

## SUPPORTING INFORMATION

### **An MCM modeling study of nitryl chloride (ClNO<sub>2</sub>) impacts on oxidation, ozone production and nitrogen oxide partitioning in polluted continental outflow**

**Theran P. Riedel<sup>1,2</sup>, Glenn M. Wolfe<sup>3,4</sup>, Kenten T. Danas<sup>2</sup>, Jessica B. Gilman<sup>5,6</sup>, William C. Kuster<sup>5,6</sup>, Daniel M. Bon<sup>5,6</sup>, Alexander Vlasenko<sup>7</sup>, Shao-Meng Li<sup>7</sup>, Eric J. Williams<sup>5,6</sup>, Brian M. Lerner<sup>5,6</sup>, Patrick R. Veres<sup>5,6</sup>, James M. Roberts<sup>5</sup>, John S. Holloway<sup>5</sup>, Barry Lefer<sup>9</sup>, Steven S. Brown<sup>5</sup>, Joel A. Thornton<sup>2</sup>**

(1) Department of Chemistry, University of Washington, Seattle, Washington, USA

(2) Department of Atmospheric Sciences, University of Washington, Seattle, Washington, USA

(3) Joint Center for Earth Systems Technology, University of Maryland Baltimore County, Baltimore, Maryland, USA

(4) Atmospheric Chemistry and Dynamics Laboratory, NASA Goddard Space Flight Center, Greenbelt, Maryland, USA

(5) NOAA Earth System Research Laboratory, Boulder, Colorado, USA

(6) Cooperative Institute for Research in Environmental Sciences, University of Colorado, Boulder, Colorado, USA

(7) Air Quality Research Division, Science and Technology Branch, Environment Canada, Canada

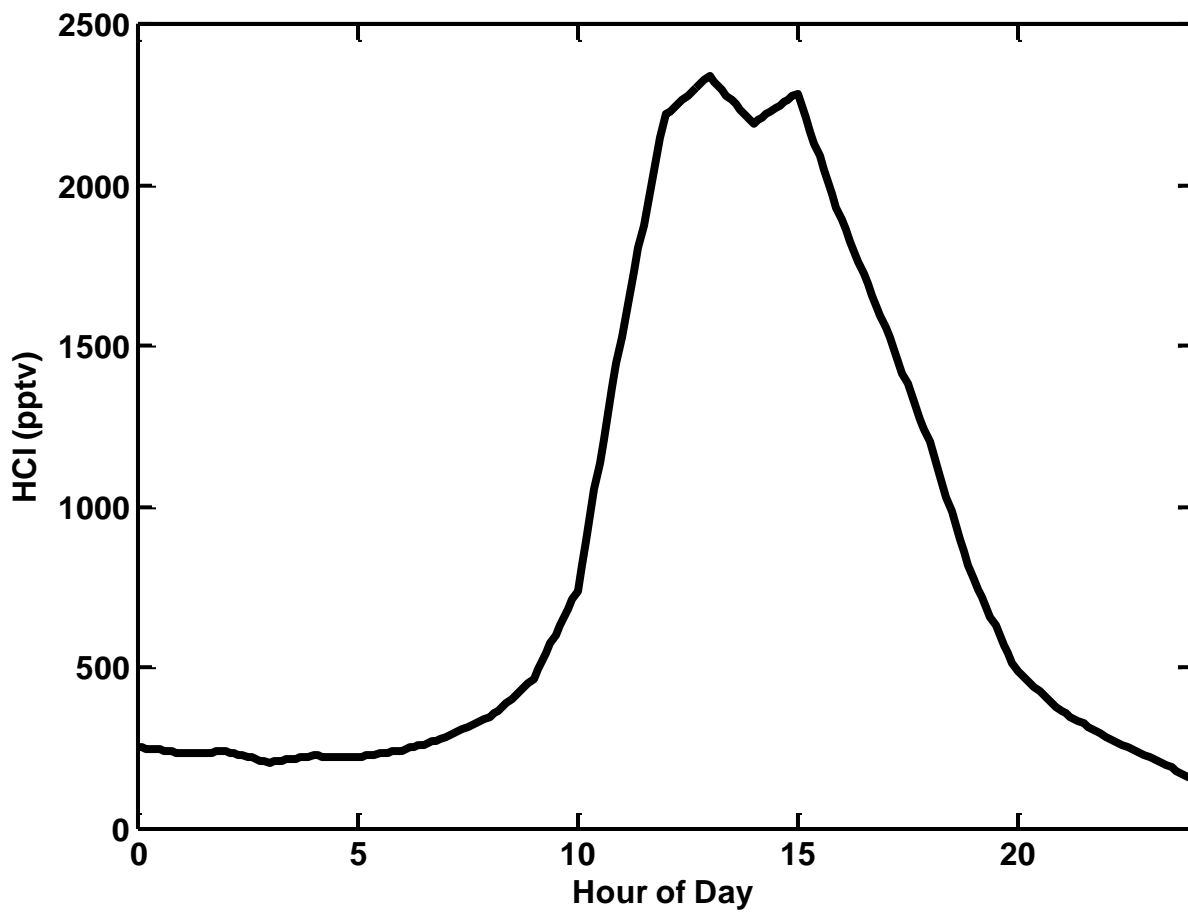
(8) Department of Chemistry and Biochemistry, University of Colorado, Boulder, Colorado, USA

