O_TAG + .2 GLYOXAL_TAG + HO2_X_TAG
GLYOXAL + OH	→	HO2 + CO + CO2	GLYOXAL_TAG + OH	→	OH + CO_TAG + HO2_X_TAG
CH3COOH + OH	→	CH3O2 + CO2 + H2O	CH3COOH_TAG + OH	→	OH + CH3O2_TAG
C2H5OH + OH	→	HO2 + CH3CHO	C2H5OH_TAG + OH	→	OH + CH3CHO_TAG + HO2_X_TAG
C3H6 + OH + M	→	PO2 + M	C3H6_TAG + OH + M	→	OH + M + PO2_TAG
C3H6 + O3	→	.54 CH2O + .19 HO2 + .33 OH + .08 CH4 + .56 CO + .5 CH3CHO + .31 CH3O2 + .25 CH3COOH	C3H6_TAG + O3	→	O3 + .54 CH2O_TAG + .5 CH3CHO_TAG + .25 CH3COOH_TAG + .31 CH3O2_TAG + .08 CH4_TAG + .56 CO_TAG + .19 HO2_X_TAG
			C3H6 + O3_X_TAG	→	C3H6
C3H6 + NO3	→	ONIT	C3H6_TAG + NO3	→	NO3 + ONIT_TAG
			C3H6 + NO3_X_TAG	→	ONIT_X_TAG + C3H6
PO2 + NO	→	CH3CHO + CH2O + HO2 + NO2	PO2_TAG + NO	→	NO + CH2O_TAG + CH3CHO_TAG + NO2_X_TAG + HO2_X_TAG
PO2 + HO2	→	POOH + O2	PO2_TAG + HO2	→	HO2 + POOH_TAG

Original reaction			VOC-tagged reaction		
			PO2 + HO2_X_TAG	→	PO2
POOH + OH	→	.5 PO2 + .5 OH + .5 HYAC + H2O	POOH_TAG + OH	→	OH + .5 HYAC_TAG + .5 PO2_TAG
C3H8 + OH	→	C3H7O2 + H2O	C3H8_TAG + OH	→	OH + C3H7O2_TAG
C3H7O2 + NO	→	.82 CH3COCH3 + NO2 + HO2 + .27 CH3CHO	C3H7O2_TAG + NO	→	NO + .27 CH3CHO_TAG + .82 CH3COCH3_TAG + NO2_X_TAG + HO2_X_TAG
C3H7O2 + HO2	→	C3H7OOH + O2	C3H7O2_TAG + HO2	→	HO2 + C3H7OOH_TAG
			C3H7O2 + HO2_X_TAG	→	C3H7O2
C3H7O2 + M	→	M + .3 CH2O + .6 HO2 + .82 CH3COCH3	C3H7O2_TAG + M	→	M + .3 CH2O_TAG + .82 CH3COCH3_TAG + .6 HO2_X_TAG
C3H7OOH + OH	→	H2O + C3H7O2	C3H7OOH_TAG + OH	→	OH + C3H7O2_TAG
CH3COCH3 + OH	→	RO2 + H2O	CH3COCH3_TAG + OH	→	OH + RO2_TAG
RO2 + NO	→	CH3CO3 + CH2O + NO2	RO2_TAG + NO	→	NO + CH2O_TAG + CH3CO3_TAG + NO2_X_TAG
RO2 + HO2	→	ROOH + O2	RO2_TAG + HO2	→	HO2 + ROOH_TAG
			RO2 + HO2_X_TAG	→	RO2
RO2 + M	→	M + .3 CH3CO3 + .2 HYAC + .5 CH3COCHO + .2 CH3OH + .1 CH2O	RO2_TAG + M	→	M + .1 CH2O_TAG + .3 CH3CO3_TAG + .5 CH3COCHO_TAG + .2 CH3OH_TAG + .2 HYAC_TAG
ROOH + OH	→	RO2 + H2O	ROOH_TAG + OH	→	OH + RO2_TAG
ONIT + OH	→	NO2 + CH3COCHO	ONIT_TAG + OH	→	OH + CH3COCHO_TAG
			ONIT_X_TAG + OH	→	NO2_X_TAG + OH
CH3COCHO + OH	→	CH3CO3 + CO + H2O	CH3COCHO_TAG + OH	→	OH + CH3CO3_TAG + CO_TAG
CH3COCHO + NO3	→	HNO3 + CO + CH3CO3	CH3COCHO_TAG + NO3	→	NO3 + CH3CO3_TAG + CO_TAG
			CH3COCHO + NO3_X_TAG	→	HNO3_X_TAG + CH3COCHO
HYAC + OH	→	CH3COCHO + HO2	HYAC_TAG + OH	→	OH + CH3COCHO_TAG + HO2_X_TAG
BIGENE + OH	→	ENEO2	BIGENE_TAG + OH	→	OH + ENEO2_TAG
ENEO2 + NO	→	CH3CHO + .5 CH2O + .5 CH3COCH3 + HO2 + NO2	ENEO2_TAG + NO	→	NO + .5 CH2O_TAG + CH3CHO_TAG + .5 CH3COCH3_TAG + NO2_X_TAG + HO2_X_TAG
MEK + OH	→	MEKO2	MEK_TAG + OH	→	OH + MEKO2_TAG
MEKO2 + NO	→	CH3CO3 + CH3CHO + NO2	MEKO2_TAG + NO	→	NO + CH3CHO_TAG + CH3CO3_TAG + NO2_X_TAG
MEKO2 + HO2	→	MEKOOH	MEKO2_TAG + HO2	→	HO2 + MEKOOH_TAG
			MEKO2 + HO2_X_TAG	→	MEKO2
MEKOOH + OH	→	MEKO2	MEKOOH_TAG + OH	→	OH + MEKO2_TAG

Original reaction			VOC-tagged reaction		
MPAN + OH + M	→	.5 HYAC + .5 NO3 + .5 CH2O + .5 HO2 + .5 CO2 + M	MPAN_TAG + OH + M	→	OH + M + .5 CH2O_TAG + .5 HYAC_TAG + .5 HO2_X_TAG
			MPAN_X_TAG + OH + M	→	.5 NO3_X_TAG + OH + M
BIGALK + OH	→	ALKO2	BIGALK_TAG + OH	→	OH + ALKO2_TAG
ALKO2 + NO	→	.4 CH3CHO + .1 CH2O + .25 CH3COCH3 + .9 HO2 + .75 MEK + .9 NO2 + .1 ONIT	ALKO2_TAG + NO	→	NO + .1 CH2O_TAG + .4 CH3CHO_TAG + .25 CH3COCH3_TAG + .75 MEK_TAG + .1 ONIT_TAG + .9 NO2_X_TAG + .1 ONIT_X_TAG + .9 HO2_X_TAG
ALKO2 + HO2	→	ALKOOH	ALKO2_TAG + HO2	→	HO2 + ALKOOH_TAG
			ALKO2 + HO2_X_TAG	→	ALKO2
ALKOOH + OH	→	ALKO2	ALKOOH_TAG + OH	→	OH + ALKO2_TAG
ISOP + OH	→	ISOPO2	ISOP_TAG + OH	→	OH + ISOPO2_TAG
ISOP + O3	→	.4 MACR + .2 MVK + .07 C3H6 + .27 OH + .06 HO2 + .6 CH2O + .3 CO + .1 O3 + .2 MCO3 + .2 CH3COOH	ISOP_TAG + O3	→	O3 + .07 C3H6_TAG + .6 CH2O_TAG + .2 CH3COOH_TAG + .3 CO_TAG + .4 MACR_TAG + .2 MCO3_TAG + .2 MVK_TAG + .06 HO2_X_TAG
			ISOP + O3_X_TAG	→	ISOP + .1 O3_X_TAG
ISOPO2 + NO	→	.08 ONITR + .92 NO2 + HO2 + .55 CH2O + .23 MACR + .32 MVK + .37 HYDRALD	ISOPO2_TAG + NO	→	NO + .55 CH2O_TAG + .37 HYDRALD_TAG + .23 MACR_TAG + .32 MVK_TAG + .08 ONITR_TAG + .92 NO2_X_TAG + .08 ONITR_X_TAG + HO2_X_TAG
ISOPO2 + NO3	→	HO2 + NO2 + .6 CH2O + .25 MACR + .35 MVK + .4 HYDRALD	ISOPO2_TAG + NO3	→	NO3 + .6 CH2O_TAG + .4 HYDRALD_TAG + .25 MACR_TAG + .35 MVK_TAG + HO2_X_TAG
			ISOPO2 + NO3_X_TAG	→	ISOPO2 + NO2_X_TAG
ISOPO2 + HO2	→	ISOPOOH	ISOPO2_TAG + HO2	→	HO2 + ISOPOOH_TAG
			ISOPO2 + HO2_X_TAG	→	ISOPO2
ISOPOOH + OH	→	.8 XO2 + .2 ISOPO2	ISOPOOH_TAG + OH	→	OH + .2 ISOPO2_TAG + .8 XO2_TAG
ISOPO2 + M	→	M + .19 MACR + .26 MVK + .3 HYDRALD + .6 HO2 + .5 CH2O	ISOPO2_TAG + M	→	M + .5 CH2O_TAG + .3 HYDRALD_TAG + .19 MACR_TAG + .26 MVK_TAG + .6 HO2_X_TAG
ISOP + NO3	→	ISOPNO3	ISOP_TAG + NO3	→	NO3 + ISOPNO3_TAG
			ISOP + NO3_X_TAG	→	ISOPNO3_X_TAG + ISOP
ISOPNO3 + NO	→	1.206 NO2 + .794 HO2 + .072 CH2O + .167 MACR + .039 MVK + .794 ONITR	ISOPNO3_TAG + NO	→	NO + .072 CH2O_TAG + .167 MACR_TAG + .039 MVK_TAG + .794 ONITR_TAG + NO2_X_TAG + .794 HO2_X_TAG
			ISOPNO3_X_TAG + NO	→	.794 ONITR_X_TAG + .206 NO2_X_TAG + NO
ISOPNO3 + NO3	→	1.206 NO2 + .072 CH2O + .167 MACR + .039 MVK + .794 ONITR + .794 HO2	ISOPNO3_TAG + NO3	→	NO3 + .072 CH2O_TAG + .167 MACR_TAG + .039 MVK_TAG + .794 ONITR_TAG + .794 HO2_X_TAG

