Supporting Information for

Impact of Chlorine Emissions from Sea-Salt Aerosol on Coastal Urban Ozone

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Table SI.1: Species included in CACM Mechanism with chlorine chemistry extensions*

NO	NITRIC OXIDE
NO2	NITROGEN DIOXIDE
O3	OZONE
HONO	NITROUS ACID
HNO3	NITRIC ACID
HNO4	PERNITRIC ACID
N2O5	NITROGEN PENTOXIDE
NO3	NITRATE RADICAL
HO2	HYDROPEROXY RADICAL
CO	CARBON MONOXIDE
CO2	CARBON DIOXIDE
H2O2	HYDROGEN PEROXIDE
NH3	AMMONIA
NIT	AEROSOL NITRATE
SO2	SULFUR DIOXIDE
SO3	SULFUR TRIOXIDE
OSD	O SINGLET D
O	O ATOM
OH	HYDROXYL RADICAL
H2O	WATER VAPOR
O2	OXYGEN
H2	HYDROGEN
M	THIRD BODY
HCL	HYDROCHLORIC ACID
CL	**ATOMIC CHLORINE**
CL2	**MOLECULAR CHLORINE**
CLO	**CHLORINE MONOXIDE**
HOCL	**HYPOCHLOROUS ACID**
CLNO	**NITROSYL CHLORIDE**
CLN2	**NITRYL CHLORIDE ($ClNO_2$)**
CLN5	**CHLORINE NITRATE ($ClONO_2$)**
OCLO	**CHLORINE DIOXIDE**
CLN3	**CHLORINE NITRITE (ClONO)**
FOCL	**FORMYL CHLORIDE (HCOCl)**
CLI1	**PRODUCT OF ISOP + CL REACTION: 4-CHLORO-3-METHYL-2-BUTANAL**
CLI2	**PRODUCT OF ISOP + CL REACTION: 4-CHLORO-2-METHYL-2-BUTANAL**
ETHE	ETHENE
OLEL	LUMPED ALKENES C3-C6
OLEH	LUMPED ALKENES >C6
ALKL	LUMPED ALKANES C3-C6
ALKM	LUMPED ALKANES C7-C12
ALKH	LUMPED ALKANES >C12
AROH	LUMPED AROMATICS WITH HIGH SOA Y
AROL	LUMPED AROMATICS WITH LOW SOA Y
PHEN	LUMPED OXYGENATED AROMATICS
BALD	LUMPED AROMATIC MONOALDEHYDES
ARAC	LUMPED AROMATIC MONOACIDS
ADAC	LUMPED AROMATIC DIACIDS

*Species in bold were added with chlorine chemistry mechanism

Table SI.1 (cont.): Species included in CACM Mechanism with chlorine chemistry extensions*

PAH	LUMPED PAH
HCHO	FORMALDEHYDE
ALD2	LUMPED ALDEHYDES
MEK	LUMPED KETONES C3-C6
KETO	LUMPED KETONES >C6
MEOH	METHANOL
ETOH	ETHANOL
ALCH	LUMPED HIGHER ALCOHOLS
ISOP	ISOPRENE
BIOL	LUMPED MONOTERPENES WITH LOW SOA Y
BIOH	LUMPED MONOTERPENES WITH HIGH SOA Y
ACID	LUMPED ORGANIC ACIDS WITH <C6
PAN1	PEROXY PENTIONYL NITRATE
PAN2	PAN
PAN3	UNSATURATED PPN
PAN4	KETO PPN
PAN5	METHYLENE-PPN
PAN6	PAN FROM GLYOXAL
PAN7	PEROXY 3-METHYL-HEPTIONYL NITRATE
PAN8	PEROXY 2-HYDROXY-3-ISOPROPYL-6-OXO-HEPTIONYL NITRATE
PAN9	PEROXY 3-ISOPROPYL-4-HYDROXY-2-BUTENIONYL NITRATE
PN10	PAN FROM GLYOXALIC ACID
MGLY	METHYL GLYOXAL
MVK	METHYL VINYL KETONE
MCR	METHACROLEIN
MTBE	METHYL TERT-BUTYL ETHER
CH4	METHANE
RO2T	TOTAL RO2 ('SUM' OF RO21 THROUGH RO249 AND CLRO21 THROUGH CLRO24)
CLRO21	**RO2 RADICAL FROM ETHE + CL**
CLRO22	**RO2 RADICAL FROM OLEL + CL**
CLRO23	**RO2 RADICAL FROM OLEH + CL**
CLRO24	**RO2 RADICAL: *OOCH2Cl FROM REACTION OF CLRO21, CLRO22, CLRO23**
CRIEG1	**CRIEGEE INTERMEDIATE FROM RO21 + CL**
CRIEG2	**CRIEGEE INTERMEDIATE FROM RO25 + CL**
RO21	PEROXY FROM CH4 OXIDATION
RO22	HYDROXY ALKYL PEROXY <C6 FROM ETHE, ETOH, OLEL, ALCH
RO23	NITRATO ALKYL PEROXY <C6 FROM ETHE, OLEL
RO24	ALDEHYDIC ALKYL PEROXY FROM ISOP, ETHE
RO25	ALKYL PEROXY <C6 FROM MEK,ISOP, ALKL, BIOH, OLEL
RO26	ACYL RADICAL FROM ALD2 OXIDATION
RO27	OXO ALKYL PEROXY <C6 FROM ISOP, MEK
RO28	ACYL PEROXY <C6 FROM ALD2,ISOP, BIOH, MEK, KETO, BIOL
RO29	HYDROXY ALKENYL PEROXY FROM ISOP
RO210	HYDROXY ALKENYL PEROXY RADICAL FROM ISOP
RO211	NITRATO ALKENYL PEROXY FROM ISOP
RO212	NITRATO ALKENYL PEROXY RADICAL FROM ISOP
RO213	OXO ALKENYL PEROXY FROM ISOP
RO214	ALKENYL PEROXY FROM ISOP
RO215	ETHER ALKYL PEROXY FROM MTBE
RO216	OXO ALKYL PEROXY FROM KETO
RO217	AROMATIC PEROXY FROM SIDE CHAIN ABSTRACTION OF PHEN
RO218	HYDROXY ALKYL PEROXY >C6 FROM OLEH, ALKM
RO219	NITRATO ALKYL PEROXY FROM OLEH
RO220	ALKYL PEROXY >C6 FROM OLEH, ALKM
RO221	AROMATIC PEROXY FROM SIDE CHAIN ABSTRACTION OF AROL
RO222	PEROXY RADICAL FROM SIDE CHAIN ABSTRACTION OF BALD
RO223	PEROXY RADICAL FROM SIDE CHAIN ABSTRACTION OF ARAC

*Species in bold were added with chlorine chemistry mechanism

Table SI.1 (cont.): Species included in CACM Mechanism with chlorine chemistry extensions