(9) Department of Earth and Atmospheric Sciences, University of Houston, Houston, Texas, USA

## Supplemental Figures and Tables

Pasadena (GC-MS)	R/V Atlantis (GC-FID)	R/V Atlantis (PTR-ToF-MS)	median (pptv)	1 $\sigma$
methanol	methanol		1220	180
ethanol			1540	200
isopropanol			320	50
ethanal	ethanal		370	150
methacrolein			10	10
propanal			90	20
butanal			20	4
ethane			3120	440
propane		propane	1940	330
i-butane		i-butane	510	70
n-butane		n-butane	1200	190
i-pentane			780	100
n-pentane		n-pentane	350	40
hexane			250	30
nonane			40	2
decane			36	2
undecane			34	4
ethene		ethene	900	100
propene		propene	250	60
cis-2-butene			10	2
1-butene		1-butene	25	5
2-methylpropene			80	20
1,3-butadiene			44	17
trans-2-butene			33	7
ethyne		ethyne	320	40
propylbenzene			15	1
isopropylbenzene			5	1
benzaldehyde			40	8
benzene	benzene	benzene	65	5
ethylbenzene			25	2
o-methylethylbenzene			4	1
1,3,5-trimethylbenzene			10	3
phenylethene			14	2
1,2,4-trimethylbenzene			25	5
o-xylene			30	3
toluene	toluene	toluene	140	13
1,2,3-trimethylbenzene			8	2
methylvinylketone			16	25
acetone	acetone		740	260
methylethylketone			53	27
alphapinene			13	8
betapinene			8	4
limonene			9	7
isoprene			30	180

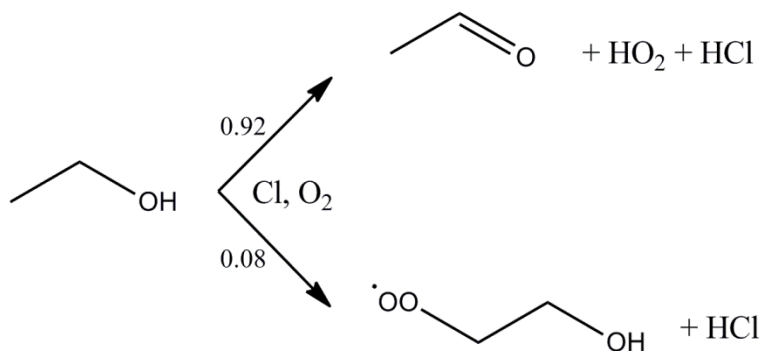
**Table S-1.** VOC measured during CalNex 2010 at the Pasadena, CA, ground site and aboard the R/V *Atlantis* and used as model constraints. Medians and standard deviations for the diurnal values used in the model are also given.