Original reaction		VOC-tagged reaction	
ISOPNO ₃ + HO ₂	→	ISOPNO ₃ _X_TAG + NO ₃	→ .794 ONITR_X_TAG + .206 NO ₂ _X_TAG + NO ₃
		ISOPNO ₃ + NO ₃ _X_TAG	→ 1.00 NO ₂ _X_TAG + ISOPNO ₃
		ISOPNO ₃ _TAG + HO ₂	→ HO ₂ + .008 CH ₂ O_TAG + .167 MACR_TAG
			+ .039 MVK_TAG + .794 ONITR_TAG + .794 HO ₂ _X_TAG
MVK + OH	→	ISOPNO ₃ _X_TAG + HO ₂	→ .206 NO ₂ _X_TAG + .794 ONITR_X_TAG + HO ₂
		ISOPNO ₃ + HO ₂ _X_TAG	→ ISOPNO ₃
		MVK_TAG + OH	→ OH + MACRO ₂ _TAG
		MVK + O ₃	→ O ₃ + .8 CH ₂ O_TAG + .04 CH ₃ CHO_TAG
MACR + OH	→		+ .95 CH ₃ COCHO_TAG + .05 CO_TAG + .06 HO ₂ _X_TAG
		MVK + O ₃ _X_TAG	→ MVK + .2 O ₃ _X_TAG
		MACR_TAG + OH	→ OH + .5 MACRO ₂ _TAG + .5 MCO ₃ _TAG
		MACR_TAG + O ₃	→ O ₃ + .7 CH ₂ O_TAG + .8 CH ₃ COCHO_TAG
MACRO ₂ + NO	→		+ .2 CO_TAG + .275 HO ₂ _X_TAG
		MACR + O ₃ _X_TAG	→ MACR + .2 O ₃ _X_TAG
		MACRO ₂ _TAG + NO	→ NO + .25 CH ₂ O_TAG + .53 CH ₃ CO ₃ _TAG
			+ .25 CH ₃ COCHO_TAG + .22 CO_TAG + .53 GLYALD_TAG
MACRO ₂ + NO ₃	→		+ .22 HYAC_TAG + NO ₂ _X_TAG + .47 HO ₂ _X_TAG
		MACRO ₂ _TAG + NO	→ NO + 0.8 ONITR_TAG + 0.8 ONITR_X_TAG
		MACRO ₂ _TAG + NO ₃	→ NO ₃ + .25 CH ₂ O_TAG + .53 CH ₃ CO ₃ _TAG
			+ .25 CH ₃ COCHO_TAG + .22 CO_TAG + .53 GLYALD_TAG
MACRO ₂ + HO ₂	→		+ .22 HYAC_TAG + .47 HO ₂ _X_TAG
		MACRO ₂ + NO ₃ _X_TAG	→ NO ₂ _X_TAG + MACRO ₂
		MACRO ₂ _TAG + HO ₂	→ HO ₂ + MACROOH_TAG
		MACRO ₂ + HO ₂ _X_TAG	→ MACRO ₂
MACROOH + OH	→	MACRO ₂ _TAG + M	→ M + .18 CH ₂ O_TAG + .26 CH ₃ CO ₃ _TAG
			+ .24 CH ₃ COCHO_TAG + .11 CO_TAG + .26 GLYALD_TAG
		MACROOH_TAG + OH	→ OH + .2 MACRO ₂ _TAG + .5 MCO ₃ _TAG
			+ .2 HO ₂ _X_TAG
MCO ₃ + NO	→	MCO ₃ _TAG + NO	→ NO + CH ₂ O_TAG + CH ₃ CO ₃ _TAG
			+ NO ₂ _X_TAG
		MCO ₃ _TAG + NO ₃	→ NO ₃ + CH ₂ O_TAG + CH ₃ CO ₃ _TAG
		MCO ₃ + NO ₃ _X_TAG	→ NO ₂ _X_TAG + MCO ₃
MCO ₃ + HO ₂	→	MCO ₃ _TAG + HO ₂	→ HO ₂ + .25 CH ₃ COOH_TAG + .75 CH ₃ COOOH_TAG

Original reaction			VOC-tagged reaction		
		+ .75 O2			+ .25 O3_X_TAG
MCO3 + M	→	M + CO2 + CH2O	MCO3 + HO2_X_TAG	→	MCO3
		+ CH3CO3	MCO3_TAG + M	→	M + CH2O_TAG + CH3CO3_TAG
MCO3 + NO2 + M	→	MPAN + M	MCO3_TAG + NO2 + M	→	NO2 + M + MPAN_TAG
			MCO3 + NO2_X_TAG + M	→	MPAN_X_TAG + M + MCO3
MPAN + M	→	MCO3 + NO2 + M	MPAN_TAG + M	→	M + MCO3_TAG
			MPAN_X_TAG + M	→	NO2_X_TAG + M
ONITR + OH	→	HYDRALD + .4 NO2 + HO2	ONITR_TAG + OH	→	OH + HYDRALD_TAG + HO2_X_TAG
			ONITR_X_TAG + OH	→	OH + .4 NO2_X_TAG
ONITR + NO3	→	HYDRALD + NO2 + HO2	ONITR_TAG + NO3	→	NO3 + HYDRALD_TAG + HO2_X_TAG
			ONITR_X_TAG + NO3	→	.5 NO2_X_TAG + NO3
			ONITR + NO3_X_TAG	→	.5 NO2_X_TAG + ONITR
HYDRALD + OH	→	XO2	HYDRALD_TAG + OH	→	OH + XO2_TAG
XO2 + NO	→	NO2 + HO2 + .5 CO	XO2_TAG + NO	→	NO + .25 CH3COCHO_TAG + .5 CO_TAG
		+ .25 GLYOXAL + .25 HYAC + .25 CH3COCHO			+ .25 GLYALD_TAG + .25 GLYOXAL_TAG + .25 HYAC_TAG
		+ .25 GLYALD			+ NO2_X_TAG + HO2_X_TAG
XO2 + NO3	→	NO2 + HO2 + 0.5 CO	XO2_TAG + NO3	→	NO3 + .25 CH3COCHO_TAG + 0.5 CO_TAG
		+ .25 HYAC + 0.25 GLYOXAL + .25 CH3COCHO			+ .25 GLYALD_TAG + 0.25 GLYOXAL_TAG + .25 HYAC_TAG
		+ .25 GLYALD			+ HO2_X_TAG
			XO2 + NO3_X_TAG	→	NO2_X_TAG + XO2
XO2 + HO2	→	XOOH	XO2_TAG + HO2	→	HO2 + XOOH_TAG
			XO2 + HO2_X_TAG	→	XO2
XO2 + M	→	M + .2 CO + .4 HO2	XO2_TAG + M	→	M + .1 CH3COCHO_TAG + .2 CO_TAG
		+ .1 GLYOXAL + .1 HYAC + .1 CH3COCHO			+ .1 GLYALD_TAG + .1 GLYOXAL_TAG + .1 HYAC_TAG
		+ .1 GLYALD			+ .4 HO2_X_TAG
XOOH + OH	→	H2O + XO2	XOOH_TAG + OH	→	OH + XO2_TAG
XOOH + OH	→	H2O + OH	XOOH_TAG + OH	→	OH
TOLUENE + OH	→	.25 CRESOL + .25 HO2 + .7 TOLO2	TOLUENE_TAG + OH	→	OH + .25 CRESOL_TAG + .7 TOLO2_TAG
					+ .25 HO2_X_TAG
CRESOL + OH	→	XOH	CRESOL_TAG + OH	→	OH + XOH_TAG
XOH + NO2	→	.7 NO2 + .7 BIGALD + .7 HO2	XOH_TAG + NO2	→	NO2 + .7 BIGALD_TAG + .7 HO2_X_TAG
			XOH + NO2_X_TAG	→	XOH + .7 NO2_X_TAG
TOLO2 + NO	→	.45 GLYOXAL + .45 CH3COCHO +.9 BIGALD	TOLO2_TAG + NO	→	NO + .9 BIGALD_TAG + .45 CH3COCHO_TAG

Original reaction		VOC-tagged reaction	
	→ + .9 NO2 + .9 HO2		→ + .45 GLYOXAL_TAG + .9 NO2_X_TAG + .9 HO2_X_TAG
TOLO2 + HO2	→ TOLOOH	TOLO2_TAG + HO2	→ HO2 + TOLOOH_TAG
		TOLO2 + HO2_X_TAG	→ TOLO2
TOLOOH + OH	→ TOLO2	TOLOOH_TAG + OH	→ OH + TOLO2_TAG
C10H16 + OH	→ TERPO2	C10H16_TAG + OH	→ OH + TERPO2_TAG
C10H16 + O3	→ .7 OH + MVK + MACR	C10H16_TAG + O3	→ O3 + MACR_TAG + MVK_TAG
	+ HO2		+ HO2_X_TAG
		C10H16 + O3_X_TAG	→ C10H16
C10H16 + NO3	→ TERPO2 + NO2	C10H16_TAG + NO3	→ NO3 + TERPO2_TAG
		C10H16 + NO3_X_TAG	→ C10H16 + NO2_X_TAG
TERPO2 + NO	→ .1 CH3COCH3 + HO2 + MVK	TERPO2_TAG + NO	→ NO + .1 CH3COCH3_TAG + MACR_TAG
	+ MACR + NO2		+ MVK_TAG + NO2_X_TAG + HO2_X_TAG
TERPO2 + HO2	→ TERPOOH	TERPO2_TAG + HO2	→ HO2 + TERPOOH_TAG
		TERPO2 + HO2_X_TAG	→ TERPO2
TERPOOH + OH	→ TERPO2	TERPOOH_TAG + OH	→ OH + TERPO2_TAG
N2O5	→ 2 HNO3	NO3NO2_X_TAG	→ HNO3_X_TAG
		NO2NO3_X_TAG	→ HNO3_X_TAG
NO3	→ HNO3	NO3_X_TAG	→ HNO3_X_TAG
NO2	→ 0.5 OH + 0.5 NO + 0.5 HNO3	NO2_X_TAG	→ 0.5 HNO3_X_TAG
DMS + OH	→ SO2	DMS_TAG + OH	→ OH
DMS + OH	→ .5 SO2 + .5 HO2	DMS_TAG + OH	→ OH + .5 HO2_X_TAG
DMS + NO3	→ SO2 + HNO3	DMS_TAG + NO3	→ NO3
		DMS + NO3_X_TAG	→ DMS + HNO3_X_TAG
HO2	→ 0.5 H2O2	HO2_X_TAG	→ dummy
HCN + OH + M	→ HO2 + M	HCN_TAG + OH + M	→ OH + M + HO2_X_TAG
CH3CN + OH	→ HO2	CH3CN_TAG + OH	→ OH + HO2_X_TAG