RO224	DIHYDROXY ALKYL PEROXY FROM OH ATTACK OF BIOL
RO225	HYDROXY NITRATO PEROXY FROM NO3 ATTACK OF BIOL
RO226	OXO HYDROXY ALDEHYDIC PEROXY FROM BIOL
RO227	HYDROXY ALKENYL PEROXY FROM BIOH
RO228	NITRATO ALKENYL PEROXY FROM BIOH
RO229	OXO ALKENYL PEROXY FROM BIOH
RO230	OXO ALDEHYDIC ALKENYL PEROXY FROM BIOH
RO231	AROMATIC PEROXY FROM SIDE CHAIN ABSTRACTION OF PAH
RO232	ALKYL PEROXY FROM ALKH
RO233	PEROXY FROM ADDITION OF O2 TO RAD2
RO234	PEROXY FROM ADDITION OF O2 TO RAD3
RO235	PEROXY FROM ADDITION OF O2 TO RAD4
RO236	PEROXY FROM ADDITION OF O2 TO RAD5
RO237	PEROXY FROM ADDITION OF O2 TO RAD6
RO238	PEROXY FROM ADDITION OF O2 TO RAD7
RO239	UNSATURATED ACYL PEROXY FROM ISOP
RO240	HYDROXY OXO ALKENYL PEROXY FROM BIOH
RO241	HYDROXY ALKYL PEROXY FROM ALKH
RO242	BICYCLIC PEROXY FROM BRIDGING OF RO233
RO243	BICYCLIC PEROXY FROM BRIDGING OF RO234
RO244	BICYCLIC PEROXY FROM BRIDGING OF RO235
RO245	BICYCLIC PEROXY FROM BRIDGING OF RO236
RO246	BICYCLIC PEROXY FROM BRIDGING OF RO237
RO247	BICYCLIC PEROXY FROM BRIDGING OF RO238
RO248	OXO ACYL PEROXY FROM FURTHER ALDEHYDE OXIDATION IN MGLY
RO249	HYDROXY KETO PEROXY RADICAL FROM MVK
RO250	ACYL PEROXY RADICAL FROM ALDEHYDIC H ATTACK OF MCR
RO251	HYDROXY ALDEHYDIC PEROXY RADICAL FROM OH DB ATTACK OF MCR
RO252	NITRATO ALDEHYDIC PEROXY RADICAL FROM NO3 DB ATTACK OF MCR
RO253	KETO ALDEHYDIC PEROXY RADICAL FROM MCR/O3 REACTION
RO254	ALDEHYDIC ACYL PEROXY RADICAL FROM RO253
RO255	ACYL PEROXY FORMED FROM FURTHER REACTION OF RPR1
RO256	HYDROXY OXO ACYL PEROXY FORMED FROM RPR3
RO257	HYDROXY UNSATURATED ACYL PEROXY FROM RPR8
RO258	ACID ACYL PEROXY RADICAL FROM RP16
RAD1	RADICAL FROM PHEN/NO3
RAD2	HEXADIENYL RADICAL FROM PHEN/OH
RAD3	HEXADIENYL RADICAL FROM AROL/OH
RAD4	HEXADIENYL RADICAL FROM AROH/OH
RAD5	HEXADIENYL RADICAL FROM BALD/OH
RAD6	HEXADIENYL RADICAL FROM ARAC/OH
RAD7	HEXADIENYL RADICAL FROM PAH/OH
RAD8	RADICAL FROM RPR4/NO3
RPR1	3-METHYL HEPTANAL
RPR2	3-HYDROXY-4-METHYL-BENZALDEHYDE
RPR3	2-HYDROXY-3-ISOPROPYL-6-OXO-HEPTANAL
RPR4	2,6-DIMETHYL-4-NITRO-PHENOL
RPR5	2-NITRO-4-METHYL-BENZALDEHYDE
RPR6	1,4-DIBENZALDEHYDE
RPR7	1-FORMYL-4-CARBOXY-BENZENE
RPR8	3-ISOPROPYL-4-HYDROXY-2-BUTENAL
RPR9	4-HYDROXY-3,5-DIMETHYL-2,4-HEXADIENDIAL
RP10	2-METHYL-BUTENALIC ACID
RP11	4,5-DIMETHYL-6-OXO-2,4-HEPTADIENAL
RP12	2-METHYL-5-FORMYL-2,4-HEXADIENDIAL
RP13	2-CARBOXYL-5-METHYL-2,4-HEXADIENDIAL
RP14	2-(DIMETHYL-PROPENAL)-BENZALDEHYDE

Table SI.1 (cont.): Species included in CACM Mechanism with chlorine chemistry extensions

RP15	2-FORMYL-ACETOPHENONE
RP16	GLYOXALIC ACID
RP17	4-HYDROXY-3,5-DIMETHYL-2,4-HEXADIENALIC ACID
RP18	2-METHYL-5-FORMYL-2,4-HEXADIENDIOIC ACID
RP19	2-(DIMETHYL-PROPENAL)-BENZOIC ACID
AP1	2-NITRATOMETHYL-6-METHYL-PHENOL
AP2	2-METHYL-2-HYDROXY-5-HEPTYLNITRATE
AP3	3-METHYL-4-HEPTYLNITRATE
AP4	1,2-DIMETHYL-3-METHYLNITRATO-BENZENE
AP5	4-METHYLNITRATO-BENZALDEHYDE
AP6	4-METHYLNITRATO BENZOIC ACID
AP7	1-METHYL-1-NITRATO-2,3-DIHYDROXY-4-ISOPROPYL-CYCLOHEXANE
AP8	1-METHYL-4-NITRATO-4-ISOPROPYL-5-HYDROXY-CYCLOHEXENE
AP9	5-ISOPROPYL-6-NITRATO-4-HEXEN-2-ONE
AP10	1-METHYL-2-METHYLNITRATO-NAPHTHALENE
AP11	8-HEXADECYLNITRATE
AP12	8-HYDROXY-11-HEXADECYLNITRATE
UR1	3-METHYL-HEPTANOIC ACID
UR2	3-HYDROXY-4-METHYL BENZOIC ACID
UR3	2-HYDROXY-3-ISOPROPYL-6-OXO-HEPTANOIC ACID
UR4	2-ISOPROPYL-5-OXO-HEXANAL
UR5	1-METHYL-3-HYDROXY-4-ISOPROPYL-1,2-CYCLOHEXANE EPOXIDE
UR6	2-HYDROXY-3-ISOPROPYL-6-METHYL-CYCLOHEXANONE
UR7	3,7-DIMETHYL-6-OXO-3-OCTENAL
UR8	3-ISOPROPYL-6-OXO-3-HEPTENOIC ACID
UR9	1-METHYL-4-ISOPROPYL-1,2CYCLO-4-HEXENE EPOXIDE
UR10	3-ISOPROPYL-6-METHYL-3-CYCLOHEXENONE
UR11	1,2-DIMETHYL-3-HYDROXY-NAPHTHALENE
UR12	1,2,3-TRIMETHYL-5-NITRO-BENZENE
UR13	3-n-PROPYL-4-NITRO-TOLUENE
UR14	2-NITRO-4-METHYL-BENZOIC ACID
UR15	1,2-DIMETHYL-3-NITRO-NAPHTHALENE
UR16	2-METHYL-2-HYDROXY-5-HEPTANONE
UR17	2-HYDROXY-3-ISOPROPYL-HEXADIAL
UR18	3-ISOPROPYL-2-PENTENDIAL
UR19	1-METHYL-2-FORMYL-NAPTHALENE
UR20	11-HYDROXY-8-HEXADECANONE
UR21	KETO-PROPANOIC ACID
UR22	2,6-DIMETHYL-3,4-DINITRO-PHENOL
UR23	3-ISOPROPYL-4-HYDROXY-2-BUTENOIC ACID
UR24	MALEIC ANHYDRIDE
UR25	3H-FURAN-2-ONE
UR26	4,5-DIMETHYL-6-OXO-2,4-HEPTADIENOIC ACID
UR27	2-CARBOXY-ACETOPHENONE
UR28	OXALIC ACID
UR29	4-HYDROXY-3,5-DIMETHYL-2,4-HEXADIENDIOIC ACID
UR30	2-METHYL-5-CARBOXY-2,4-HEXADIENDIOIC ACID
UR31	2-(DIMETHYL-PROPENOIC ACID)-BENZOIC ACID
UR32	3-METHYL-4-HEPTANONE
UR33	2-ISOPROPYL-5-OXO-2-HEXENAL
UR34	8-HEXADECANONE

Table SI.2: Gas-phase chlorine chemistry mechanism: rate constants are given $k = \mathbf{A}/T \times \exp(\mathbf{E/R}T)$ in ppm min^{-1}, where T is the ambient temperature in K.

