



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

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Nitryl chloride (ClNO<sub>2</sub>) is produced efficiently at night by reactions of dinitrogen pentoxide (N<sub>2</sub>O<sub>5</sub>) on chloride containing particles. Levels of ClNO<sub>2</sub> exceeding 1 ppbv have been measured in several field campaigns near polluted regions. ClNO<sub>2</sub> is photolyzed during the day to liberate highly reactive chlorine atoms. We have incorporated ClNO<sub>2</sub> production, photolysis, and subsequent chlorine atom reactions into a Master Chemical Mechanism (MCM version 3.2) model framework. Chlorine atom reactions with alkenes and alcohols, not presently part of the MCM, have also been added. Using observational constraints from the CalNex 2010 field study, we assess the dominant reactive sources and sinks of chlorine atoms over the course of a model day, and the impact of this radical source on HO<sub>x</sub> and NO<sub>x</sub> abundance and partitioning, VOC lifetimes, and ozone production. Relative to model runs excluding ClNO<sub>2</sub> formation, the presence of ClNO<sub>2</sub> increases OH, HO<sub>2</sub>, and RO<sub>2</sub> by a factor of 2 in the morning with a 10 - 20% perturbation to the total primary HO<sub>x</sub> production rate. Consistent with these changes, the formation of acyl peroxy nitrates is increased by 50% in the morning, and gross ozone production is enhanced by 10 - 20% (equivalent to about 12 ppb) compared to a model without ClNO<sub>2</sub> formation included. We also include a discussion of the impact of Cl-atom chemistry on VOC, and in particular, on possible chlorine-containing VOC oxidation products which might act both as tracers of Cl-atom chemistry and as Cl-atom sources via subsequent reaction with OH.