2 Supplementary figures

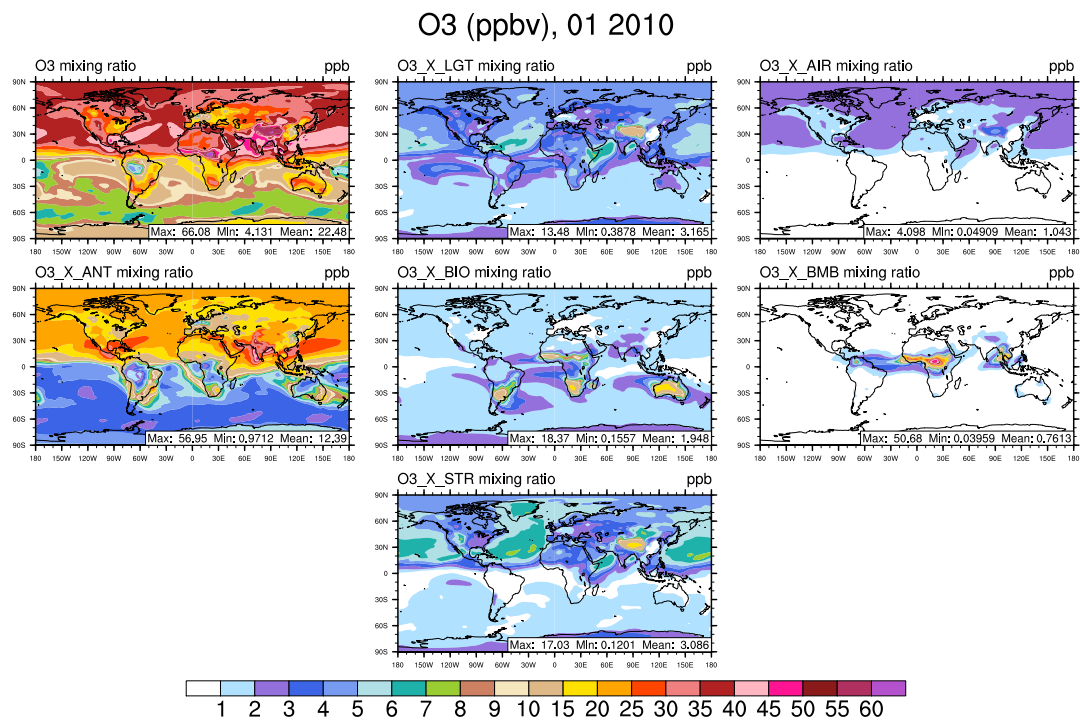


Figure S1. Surface ozone in January from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), lightning (LGT), and transport from the stratosphere (STR).

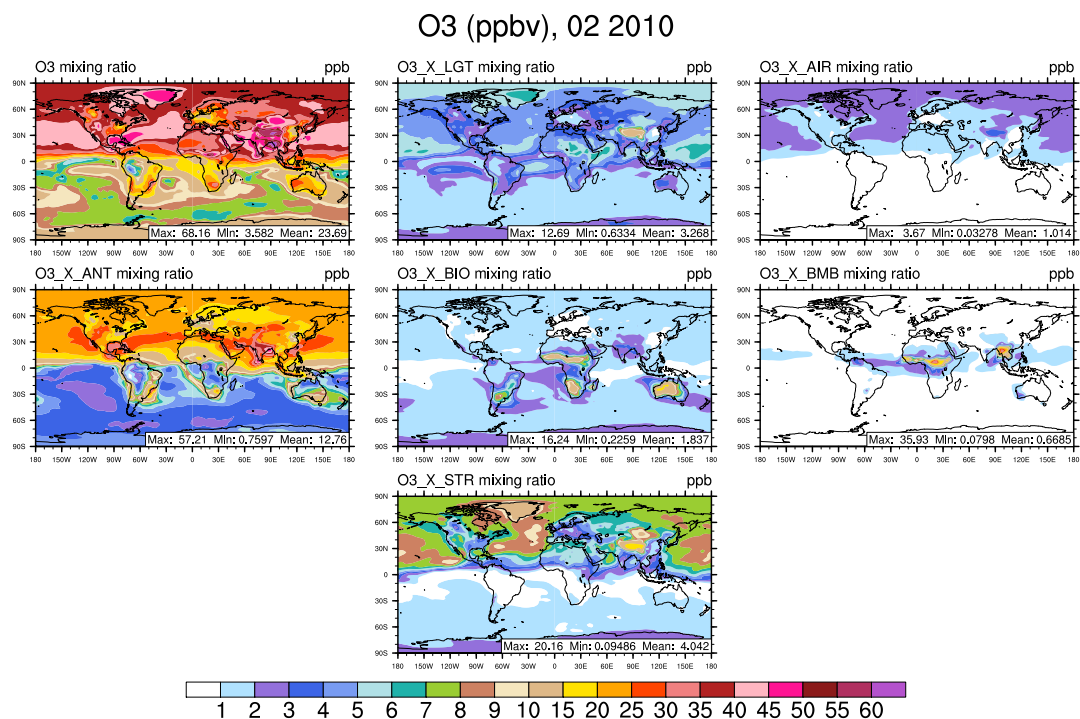


Figure S2. Surface ozone in February from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

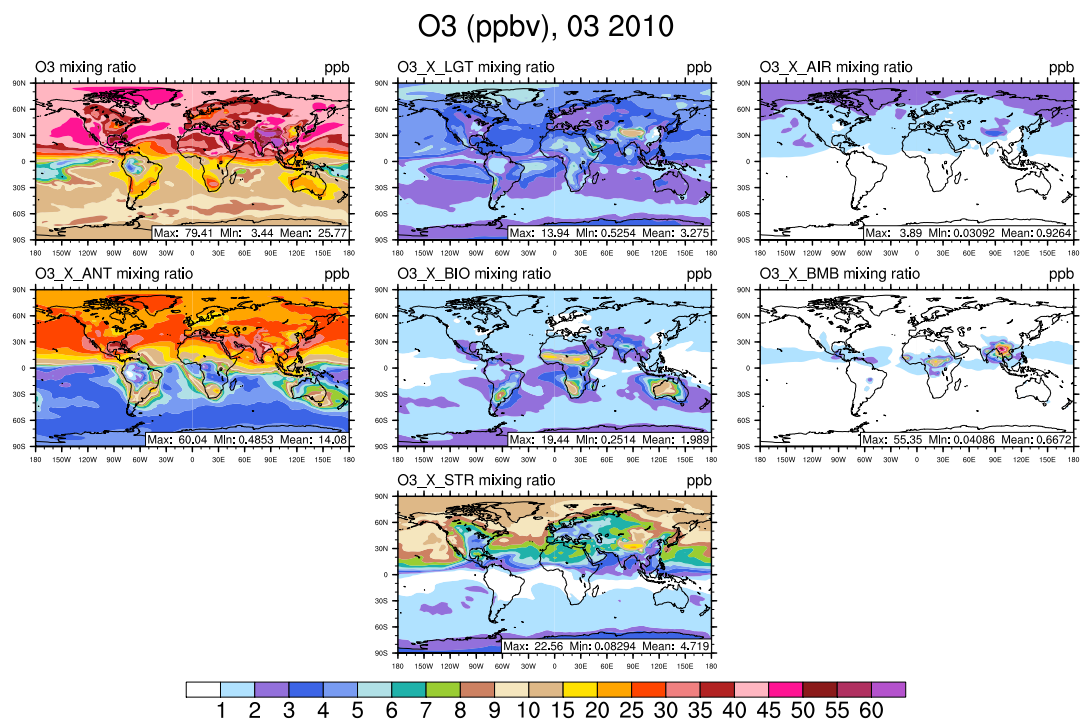


Figure S3. Surface ozone in March from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

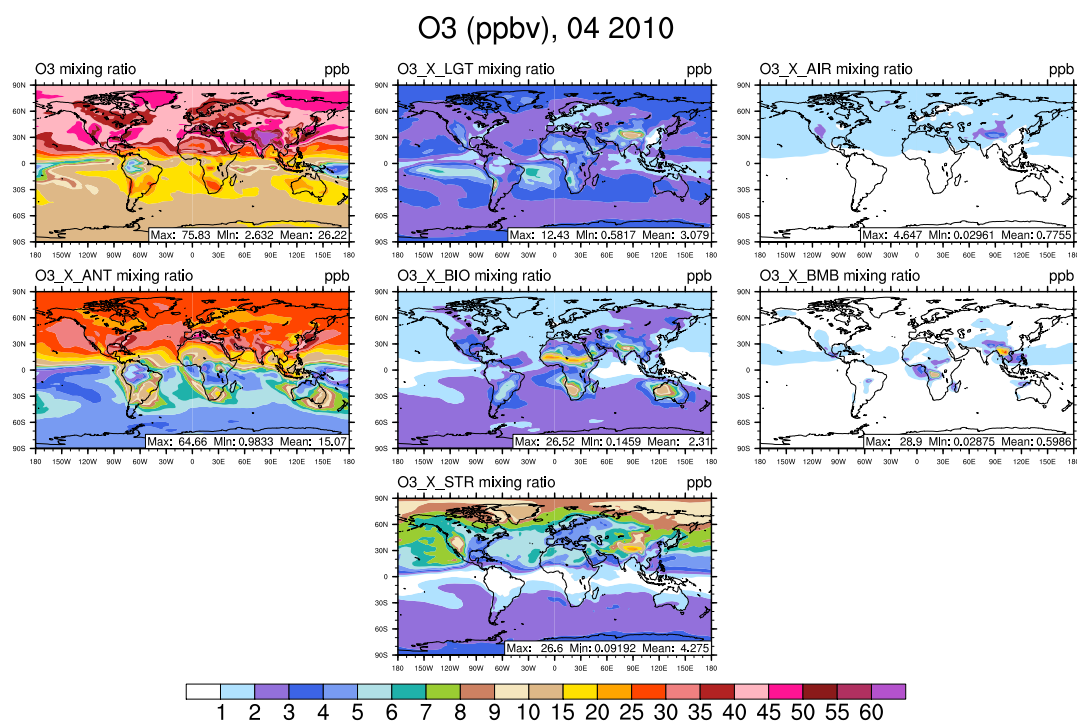


Figure S4. Surface ozone in April from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