Reaction			A	E/R	Reference	
HOCl + hv	→	OH + Cl				Photolysis
Cl_2 + hv	→	Cl + Cl				Photolysis
ClNO + hv	→	Cl + NO				Photolysis
$ClNO_2$ + hv	→	Cl + NO_2				Photolysis
$ClONO_2$ + hv	→	0.9 Cl + 0.9 NO_3 + 0.1 ClO + 0.1 NO_2				Photolysis
OClO + hv	→	ClO + $O(^3P)$				Photolysis
ClONO + hv	→	Cl + NO_2				Photolysis
HCOCl + hv + O_2	→	Cl + HO_2 + CO				Photolysis
Cl_2 + OH	→	Cl + HOCl	1.59×10^6	-1200	(*48*)	
Cl + OClO	→	ClO + ClO	1.41×10^7	700	(*48*)	
Cl + O_3	→	ClO + O_2	1.28×10^7	-260	(*48*)	
Cl + H_2 + O_2	→	HCl + HO_2	1.72×10^7	-2310	(*48*)	
Cl + H_2O_2	→	HCl + HO_2	4.85×10^6	-980	(*48*)	
Cl + HO_2	→	HCl + O_2	$7.93 \times 10_6$	170	(*48*)	
Cl + HO_2	→	ClO + OH	1.81×10^7	-450	(*48*)	
Cl + HOCl	→	Cl_2 + OH	1.10×10^6	-130	(*49*)	
ClO + O_3	→	Cl + 2 O_2	6.61		(*48*)	upper limit @ 298 K
ClO + O_3	→	OClO + O_2	0.44		(*48*)	upper limit @ 298 K
ClO + HO_2	→	HOCl + O_2	2.03×10^5	710	(*48*)	
ClO + ClO	→	Cl_2 + O_2	4.40×10^5	-1590	(*48*)	
ClO + ClO	→	Cl + Cl + O_2	1.32×10^7	-2450	(*48*)	
ClO + ClO	→	Cl + OClO	1.54×10^5	-1370	(*48*)	
ClO + OH	→	0.93 Cl + 0.93 HO_2 + 0.07 HCl + 0.07 O_2	3.39×10^6	270	(*48*)	
OClO + OH	→	HOCl + O_2	1.98×10^5	800	(*48*)	
HCl + OH	→	Cl + H_2O	7.93×10^5	-240	(*48*)	
HOCl + OH	→	ClO + H_2O	2.20×10^5		(*48*)	
ClO + SO_2	→	Cl + SO_3	1.76		Estimated	
Cl + ClNO + *M*	→	ClNO + M	function		(*49*)	
Cl + ClNO	→	Cl_2 + NO	2.55×10^7	100	(*49*)	
Cl + NO_2 + *M*	→	ClONO + M	function		(*49*)	
Cl + NO_2 + *M*	→	$ClNO_2$ + M	function		(*49*)	
Cl + NO_3	→	ClO + NO_2	1.06×10^7		(*48*)	
Cl + HNO_3	→	HCl + NO_3	88.1		(*48*)	upper limit @ 298 K
Cl + $ClONO_2$	→	Cl_2 + NO_3	2.86×10^6	135	(*48*)	
ClO + NO	→	Cl + NO_2	2.73×10^6	295	(*48*)	
ClO + NO_2 + *M*	→	$ClONO_2$ + M	function		(*49*)	
ClO + NO_3	→	0.74 Cl + NO_2 + 0.74 O_2 + 0.26 OClO	2.03×10^5		(*48*)	
HCl + NO_3	→	Cl + HNO_3	22.0		(*48*)	upper limit @ 298 K
$ClNO_2$ + OH	→	HOCl + NO_2	1.06×10^6	-1250	(*48*)	
OClO + NO	→	ClO + NO_2	1.50×10^5		(*48*)	
ClNO + OH	→	HOCl + NO	3.96×10^6	-1130	Estimated	
ClNO + OH	→	Cl + HONO	4.05×10^4	240	Estimated	

Table SI.2 (cont.): Gas-phase chlorine chemistry mechanism: rate constants are given $k = \mathbf{A}/T \times \exp(\mathbf{E/R}T)$ in ppm min^{-1}, where T is the ambient temperature in K.

Cl + CH_4	→	HCl + RO21 + RO2T	4.23×10^6	-1360	(*50*)	
Cl + ALKL	→	HCl + RO25 + RO2T	9.69×10^7		(*51*)	Using 2-dimethylbutane via SSR and Table 3 of (*51*)
Cl + ALKM	→	HCl + RO220 + RO2T	1.76×10^8		(*51*)	Using 3,5 dimethylheptane via SSR
Cl + ALKH	→	HCl + RO232 + RO2T	3.96×10^8		(*51*)	Using n-hexadecane via SSR
Cl + HCHO	→	HCl + HO_2 + CO	3.66×10^7		(*48*)	
Cl + ALD2	→	HCl + RO26 + RO2T	5.29×10^7		(*48*)	Using propanal (C_2H_5CHO) value (n-pentanal (*) not available/found)
Cl + MeOH	→	HCl + HCHO + HO_2	2.42×10^7		(*48*)	
Cl + EtOH	→	HCl + ALD2 + HO_2	3.96×10^7		(*48*)	
Cl + ALCH	→	HCl + RO22 + RO2T	6.61×10^7		(*48*)	Using n-propanol (n-C_3H_7OH) Value (2-hexanol value not available/found
Cl + MTBE	→	HCl + RO215 + RO2T	6.17×10^7		(*55*)	
Cl + MEK	→	HCl + RO27 + RO2T	3.08×10^7		(*56*)	Using 3-methyl-2-butanone Value (2-pentanone value not available/found)
Cl + KETO	→	HCl + RO216 + RO2T	4.85×10^7		(*56*)	Using 5-methyl-2-hexanone Value (2-heptanone value not available/found)
Cl + ETHE	→	CLRO21 + RO2T	1.72×10^6	966	(*54*)	Using value from (*54*) with Erratum
Cl + OLEL	→	CLRO22 + RO2T	1.76×10^7	745	(*54*)	Using 1-pentene value from (*54*) with Erratum
Cl + OLEH	→	CLRO23 + RO2T	1.76×10^7	745		Using same value as above (no higher alkene data found)
CLRO21 + NO	→	NO_2 + HCHO + CLRO24 + RO2T				Using same value as reaction 113 (RO22 + NO): (*24*)
CLRO21 + HO_2	→	OH + HCHO + CLRO24 + RO2T				Using same value as reaction 94: (*24*)
CLRO21 + RO2T	→	O_2 + HCHO + CLRO24 + RO2T + ALD2 + HO_2				Using same value as reaction 96: (*24*)
CLRO22 + NO	→	NO_2 + ALD2 + CLRO24 + RO2T				Using same value as reaction 113 (RO22 + NO) : (*24*)
CLRO22 + HO_2	→	OH + ALD2 + CLRO24 + RO2T				Using same value as reaction 94: (*24*)
CLRO22 + RO2T	→	O_2 + ALD2 + CLRO24 + RO2T + ALD2 + HO_2				Using same value as reaction 96: (*24*)
CLRO23 + NO	→	NO_2 + ALD2 + CLRO24 + RO2T				Using same value as reaction 170 (RO218 + NO) : (*24*)
CLRO23 + HO_2	→	OH + ALD2 + CLRO24 + RO2T				Using same value as reaction 94: (*24*)
CLRO23 + RO2T	→	O_2 + ALD2 + CLRO24 + RO2T + ALD2 + HO_2				Using same value as reaction 96: (*24*)
CLRO24 + NO	→	NO_2 + HCOCl + HO_2				Using same value as reaction 95: (*24*)
CLRO24 + HO_2	→	OH + HCOCl + HO_2				Using same value as reaction 94: (*24*)
CLRO24 + RO2T	→	O_2 + HCOCl + HO_2 + RO2T				Using same value as reaction 96: (*24*)
Cl + RO21	→	ClO + HCHO + HO_2	3.52×10^7		(*49*)	
Cl + RO21	→	HCl + CRIEG1	3.52×10^7		(*49*)	
Cl + RO25	→	HCl + CRIEG2	3.39×10^7		(*49*)	
Cl + RO25	→	ClO + ALD2 + HO_2	3.26×10^7		(*49*)	
ClO + RO21	→	Cl + HCHO + HO_2 + O_2	1.46×10^6	-115	(*49*)	
CRIEG1 + NO	→	HCHO + NO_2	3.08×10^6		Estimated	
CRIEG1 + NO_2	→	HCHO + NO_3	3.08×10^5		Estimated	
CRIEG1 + H_2O	→	ACID	1.76		Estimated	
CRIEG2 + SO_2	→	ALD2 + SO_3	3.08×10^4		Estimated	
CRIEG2 + NO	→	ALD2 + NO_2	3.08×10^6		Estimated	
CRIEG2 + NO_2	→	ALD2 + NO_3	3.08×10^5		Estimated	
CRIEG2 + H_2O	→	ACID	1.76		Estimated	
Cl + ISOP + *NO*	→	NO2 + 0.42 HCOCL + 0.21 MVK + 0.21 MCR + 0.58 HO_2 + 0.29 CLI1 + 0.29 CLI2	2.25×10^8		Estimated	Products: personal communication with Dr. Barbara J. Finlayson-Pitts
HNO_3 + hv	→	OH + NO_2				Photolysis

