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Mitigating PFAS pollution: kinetic study of model compounds

Aim

The aim of this thesis is to investigate the thermal decomposition chemistry of PFAS compounds by means of computer-aided construction of microkinetic models

Justification

Per- and polyfluoroalkyl substances (PFAS) are a very large class of man-made chemicals that are characterized by carbon-fluorine bonds, which are amongst the strongest existing chemical bonds. PFAS They are found in everyday items such as food packaging, non-stick stain repellent, and waterproof products, including clothes and other products used by outdoor enthusiasts. PFAS are also widely used in industrial applications and for firefighting. However, PFAS can enter the environment during production, or through the wide variety of waste streams where they can end up. As they are persistent in the environment and the human body, safe and ultimate disposal is challenging. Selecting the appropriate method for ultimate disposal of PFAS is further complicated by the volatility of PFAS, their water solubility, environmental mobility, and persistence

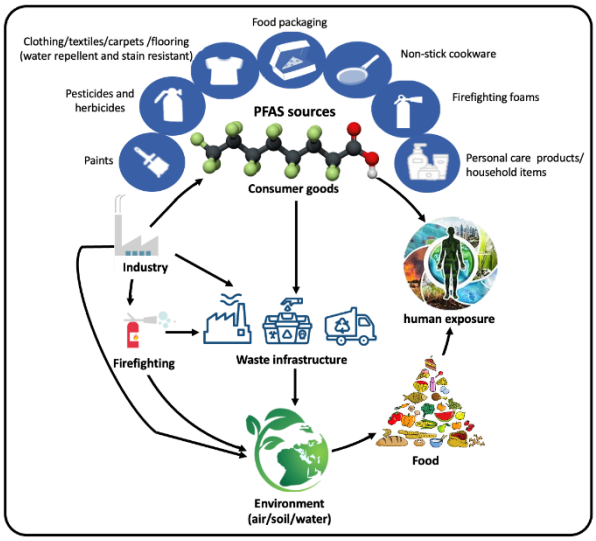

Figure 1: Exposure pathways of PFAS

Computer-aided model development for the disposal process could nowadays be feasible. Kinetic models of the pyrolysis of PFAS compounds can be studied with Genesys, an in-house automatic model generation framework. However, data on the thermochemistry and kinetics of PFAS are currently lacking. To fill this data gap, quantum chemistry calculations will be done, from which group additive values will be regressed. A microkinetic model for the pyrolysis of selected model compounds of PFAS will be constructed and validated against in-house data.

Program

- Literature survey on the destruction methods of PFAS and selected PFAS model compounds.
- Extension of databases with thermodynamic and kinetic parameters PFAS molecules obtained from quantum chemical calculations.
- Automatic construction of a microkinetic model with Genesys for selected PFAS model compounds.
- Performing simulations and validating the new kinetic models against in-house pyrolysis data.