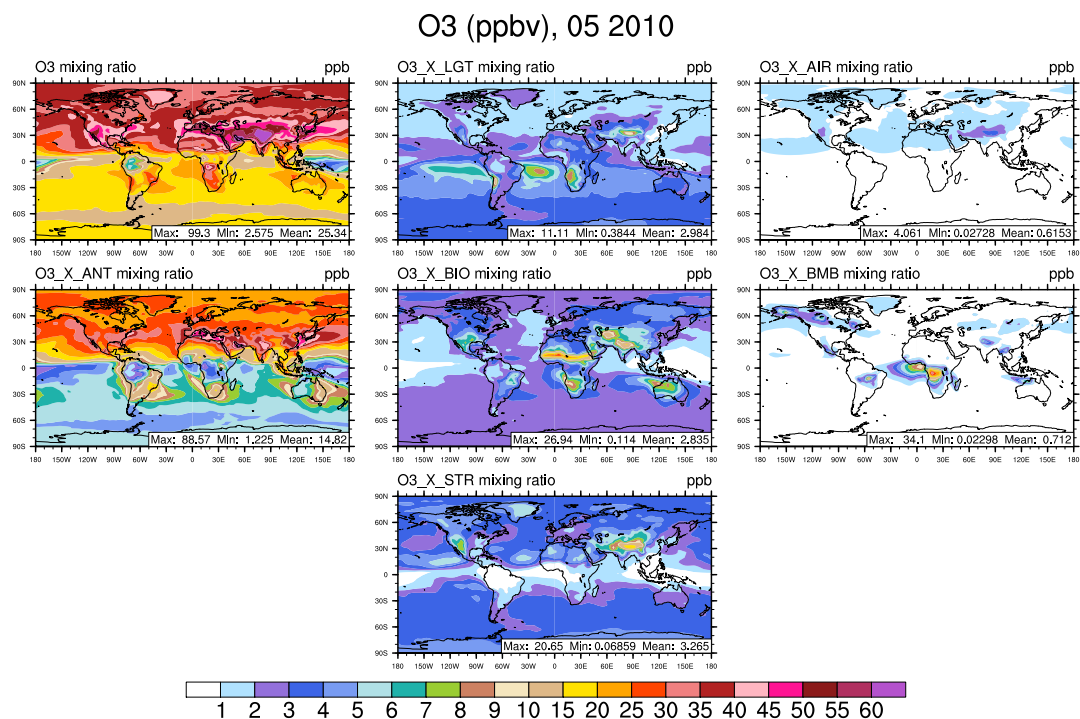


Figure S5. Surface ozone in May from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

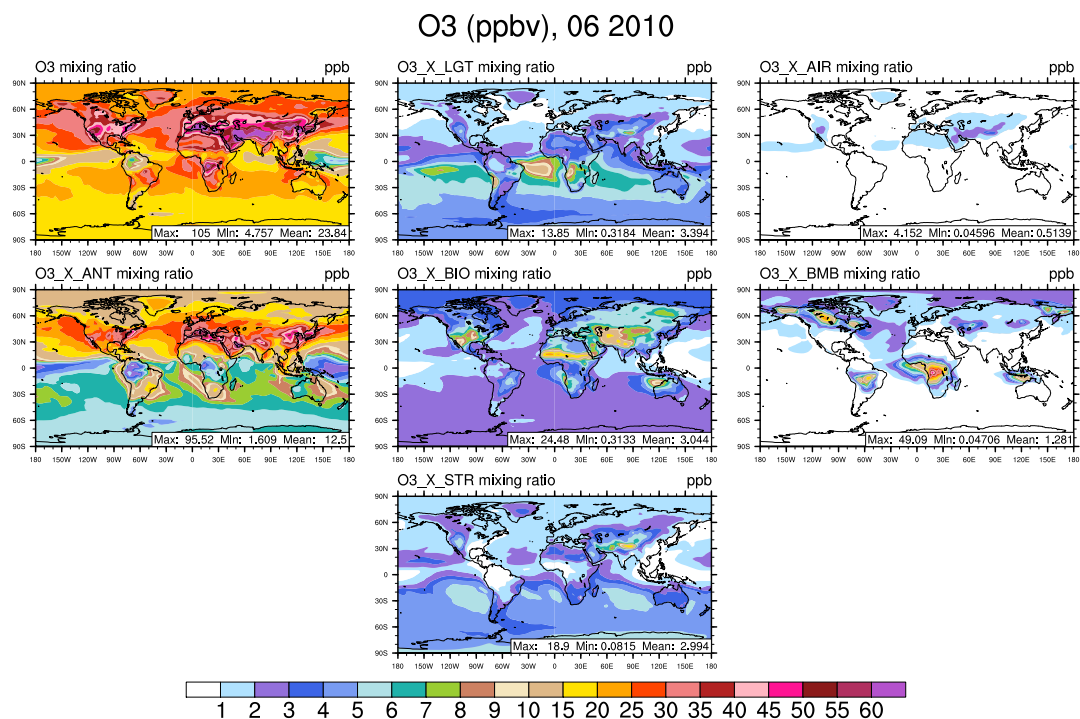


Figure S6. Surface ozone in June from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

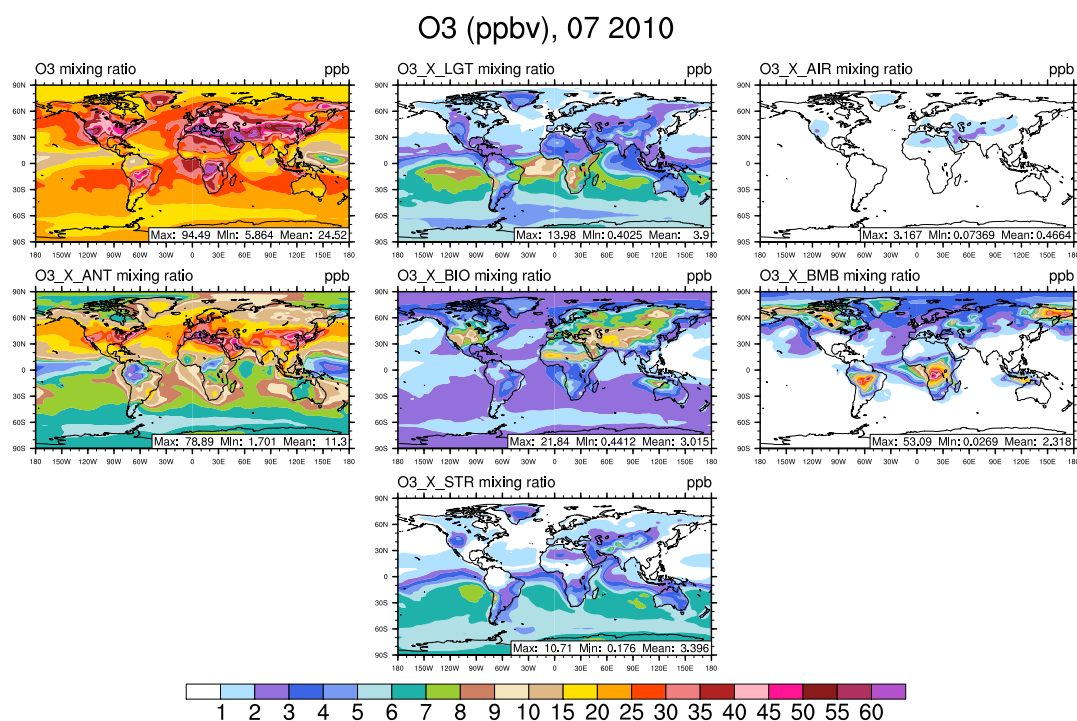


Figure S7. Surface ozone in July from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

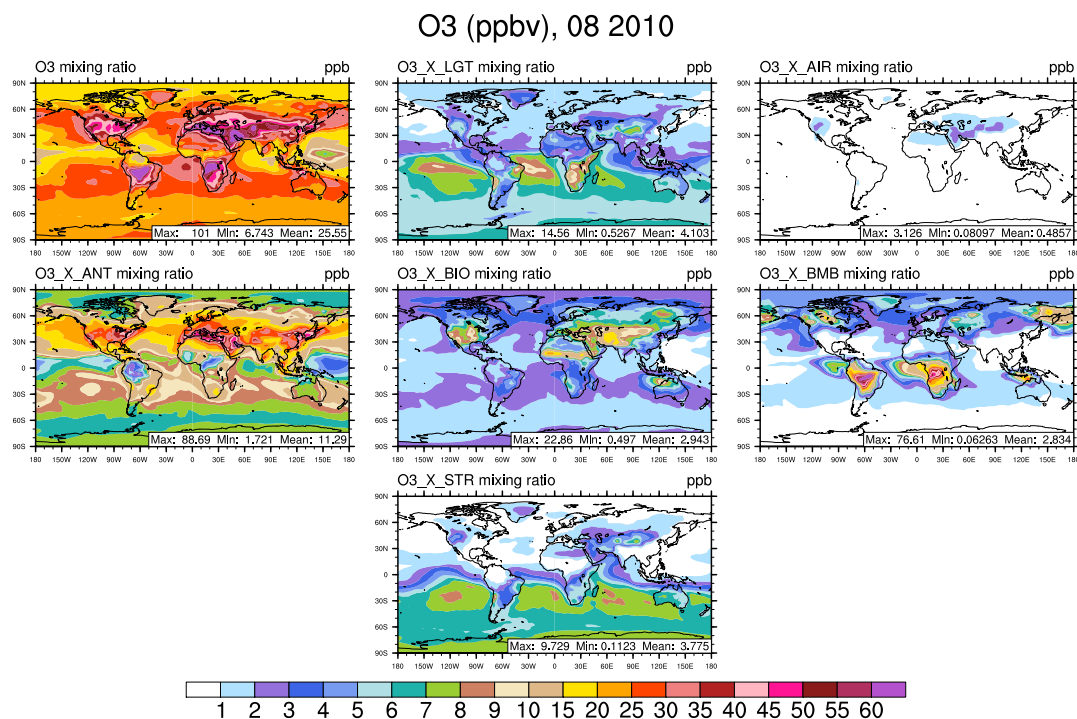


Figure S8. Surface ozone in August from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