Table SI.3: Distribution of reactive chlorine species in the troposphere

Species		Source	% of tropospheric reactive chlorine*	Globally averaged concentration*	Approximate lifetime τ_{OH} **
CH_3Cl	methyl chloride (chloromethane)	Anthropogenic and natural	43%	540 ppt	~10 months
CH_3CCl_3	methyl chloroform (1,1,1 trichloroethane)	Mainly Anthropogenic	29%	120 ppt	~ 3 years
$CHCl_3$	chloroform (trichloromethane)	Mostly natural	4%	16 ppt	~ 4 months
CH_2Cl_2	methylene chloride (dichloromethane)	Mainly anthropogenic	3%	18 ppt	~ 2 months
C_2Cl_4	Perchloroethylene (Tetrachloroethene)	Mostly anthropogenic	2%	6 ppt	~ 3 months
Other organo-chlorine species			11%		
Sum of % total reactive chlorine			93%		

* Adapted from Khalil *et al.,* 1999

** $\tau_{OH:}$ Lifetime with respect to a typical diurnal average [OH] = 1×10^6 molecule cm^{-3} at 298 K and 1 atm.

Table SI.4: Summary of ozone metrics at 36 stations of the South Coast Air Basin of California (all values in units of ppb)

Monitoring Stations		Peak [O_3]	Δ Peak 1-hr [O_3]				Max Δ 1-hr [O_3]			
		Base Case	Case 1	Case 2	Case 3	Case 4	Case 1	Case 2	Case 3	Case 4
ANAH	Anaheim	65.9	2.6	3.6	87.2	253.8	3.6	4.2	87.2	270.0
AZUS	Azusa	93.6	2.2	3.0	96.3	498.0	2.7	3.5	117.4	532.1
BANN	Banning	352.0	2.1	2.2	52.7	-71.8	3.5	3.1	60.2	111.1
BURK	Burbank	127.0	3.8	3.5	83.0	267.7	4.7	4.4	85.5	302.2
CELA	Central LA	102.5	3.0	4.5	70.6	323.8	3.6	4.5	74.8	369.9
CLAR	Claremont	151.3	2.7	3.1	119.7	232.9	3.2	4.0	127.2	271.1
COST	Costa Mesa	116.3	3.5	2.1	10.4	39.0	4.5	5.3	21.4	103.3
CRES	Crestline	242.7	2.1	2.7	70.6	-1.7	2.7	3.0	70.6	99.3
ELRO	El Rio	40.0	0.0	0.0	0.0	0.0	0.3	0.1	1.2	0.0
FONT	Fontana	181.0	1.6	2.2	102.5	224.1	2.8	3.3	107.8	251.3
GLEN	Glendora	126.4	4.1	3.2	132.8	440.3	4.2	4.2	136.3	478.4
HAWT	Hawthorne	82.0	0.7	0.0	8.9	33.2	1.4	1.4	16.0	85.5
HEME	Hemet	353.3	2.2	2.3	40.6	-112.0	2.2	2.3	40.6	58.7
HESP	Hesperia	336.6	-0.5	0.9	3.5	-126.7	2.2	1.9	50.4	42.0
LAHB	La Habra	50.1	2.4	2.4	87.6	327.1	2.4	2.4	90.9	343.5
LGBH	North Long Beach	50.7	1.3	1.7	26.4	163.7	1.3	1.7	28.9	190.6
LSAL	Los Alamitos	82.5	2.2	3.5	58.1	230.4	2.7	4.4	58.1	268.6
LYNN	Lynwood	67.5	0.7	-1.2	23.5	181.3	0.8	1.2	35.5	207.9
NEWL	Newhall	134.8	1.5	1.7	102.3	113.7	1.6	1.7	102.3	158.0
NORC	Norco	195.7	2.8	2.9	64.8	99.3	3.4	3.5	107.7	161.5
PASA	Pasadena	55.0	2.1	2.9	105.1	484.4	4.9	5.2	113.8	484.7
PERI	Perris	307.1	3.0	2.9	65.1	-70.7	3.5	3.5	68.5	52.1
PICO	Pico Rivera	84.6	2.5	2.2	64.6	309.4	2.6	2.6	76.0	355.8
PIRU	Piru	95.1	1.1	1.3	69.8	87.4	2.1	2.4	72.6	99.9
PLSP	Palm Springs	205.7	3.3	3.1	85.0	48.2	3.3	3.1	85.0	140.9
POMA	Pomona	129.4	2.9	3.1	98.3	306.3	2.9	3.6	114.6	347.9
RDLD	Redlands	326.5	2.9	3.1	80.1	98.6	3.4	4.9	80.1	104.3
RESE	Reseda	118.8	3.3	3.1	89.2	159.5	3.3	3.2	92.4	203.0
RIVR	Riverside	285.9	2.5	2.3	74.8	38.3	2.6	2.6	97.6	115.6
SIMI	Simi Valley	82.2	2.0	2.1	76.6	165.5	2.8	2.5	88.7	181.2
SNBO	San Bernardino	313.7	3.4	3.3	88.9	86.9	3.4	3.3	90.1	136.0
THSO	Thousand Oaks	38.2	1.6	1.3	47.5	163.0	1.6	1.3	47.5	181.1
TORO	El Toro	166.3	4.0	3.1	46.1	166.9	7.7	7.4	57.1	232.9
UPLA	Upland	162.6	2.6	2.7	108.8	186.0	2.9	3.6	117.8	228.1
WHIT	Whittier	68.7	1.9	2.4	77.0	327.6	1.9	2.4	83.3	365.9
WSLA	West LA	81.1	3.2	3.2	23.1	85.3	3.2	3.6	23.1	127.8
	Station-wide*		2.2	2.3	53.3	238.3	7.7	7.4	136.3	532.1
	Domain		3.9	3.8	62.7	195.1	12.7	13.7	139.2	538.1
	Domain over 80 ppb						12.5	11.5	139.2	538.1
	Domain over 90 ppb						11.7	9.6	139.2	538.1
	Station-wide peak (location)	353.3 HEME	355.5 HEME	355.6 HEME	406.6 RDLD	591.6 AZUS				
	Domain peak	406.2	410.1	410.0	468.9	601.3				