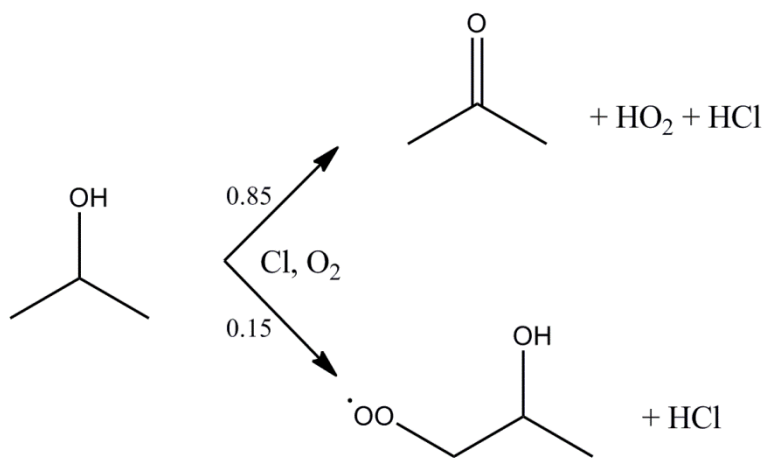
**Figure S-1.** Hydrochloric acid (HCl) diurnal profile used in the model.



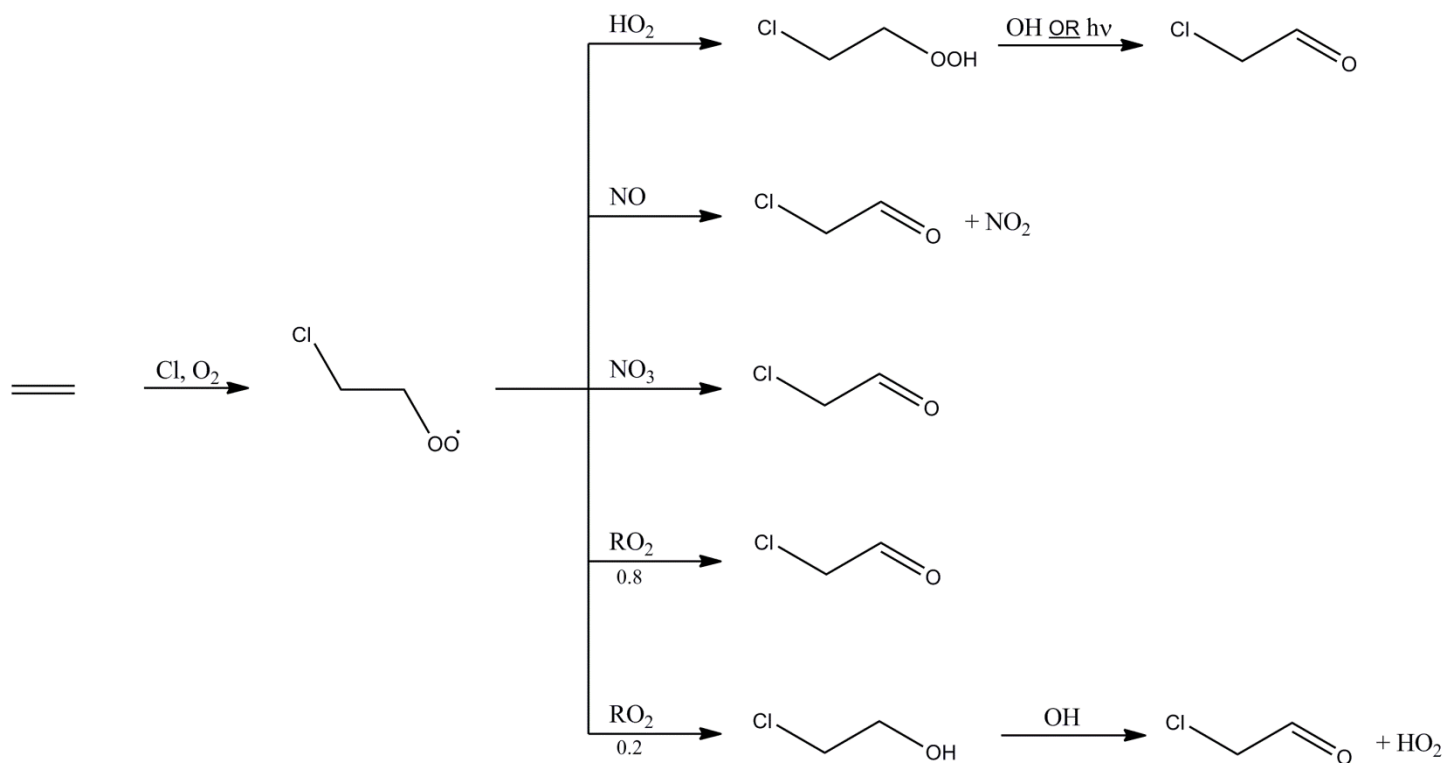
**Figure S-2.** Methanol oxidation mechanism by atomic chlorine added to the model reactions.