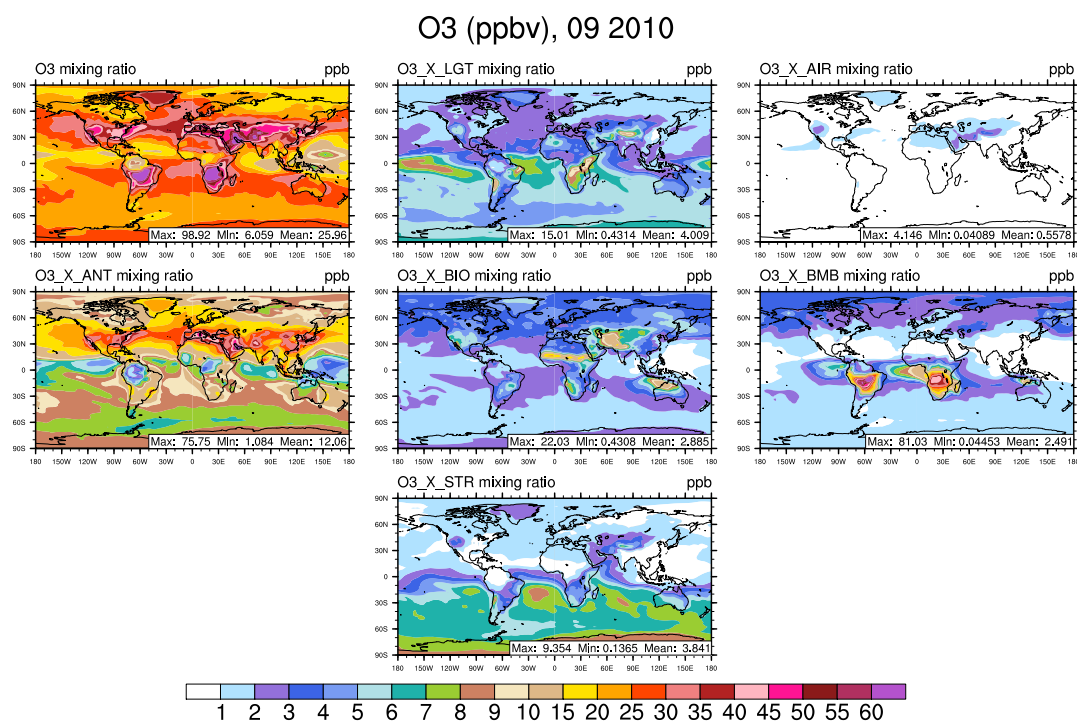


Figure S9. Surface ozone in September from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

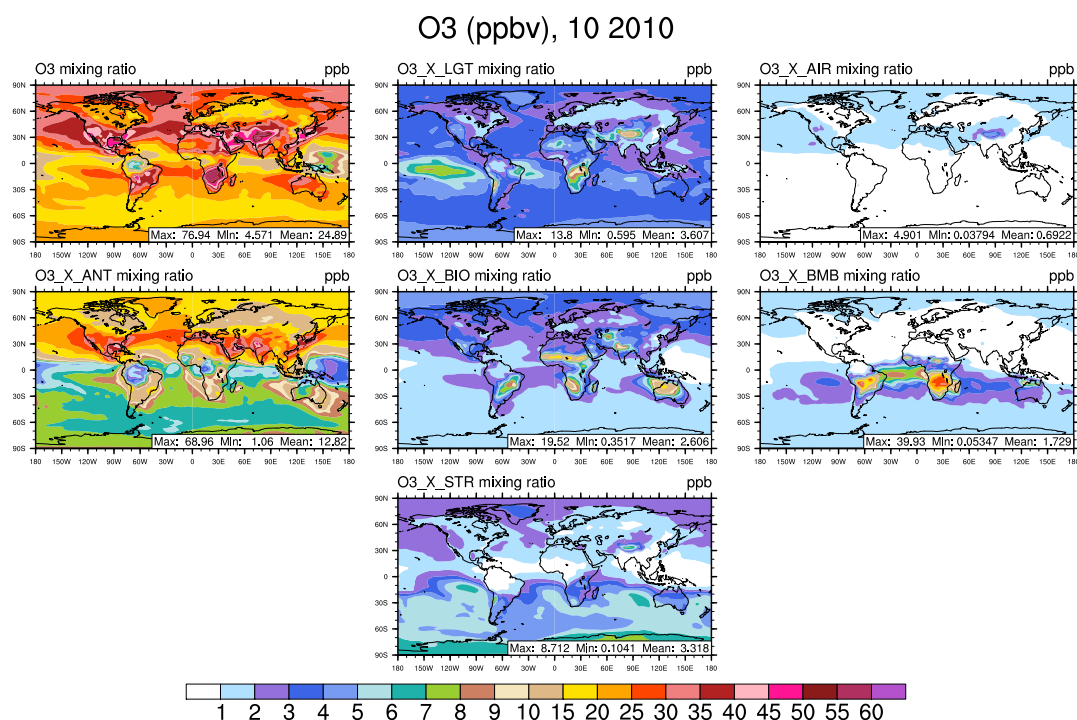


Figure S10. Surface ozone in October from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

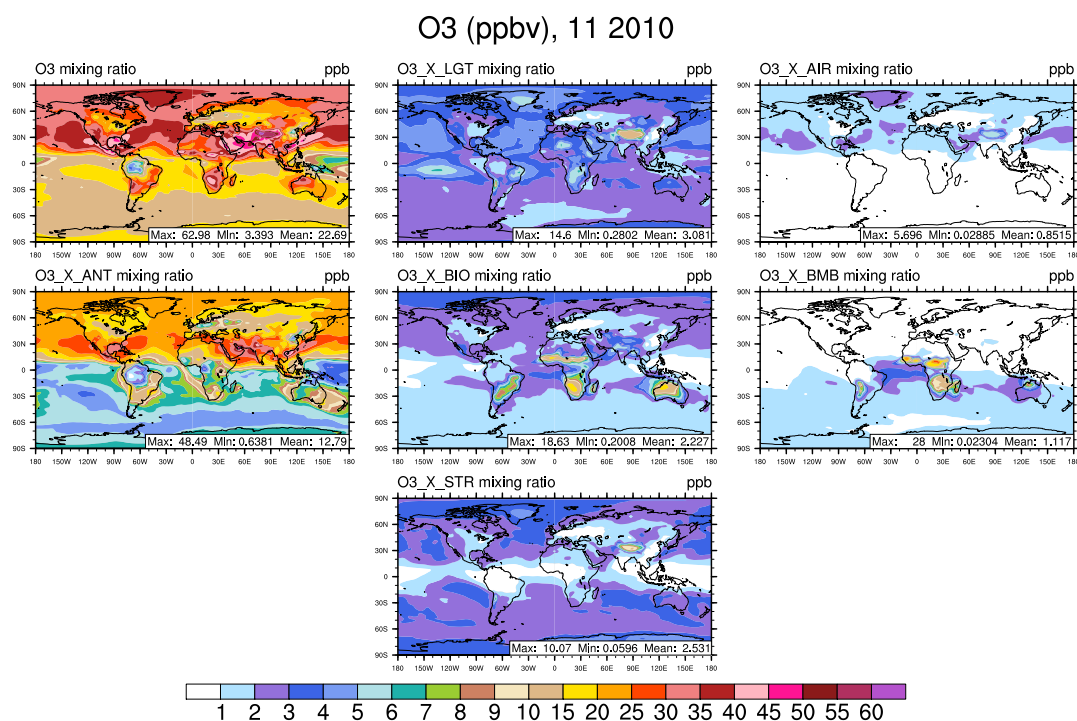


Figure S11. Surface ozone in November from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

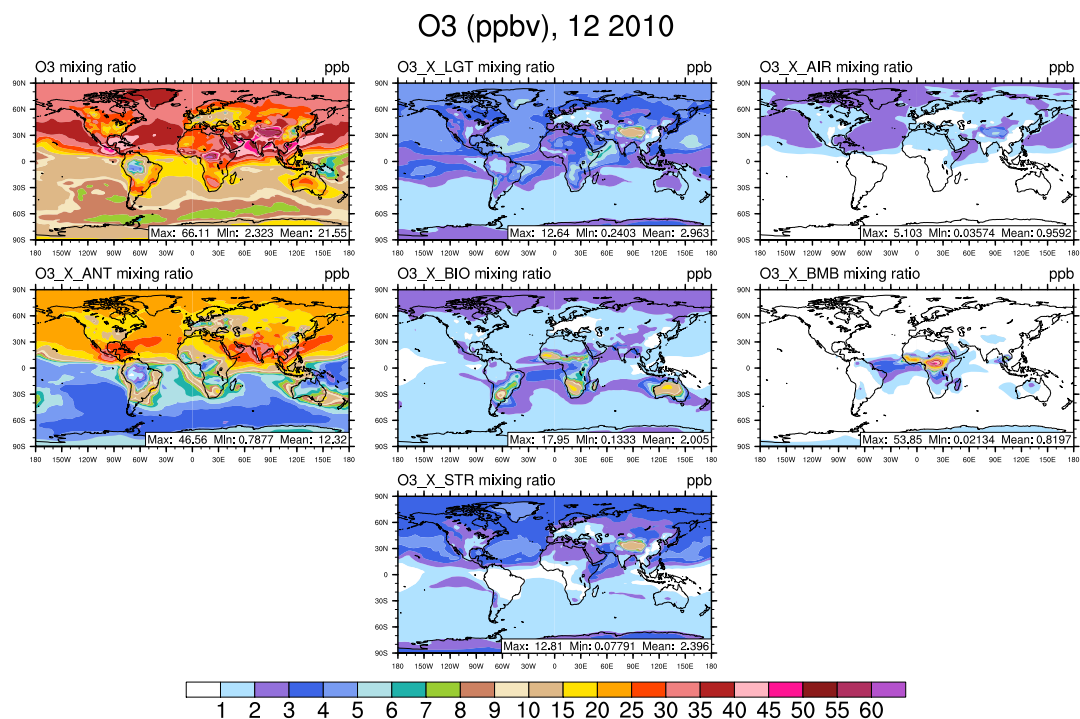


Figure S12. Surface ozone in December from the NO_x-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to NO_x precursors emitted by lightning (LGT), aircraft (AIR), anthropogenic sources (ANT), biogenic sources (BIO), biomass burning (BMB), and transport from the stratosphere (STR).