Case Numbers – 1: Case Cl Chem; 2: Case Cl Chem & NO_3 Reaction; 3: Case [Cl_2] =150 ppt; 4: Case [Cl_2] =1500 ppt
All values correspond to ground-level model predictions for September 9, 1993.

* Δ 1-hr peak station-wide [O_3] (not necessarily same location) and maximum of 1-hr Δ [O_3] at any station at any time

Table SI.5: Comparison of several [OH], [Cl_2], and [Cl] metrics as predicted by the simulations

Maximum individual-cell 1-hr average concentrations/mixing ratios *

Species		Base	Case 1	Case 2	Case 3	Case 4
[OH]	molecule cm^{-3}	1.70×10^7	1.70×10^7	1.70×10^7	1.78×10^7	2.91×10^7
[Cl_2]	ppt		11.99	637.10	150.00	1500.00
[Cl]	molecule cm^{-3}		3.44×10^4	3.13×10^4	4.56×10^5	1.65×10^7

Maximum domain-averaged 1-hr average concentrations/mixing ratios **

Species		Base	Case 1	Case 2	Case 3	Case 4
[OH]	molecule cm^{-3}	5.58×10^6	5.62×10^6	5.63×10^6	7.25×10^6	1.02×10^7
[Cl_2]	ppt		1.45	74.74	150.00	1500.00
[Cl]	molecule cm^{-3}		1.94×10^3	1.79×10^3	6.74×10^4	1.75×10^6

Maximum individual-cell 24-hr average concentrations/mixing ratios ***

Species		Base	Case 1	Case 2	Case 3	Case 4
[OH]	molecule cm^{-3}	3.97×10^6	3.98×10^6	3.98×10^6	4.18×10^6	6.41×10^6
[Cl_2]	ppt		4.35	238.00	150.00	1500.00
[Cl]	molecule cm^{-3}		5.46×10^3	6.70×10^3	6.29×10^4	2.06×10^6

Domain-averaged 24-hr average concentrations/mixing ratios

Species		Base	Case 1	Case 2	Case 3	Case 4
[OH]	molecule cm^{-3}	1.51×10^6	1.53×10^6	1.53×10^6	1.95×10^6	3.01×10^6
[Cl_2]	ppt		0.68	27.35	150.00	1500.00
[Cl]	molecule cm^{-3}		3.82×10^2	4.25×10^2	1.82×10^4	4.23×10^5

Case Numbers – 1: Case Cl Chem; 2: Case Cl Chem & NO_3 Reaction; 3: Case [Cl_2] =150 ppt; 4: Case [Cl_2] =1500 ppt

All values correspond to ground-level model predictions for September 9, 1993.

* Values do not necessarily correspond to the same cell for this parameter or the same hour.

** Values do not necessarily correspond to the same hour.

*** Values do not necessarily correspond to the same cell.

Table SI.6: Comparison of additional [OH], [Cl_2], and [Cl] metrics as predicted by the simulations

Maximum individual cell 3-hr (6:00 AM – 9:00 AM) average concentrations*

Species		Base	Case 1	Case 2	Case 3	Case 4
[OH]	molecule cm^{-3}	4.41×10^6	4.38×10^6	4.41×10^6	5.00×10^6	1.09×10^7
[Cl_2]	ppt		11.75	592.30	150.00	1500.00
[Cl]	molecule cm^{-3}		3.44×10^4	3.13×10^4	4.97×10^4	1.19×10^6

Domain-averaged 3-hr (6:00 AM – 9:00 AM) average concentrations

Species		Base	Case 1	Case 2	Case 3	Case 4
[OH]	molecule cm^{-3}	8.45×10^5	8.68×10^5	8.70×10^5	1.05×10^6	2.05×10^6
[Cl_2]	ppt		0.39	16.68	150.00	1500.00
[Cl]	molecule cm^{-3}		1.05×10^3	1.24×10^3	9.87×10^3	1.03×10^5

Maximum individual-cell 8-hr (9:00 AM – 5:00 PM) average concentrations*

Species		Base	Case 1	Case 2	Case 3	Case 4
[OH]	molecule cm^{-3}	1.70×10^7	1.70×10^7	1.70×10^7	1.78×10^7	2.91×10^7
[Cl_2]	ppt		6.28	25.10	150.00	1500.00
[Cl]	molecule cm^{-3}		2.27×10^4	2.13×10^4	4.65×10^5	1.65×10^7

Domain-averaged 8-hr (9:00 AM – 5:00 PM) average concentrations

Species		Base	Case 1	Case 2	Case 3	Case 4
[OH]	molecule cm^{-3}	3.98×10^6	4.02×10^6	4.02×10^6	5.18×10^6	7.89×10^6
[Cl_2]	ppt		0.24	0.46	150.00	1500.00
[Cl]	molecule cm^{-3}		7.16×10^2	7.55×10^2	4.97×10^4	1.19×10^6

Case Numbers – 1: Case Cl Chem; 2: Case Cl Chem & NO_3 Reaction; 3: Case [Cl_2]=150 ppt; 4: Case [Cl_2]=1500 ppt

All values correspond to ground-level model predictions for September 9, 1993.

* Values do not necessarily correspond to the same cell.

Figure SI.1: Master domain of CIT Airshed Model (150 × 400 km)