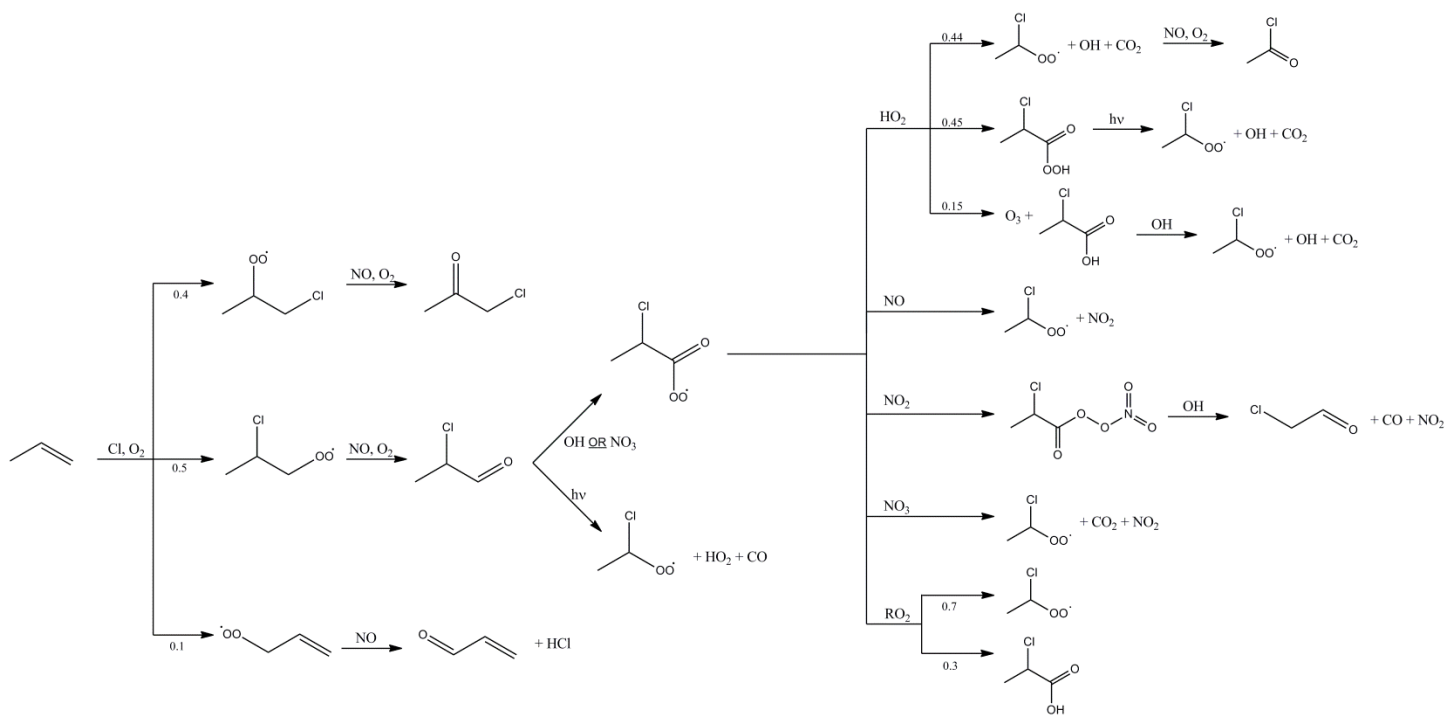
**Figure S-3.** Ethanol oxidation mechanism by atomic chlorine added to the model reactions.