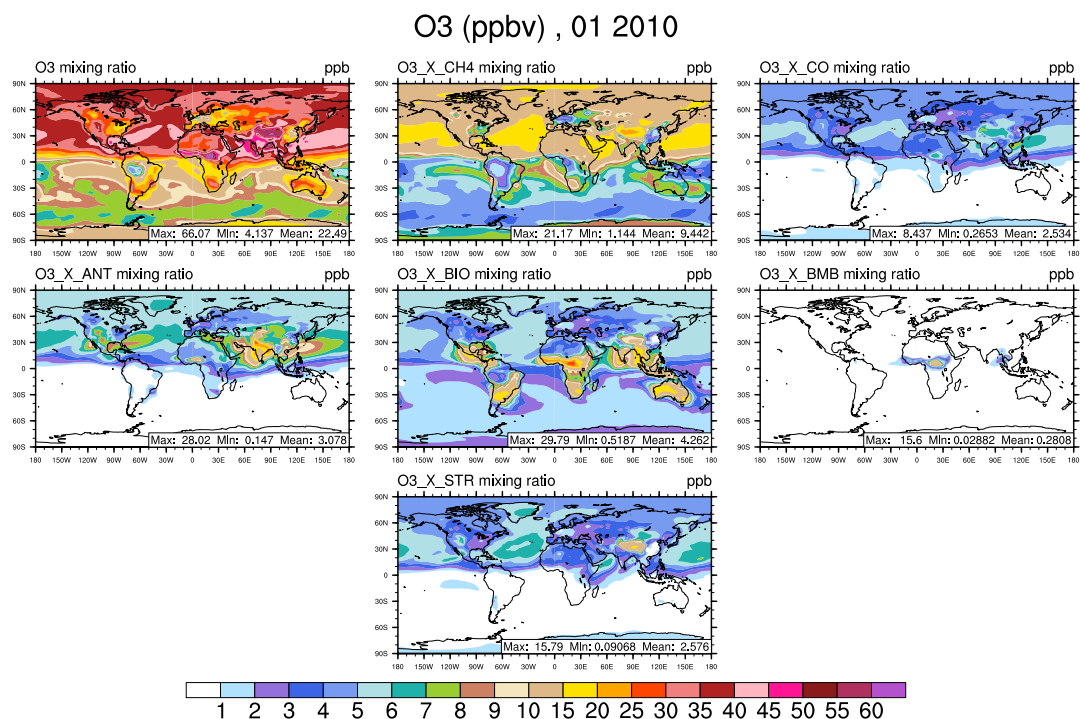


Figure S13. Surface ozone in January from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

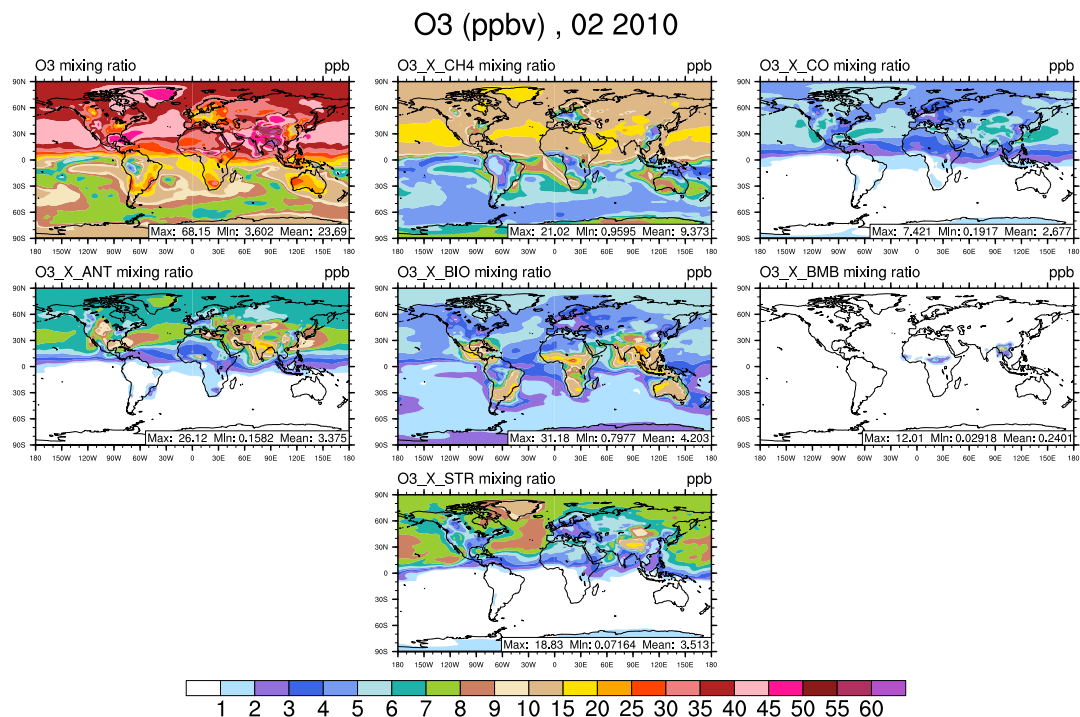


Figure S14. Surface ozone in February from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

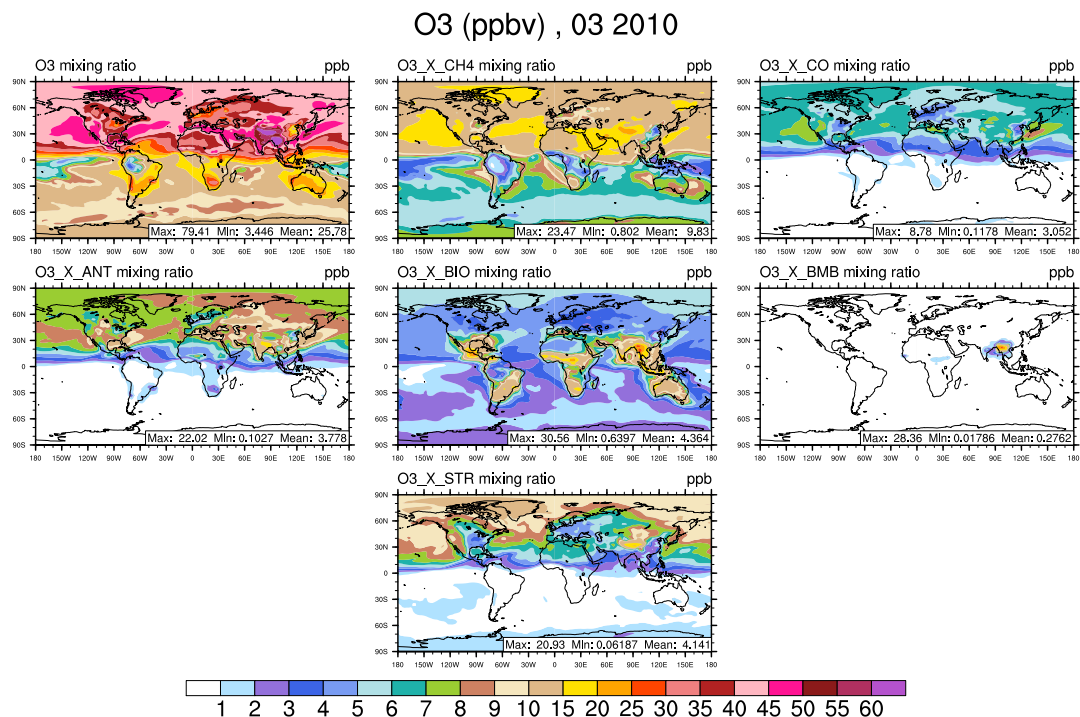


Figure S15. Surface ozone in March from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

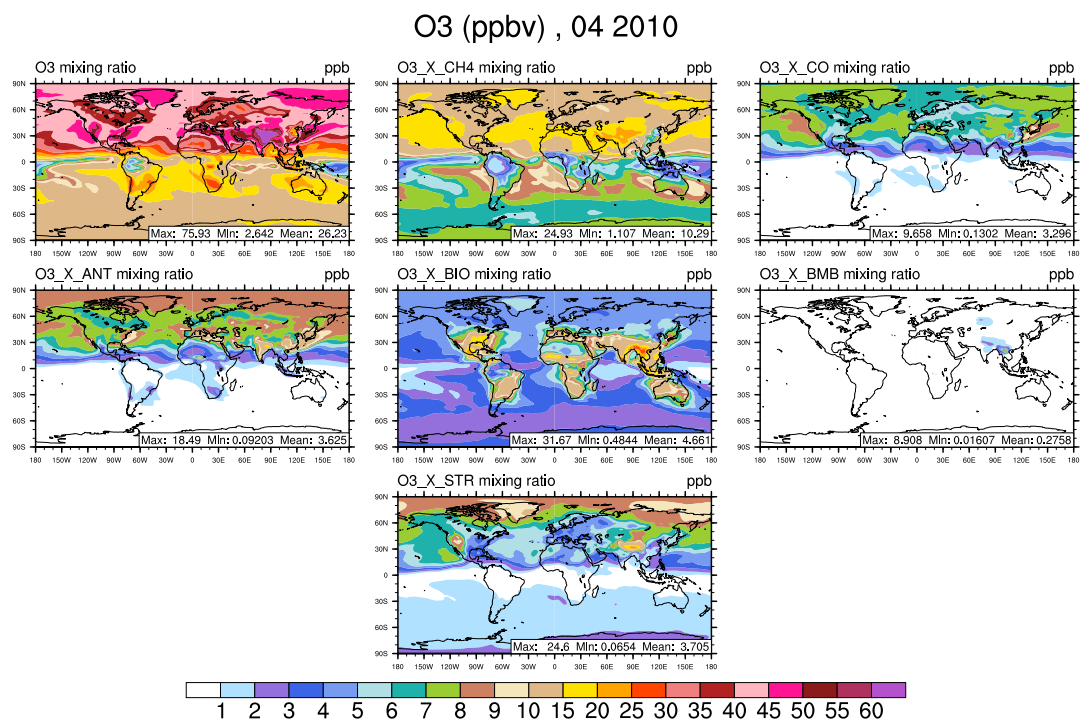


Figure S16. Surface ozone in April from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