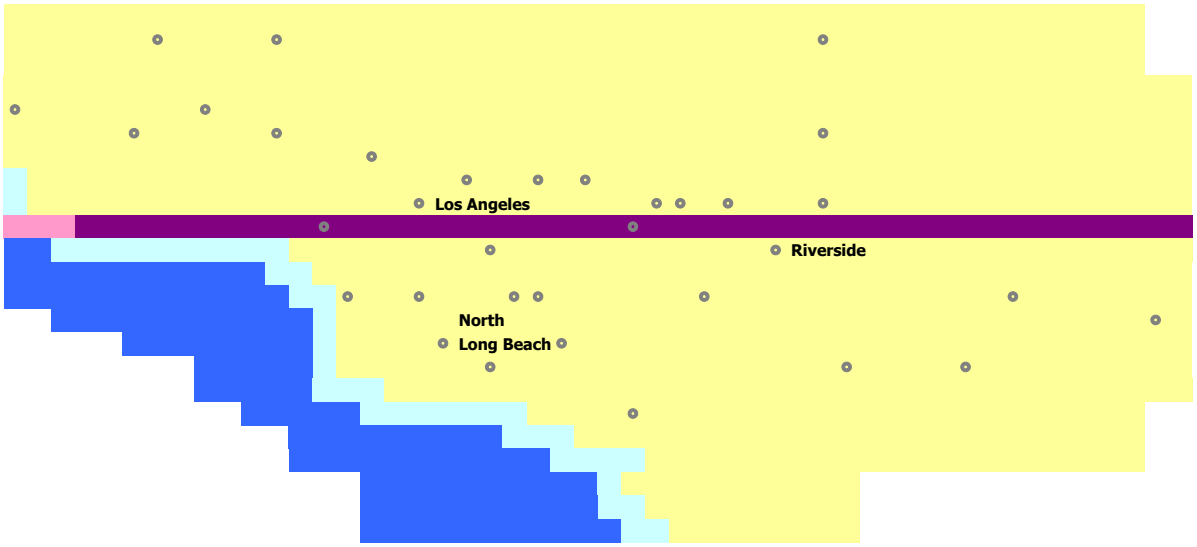

Figure SI.2: Computational domain of CIT Airshed Model (994/1150 cells within a 115 × 250 km subset of the master domain). Yellow, light blue and dark blue cells represent land, surf and open-ocean regions. Grey circles represent monitoring stations. The violet "strip" denotes a region used to show "slices" of contour plots in Figures SI.5 – SI.7.

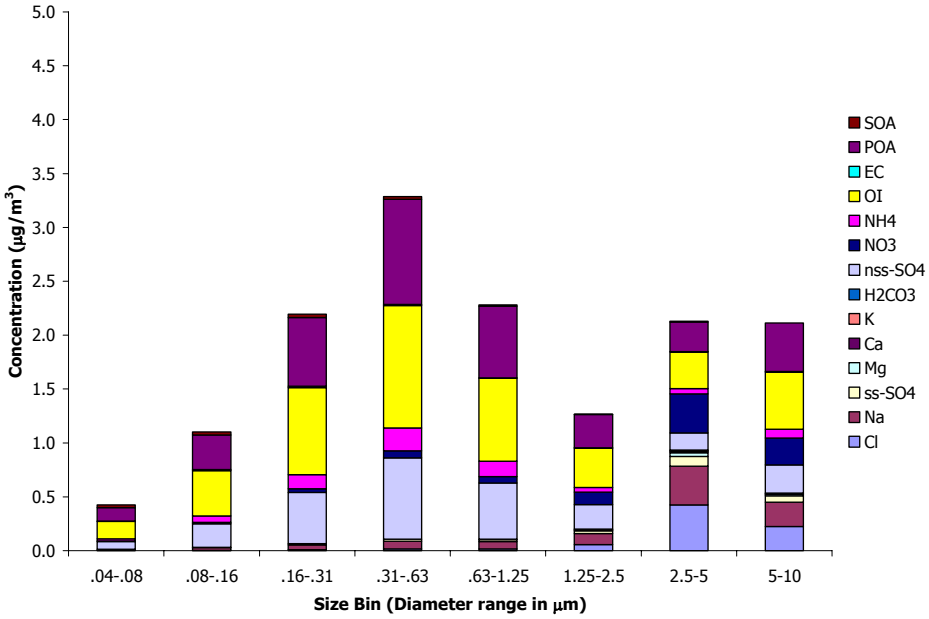

Figure SI.3: Typical model-predicted 24-hour-average open-ocean aerosol distribution for September 9, 1993

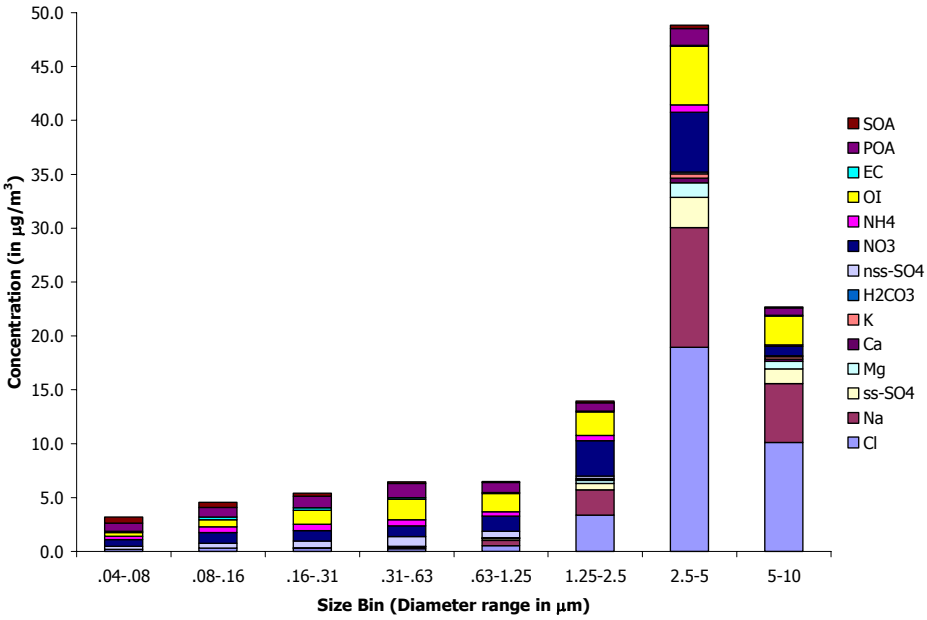

Figure SI.4: Typical model-predicted 24-hour-average coastal aerosol distribution for September 9, 1993

