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Detailed photochemical simulation of Nitryl Chloride chemistry: impacts of temperature and emission profiles

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A detailed photochemical box model utilizing the near-explicit Master Chemical Mechanism was extended to simulate heterogenous $ClNO_2$ formation including condensed-phase reactions. The model has been validated against $ClNO_2$ observations in an urban and rural environment and is employed to: (1) Evaluate the impact of nitryl chloride ($ClNO_2$) chemistry on the formation of HO_x, and abundance of NO_x, O_3, and VOCs in a range of typical urban background environments; (2) Assess the influence of temperature variations upon the production and impact of $ClNO_2$ chemistry as this is of particular importance in future climate with potentially different global temperatures; and (3) Assess the impacts of potential changes in emission patterns to evaluate the interaction of this chemistry with changing source terms i.e. human behaviour. The simulations demonstrate that the formation of $ClNO_2$ enhances the production of OH, HO_2, $CH3O_2$, HNO_3, HCHO and O_3, and decreases the NO, NO_2, and H_2O_2 levels under typical mid-latitude continental boundary layer conditions. Moreover, the model shows that the production of $ClNO_2$ and its impact on air quality is highly sensitive to atmospheric temperature in all seasons.