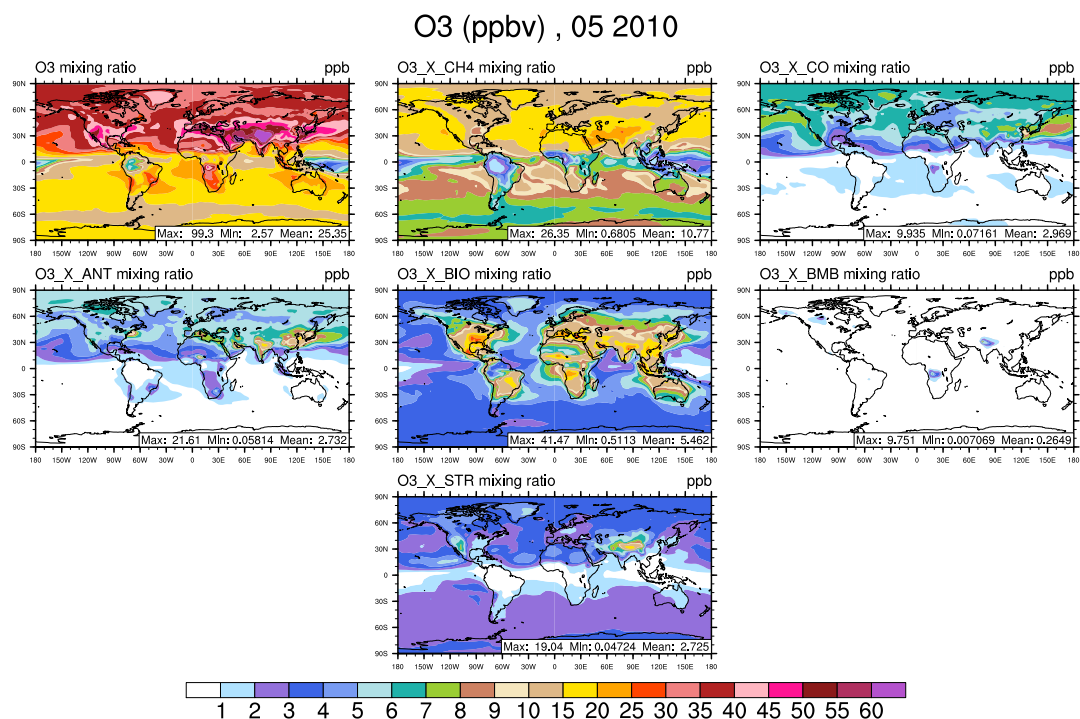


Figure S17. Surface ozone in May from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

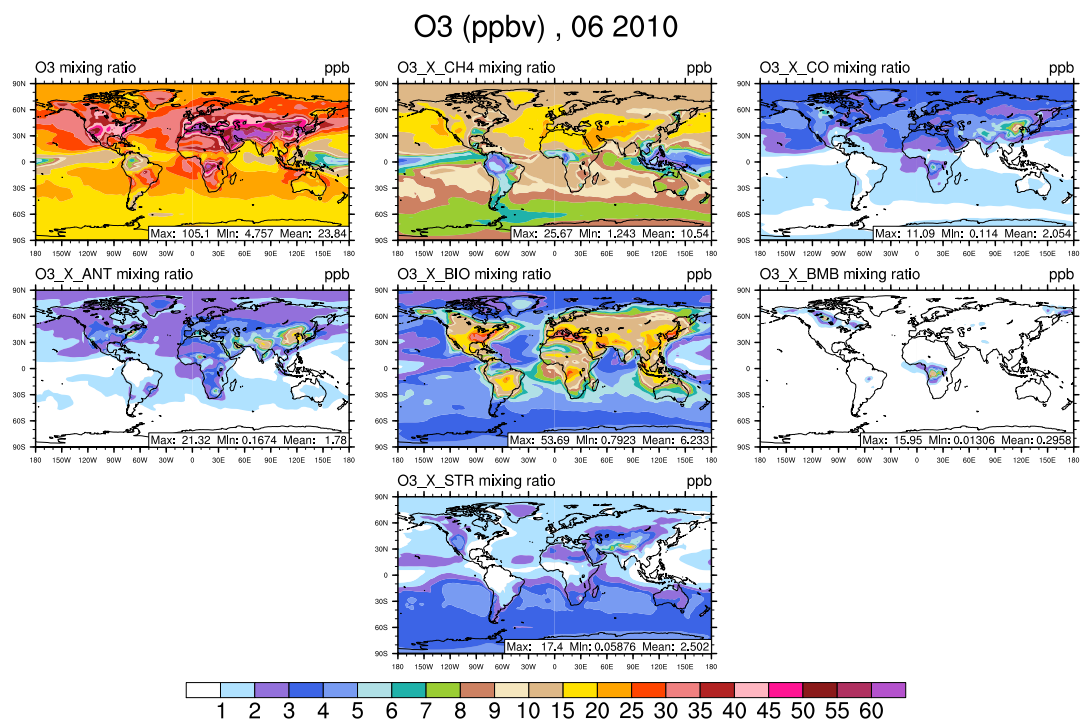


Figure S18. Surface ozone in June from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

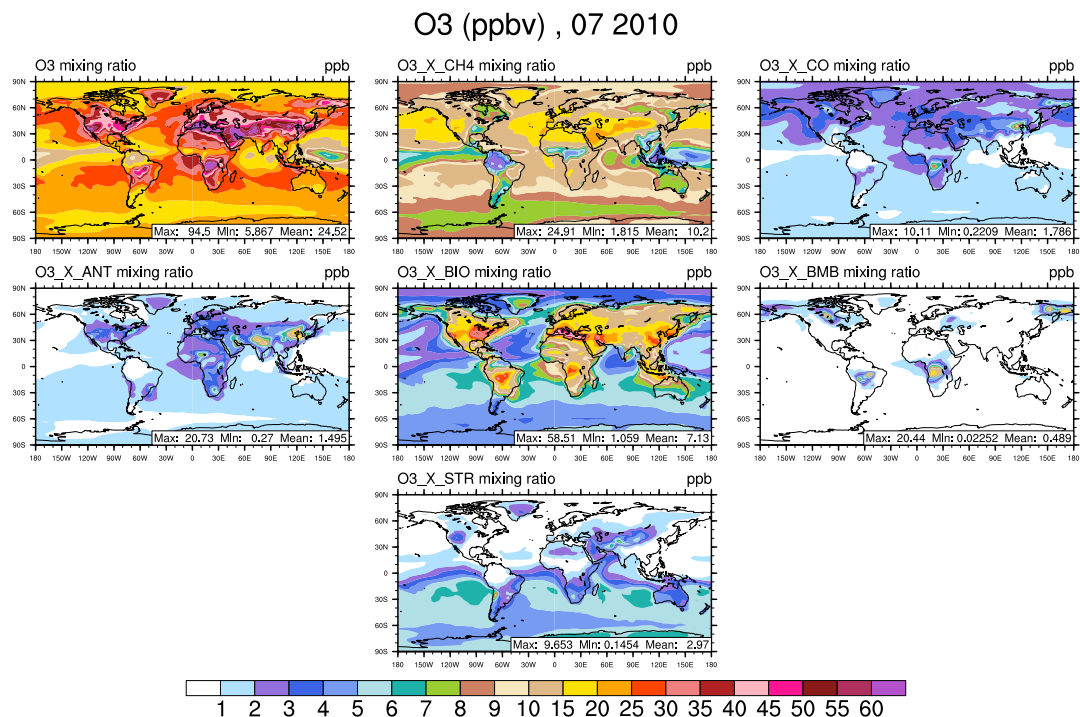


Figure S19. Surface ozone in July from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

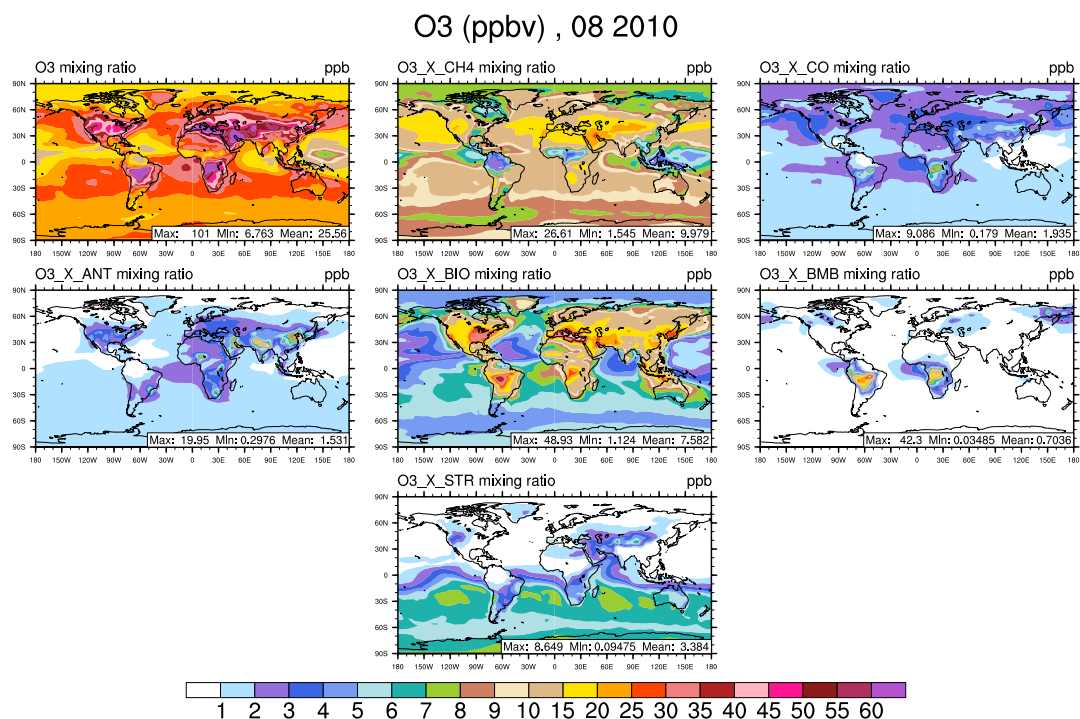


Figure S20. Surface ozone in August from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