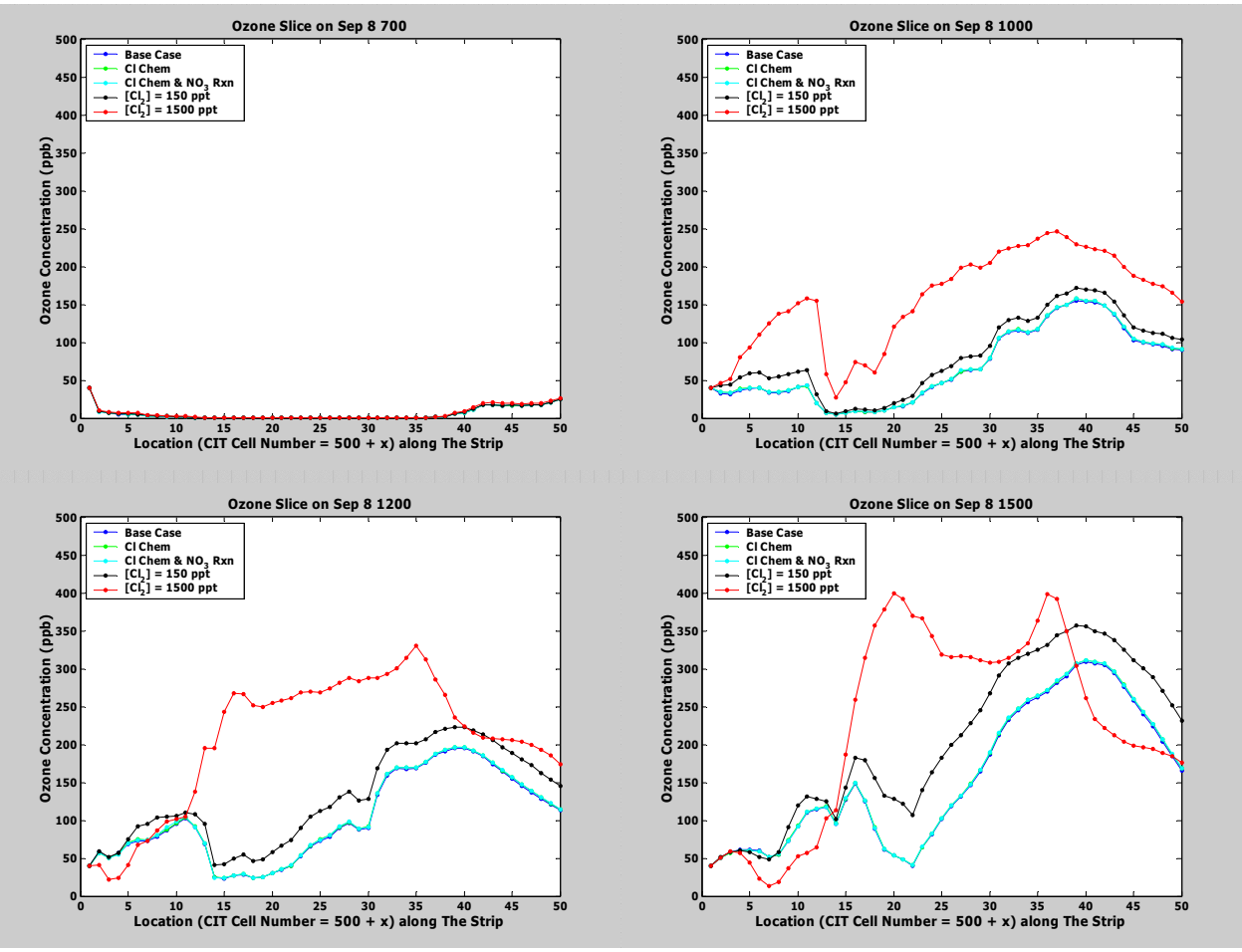

Figure SI.5: Model-predicted ozone contour slices for September 8, 1993 at 700, 1000, 1200 and 1500 hours (PST). Illustrated are cross-sections of ozone concentration contours (for each simulation in the study) along a strip of cells shown in Figure SI.2. The strip of cells begins in the western boundary of the domain in the Pacific Ocean in CIT Cell Number 500 and extends westward above the Santa Monica Mountains, passes through Central Los Angeles, continues towards Riverside and exits through the San Bernardino National Forest.

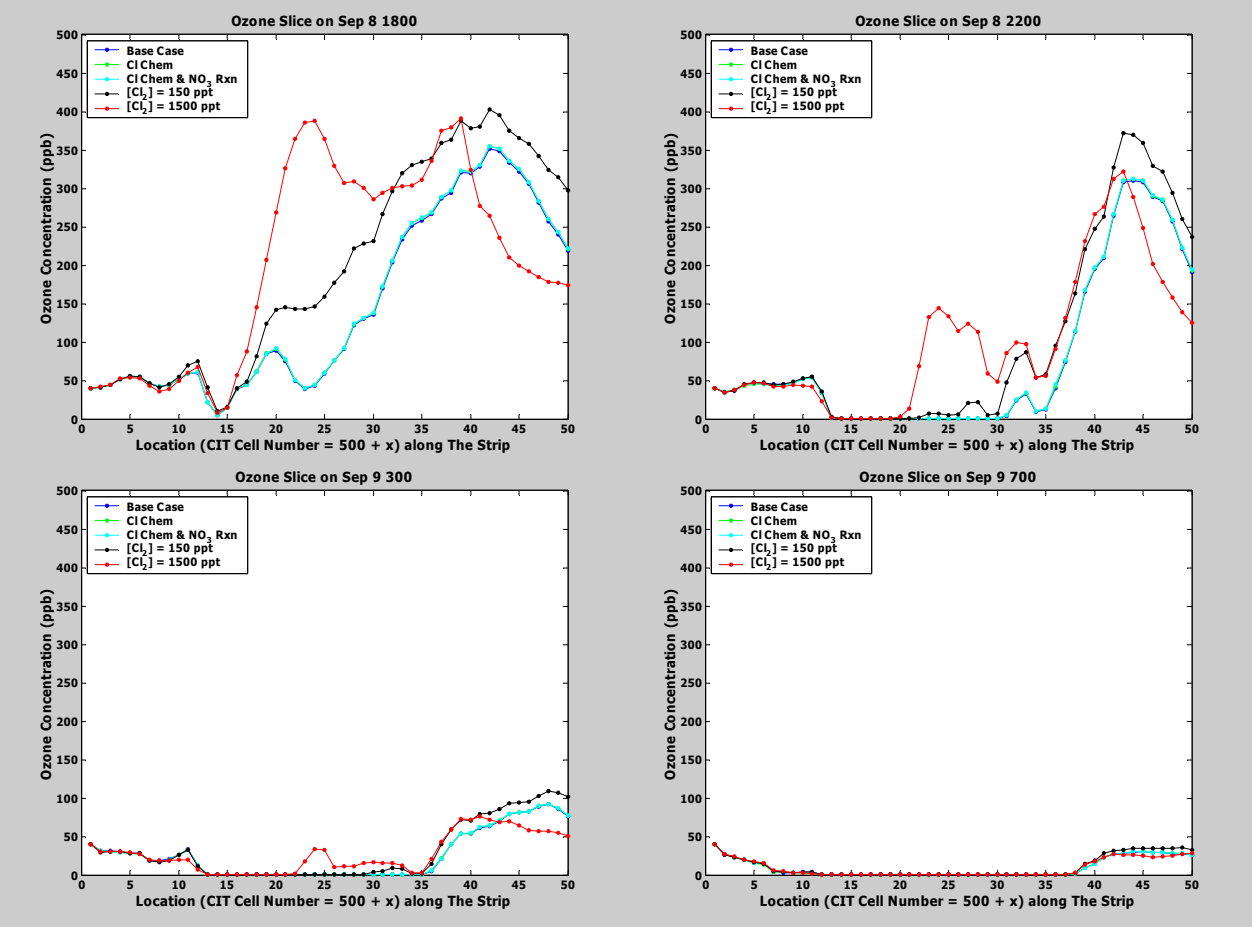

Figure SI.6: Model-predicted ozone contour slices for September 8, 1993 at 1800 and 2200 hours (PST) and for September 9, 1993 at 300 and 700 hours (PST). Illustrated are cross-sections of ozone concentration contours (for each simulation in the study) along a strip of cells shown in Figure SI.2. Geographical description can be found on caption of Figure SI.5.