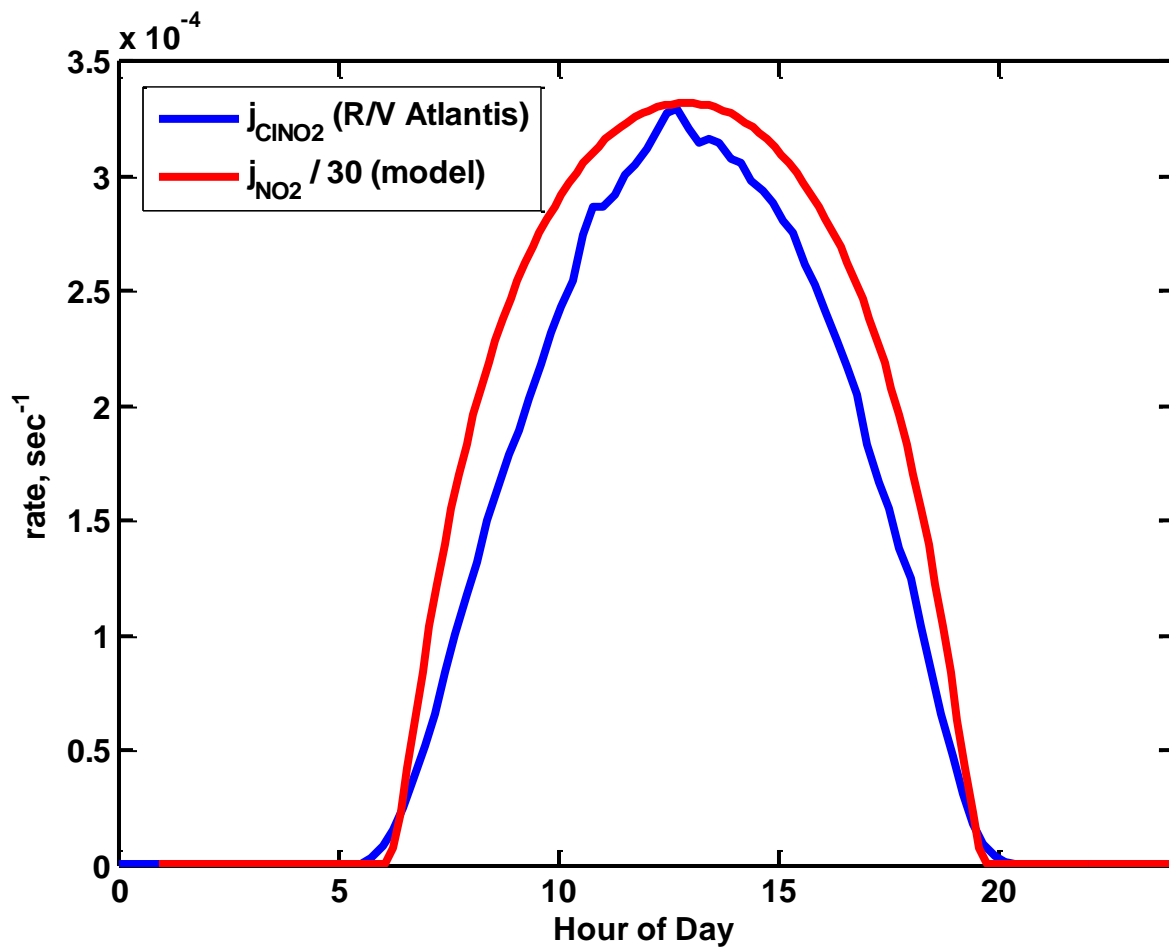
**Figure S-4.** Isopropanol oxidation mechanism by atomic chlorine added to the model reactions.