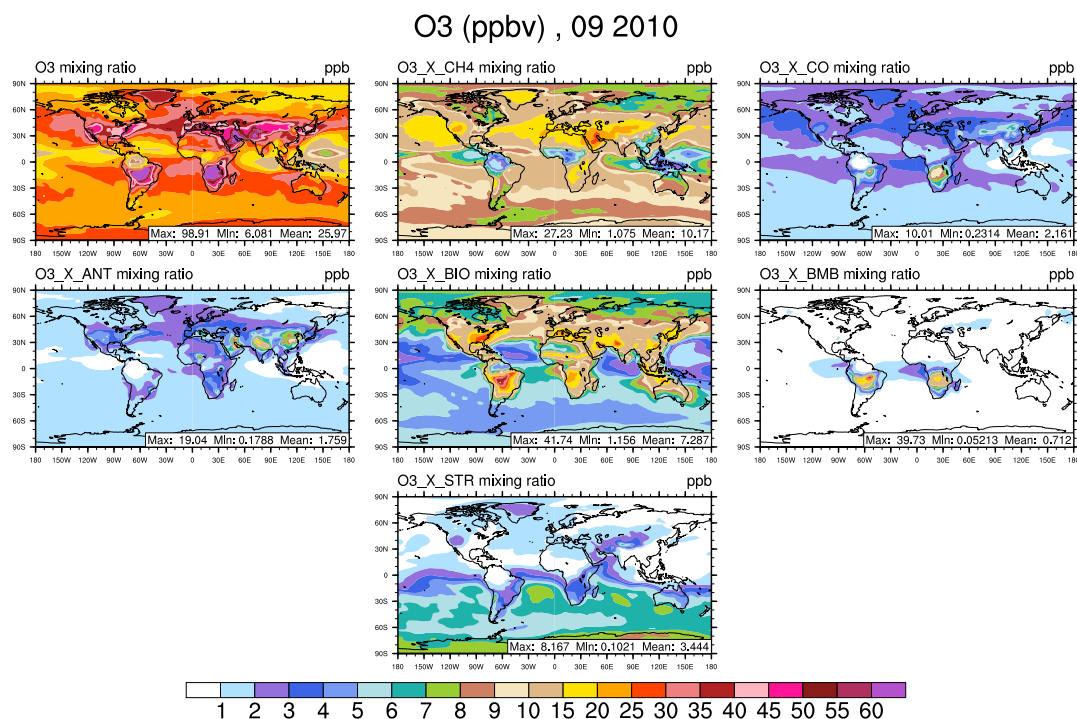


Figure S21. Surface ozone in September from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

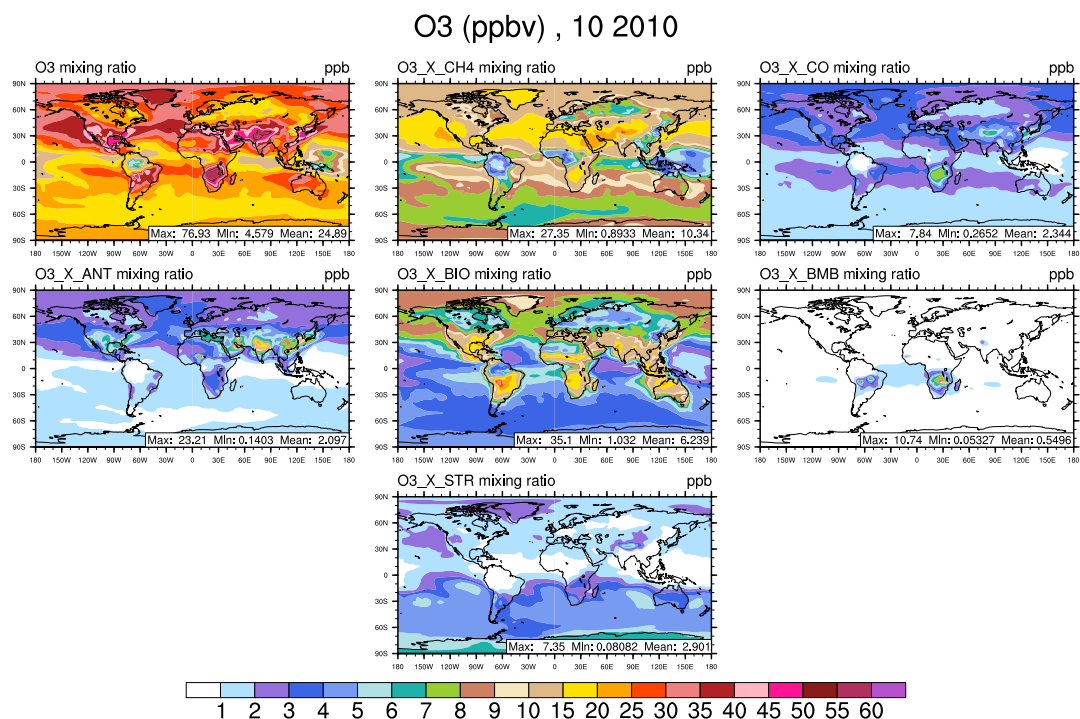


Figure S22. Surface ozone in October from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

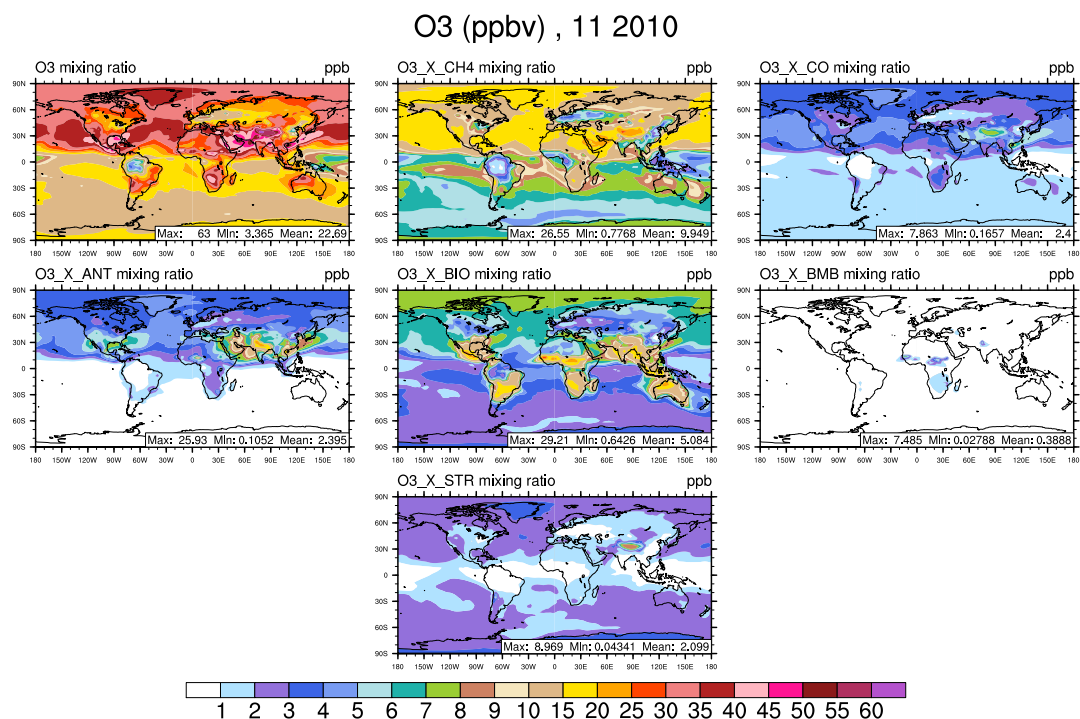


Figure S23. Surface ozone in November from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).

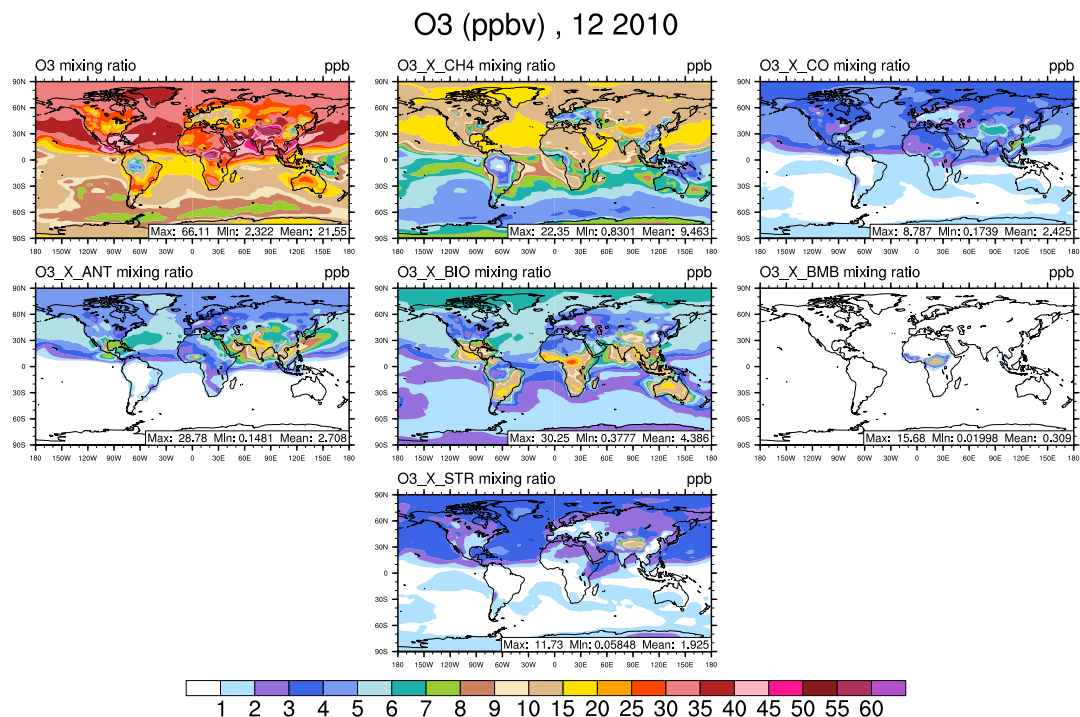


Figure S24. Surface ozone in December from the VOC-tagging run. Total surface ozone is shown in the top-left panel. Other panels show the contribution to surface ozone due to methane (CH₄), all CO emissions (CO), anthropogenic NMVOC sources (ANT), biogenic NMVOC sources (BIO), biomass burning NMVOC sources (BMB), and transport from the stratosphere (STR).