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Computational Modelling of PFAS destruction pathways

Reema Aroos, Gabriel da Silva

Department of Chemical Engineering, University of Melbourne, Victoria 3010, Australia

faroos@student.unimelb.edu.au

ABSTRACT

Per- and polyfluoroalkyl substances (PFAS) are widely used in a range of industrial applications, including non-stick coatings, paints, and aqueous film-forming foams (AFFF). Owing to their highly persistent nature, these compounds have increasingly emerged as environmental pollutants of significant concern. PFAS waste streams are destroyed through thermal processes, such as pyrolysis and incineration, although the mechanism of PFAS combustion and their breakdown products remains poorly understood. Herein we carry out simulations of premixed PFAS-doped flames, as well as isothermal Plug Flow Reactor (PFR) simulations, using a detailed chemical kinetic model for short chain perfluorocarboxylic and sulfonic acids. This work describes extension of our previously developed model from 1127 to 1445 reactions, to include C4 acids, as well as sodium and potassium perfluorocarboxylate salts, which break down to form a perfluoroalkene and NaF/KF – these reactions become relevant in treatment of PFAS ladden biosolids. The results from the simulation studies have shown that the breakdown of these species results in the generation of HFCs and fluorocarbon (FC) gases with high global warming potential (GWP), such as CHF_3, CF_4 and C_2F_6 . However, addition of alkali elements was observed to influence the breakdown of these FC gases. Perfluorinated carboxylate salts decomposed to Na and K atoms, which can then subsequently abstract F atoms from FCs like CF_4 and thereby aiding in their breakdown., Pyrolysis conditions were also found to favor the formation of HFC and FC gases, which can be attributed to a limited O/H radical pool arising from the absence of oxygen, compared to other treatment methods, and the presence of oxygen, or even water vapor, significantly suppresses the formation of these species. In addition, the influence of molecular structure was investigated by comparing different isomers. Specifically, reactions of both a linear form of perfluorobutanoic acid (PFBA) and a branched isomer (iso-PFBA) were incorporated into the kinetic model. Notable differences were observed between the two, with the branched isomer exhibiting significantly higher formation of C_2F_6 in the temperature range of 1000–1300 K under thermal oxidation conditions. These findings suggest that insights obtained from such simulation studies can contribute to the optimization of industrial PFAS destruction processes.

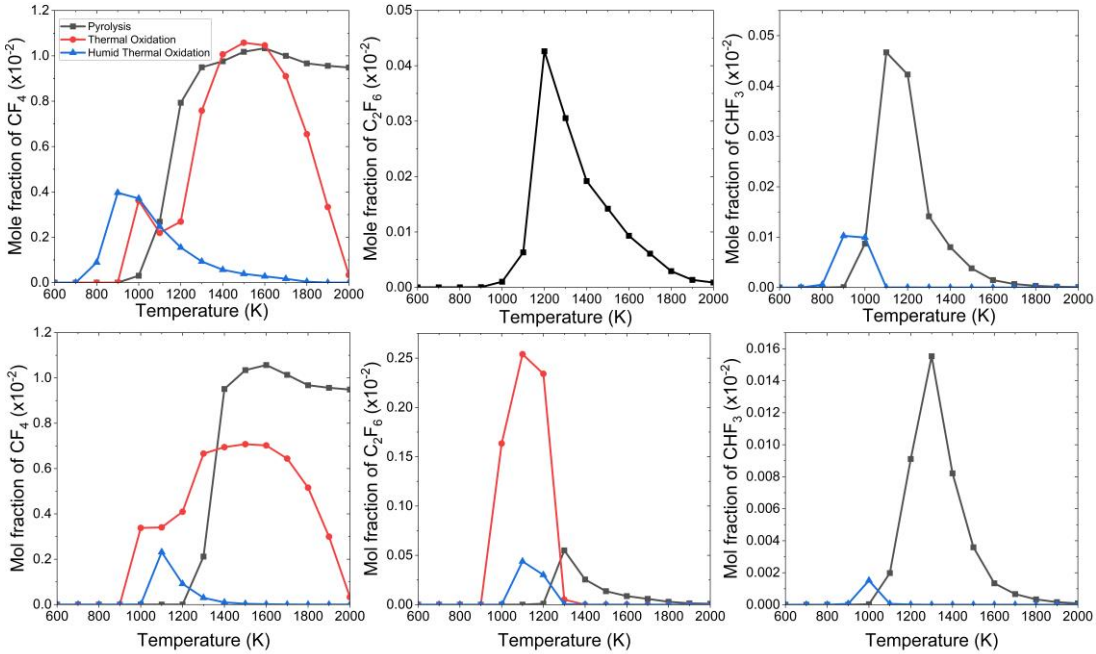

Figure 1 Mole fraction of persistent HFC and FC gases at various temperatures from PFBA (first row) and iso-PFBA (second row) pyrolysis, thermal oxidation (presence of oxygen), and humid thermal oxidation (presence of oxygen and water) at 600 – 2000 K. Mole fraction profiles are omitted in cases where they are always below 1×10^{-5}

KEY WORDS

Perfluoroalkyl substances, PFAS, kinetic modelling, combustion, incineration, pyrolysis

BIOGRAPHY

Ms Reema Aroos is a PhD student from the University of Melbourne researching on the thermal decomposition pathways of PFAS compounds, and aims to expand the existing kinetic models to include more subset of reactions in order to create a model that better reflects industrial processes. Previously, she worked in the petrochemical industry – first at Viva Energy and then at ConocoPhillips Australia as a chemist. She holds a Chemical Engineering degree from Monash University and also completed a masters of research (chemistry) at University of Melbourne – as a part of which she undertook her industrial placement at Qenos.

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