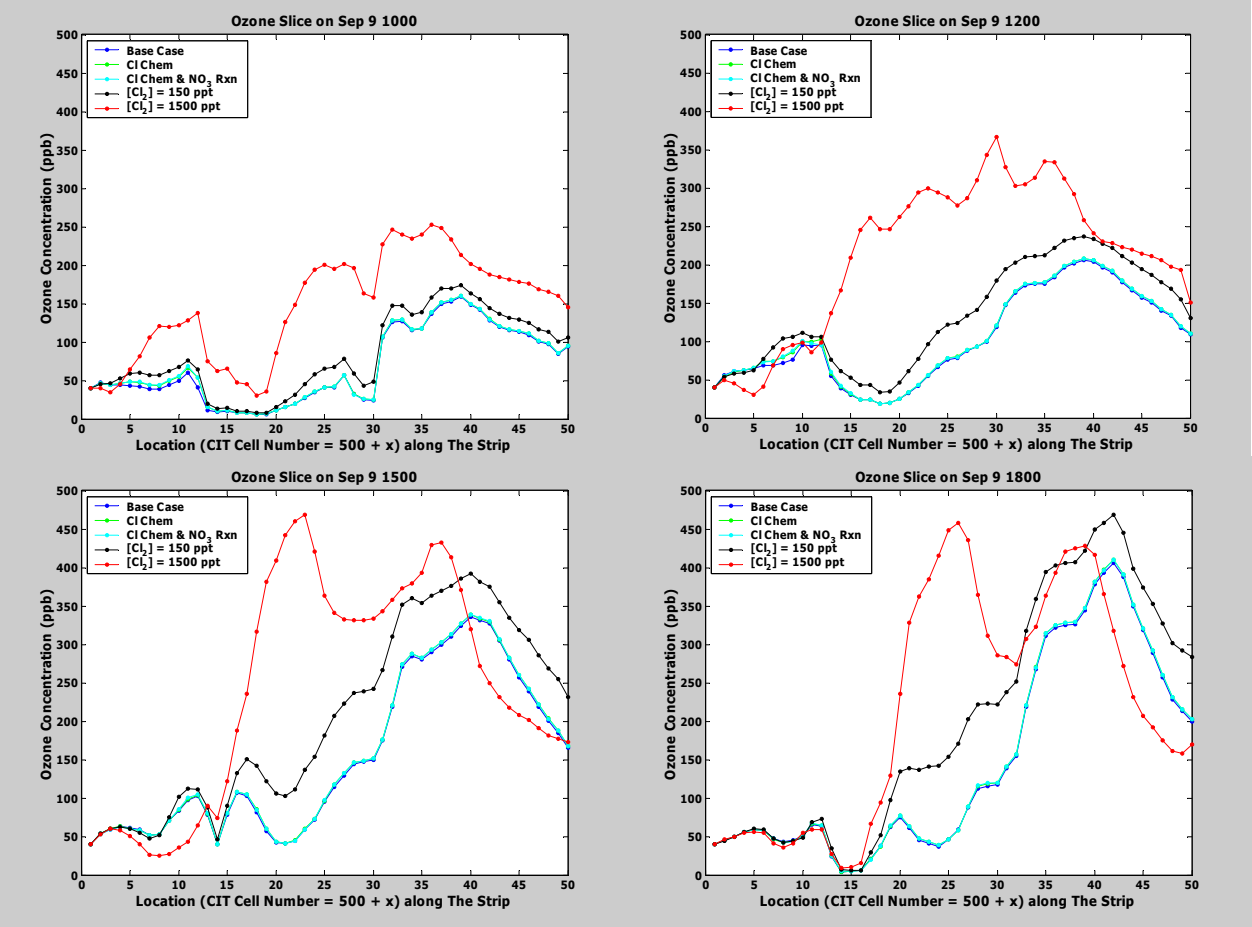

Figure SI.7: Model-predicted ozone contour slices for September 9, 1993 at 1000, 1200, 1500 and 1800 hours (PST). Illustrated are cross-sections of ozone concentration contours (for each simulation in the study) along a strip of cells shown in Figure SI.2. Geographical description can be found on caption of Figure SI.5.

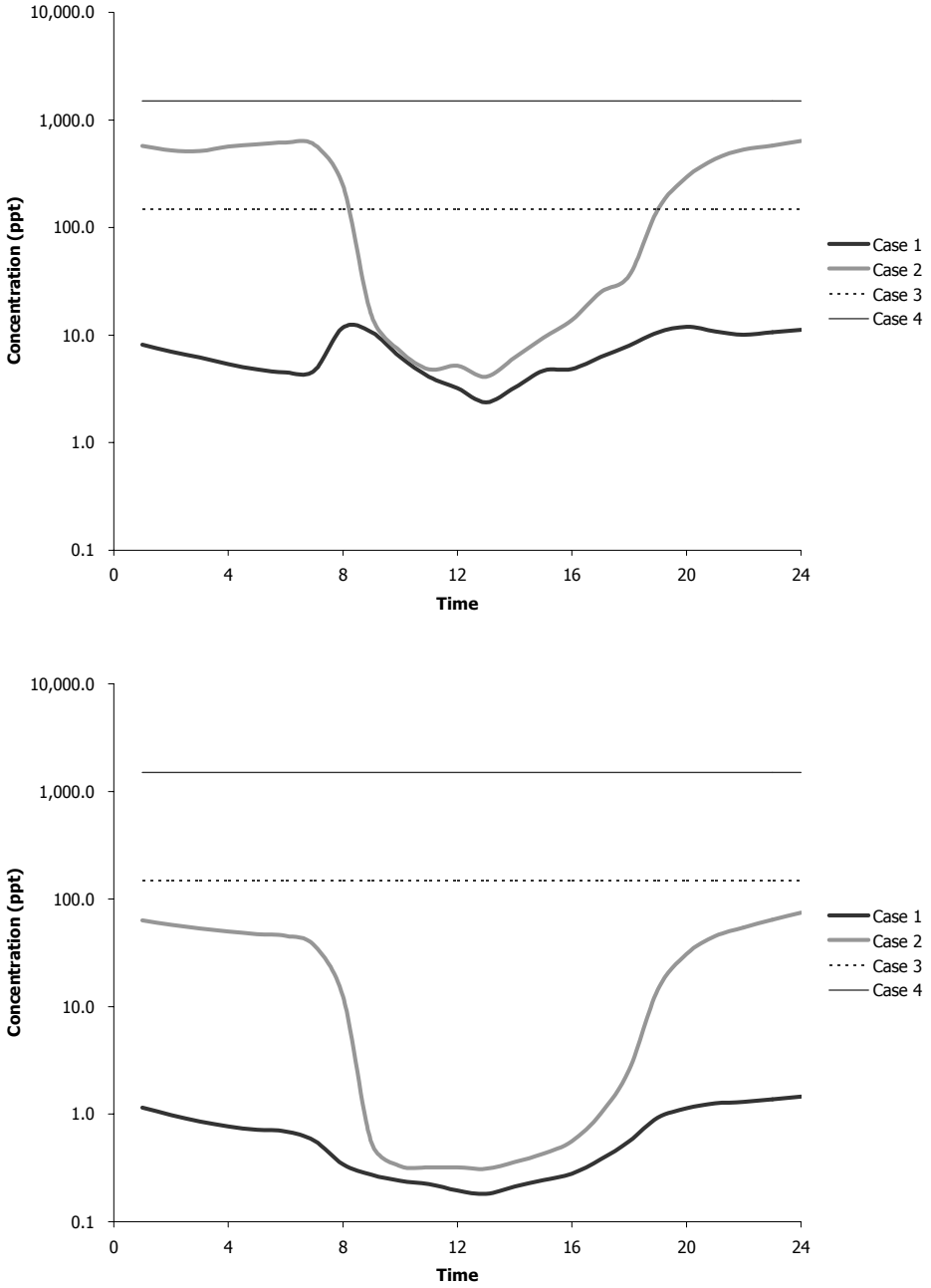

Figure SI.8: Model-predicted Cl_2 time series: (top) maximum ground-level individual-cell 1-hr average Cl_2 concentrations and (bottom) domain-averaged ground-level 1-hr average Cl_2 concentrations for September 9, 1993
Case Numbers – 1: Case Cl Chem; 2: Case Cl Chem & NO_3 Reaction; 3: Case $[Cl_2]$ =150 ppt; 4: Case $[Cl_2]$ =1500 ppt
** Values do not necessarily correspond to the same cell