



Implications of VOC Oxidation in Atmospheric Chemistry: Development of a Comprehensive AI Model for Predicting Reaction Rate Constants

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Abstract. Volatile Organic Compounds (VOCs) significantly influence global atmospheric chemistry through oxidative reactions with oxidants. These reactions produce key precursors to the formation of atmospheric fine particulate matter (PM_{2.5}) and ozone (O₃), which in turn play a crucial role in regulating O₃ pollution and reducing PM_{2.5} concentrations. With the increasing diversity of VOCs, the need for advanced modeling techniques to accurately estimate the atmospheric oxidation reaction rate constants (k_i , where $i \in \{•OH, •Cl, NO_3, \text{ or } O_3\}$) has become more urgent. Here we introduce Vreact, a Siamese message passing neural networks (MPNN) architecture that jointly models VOC–oxidant reactivity. The model simultaneously predicts $\log_{10}k_i$ values and achieves a mean squared error (MSE) of 0.299 and a coefficient of determination (R²) of 0.941 on the internal test set. This framework overcomes the single-oxidant constraint of traditional models, enabling unified and scalable prediction of VOC oxidation kinetics across multiple oxidants. An interactive web tool (<http://vreact.cn/wind.site:8001>) is provided to facilitate non-expert access to reactivity screening. Vreact offers valuable insights into the formation and evolution of atmospheric pollutants, and serves as a critical resource for developing effective control and emission strategies, ultimately supporting global efforts to mitigate air pollution and improve public health.

1 Introduction

The rapid advancement in data-driven methodologies has revolutionized various fields, such as protein structure prediction (Abramson et al., 2024), molecular generation (Zhang et al., 2023), organic reaction prediction (Burés and Larrosa, 2023), and bioinformatics (Theodoris et al., 2023). Environmental challenges, particularly those associated with atmospheric chemistry and climate change, have also benefited from these innovations. As pollutants evolve under both anthropogenic and natural influences, the understanding of their chemical and physical properties has become increasingly vital for addressing global air quality and climate issues. Volatile Organic Compounds (VOCs) are organic chemicals that readily

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