**Figure S-5.** Ethene oxidation mechanism by atomic chlorine added to the model reactions.



**Figure S-6.** Propene oxidation mechanism by atomic chlorine added to the model reactions.



**Figure S-7.** Photolysis frequency comparison between  $j_{\text{ClNO}_2}$  as measured aboard the R/V *Atlantis* and modeled clear sky  $j_{\text{NO}_2}/30$  which used in the model as a proxy for  $j_{\text{ClNO}_2}$ .

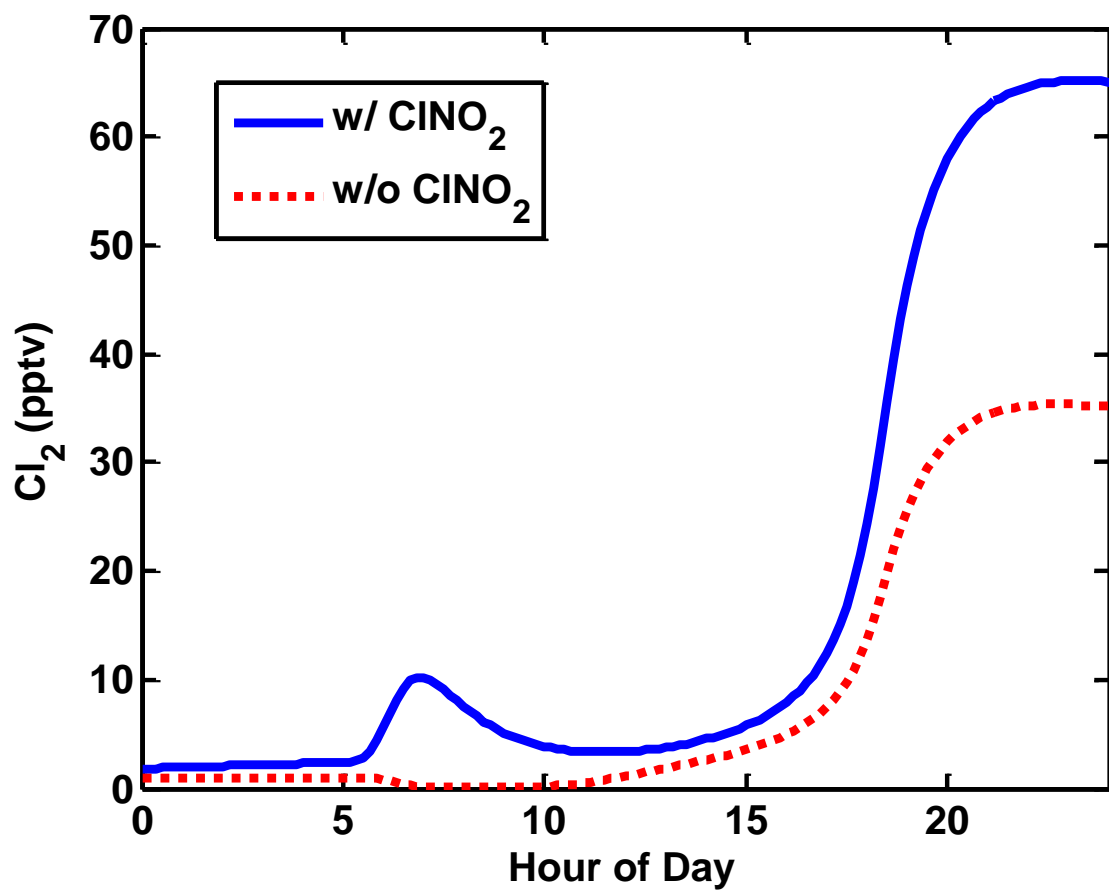
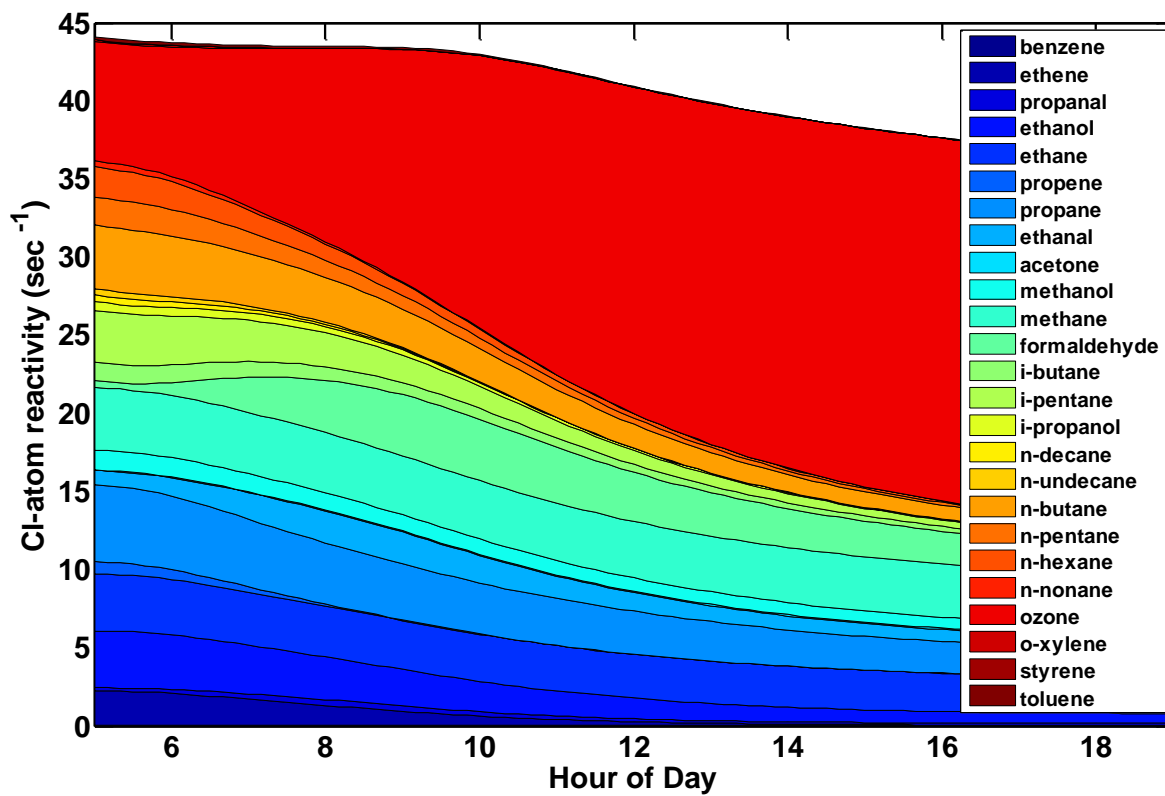


Figure S-8. Effects of  $\text{ClNO}_2$  on the molecular chlorine ( $\text{Cl}_2$ ) levels during a model run.



**Figure S-9.** Predicted Cl-atom reactivity over the course of a model day.