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ע״ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar

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Experimental investigation and multiscale modeling of plastic pyrolysis with a neural network-inspired pyrolysis kinetic model and coarse grained DEM-CFD

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MSc Seminar

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Plastic is a versatile material that is widely used in industries, including construction, packaging, and the automotive industry. Pyrolysis is an efficient technology in the decomposition of plastic into gas, oil, and wax products at elevated temperatures under oxygen-limited or anoxic conditions. Understanding the pyrolysis kinetics and multiple-scale transport phenomena is crucial for optimizing the design and operation of fluidized bed pyrolyzers. In this work, both experimental investigation and multiscale modeling were conducted to study plastic pyrolysis in a fluidized bed reactor.

In the first work, a neural network-inspired pyrolysis kinetic model for high-density polyethylene (HDPE) was developed using experimental data obtained from thermogravimetric analyzer (TGA) and pyrolysis-GC-MS experiments. A coarse-grained discrete element method (DEM) -CFD fluidization model for sand-HDPE binary mixtures was developed and validated with fluidization experiments. Additionally, a multiscale model was developed for plastic pyrolysis in a fluidized bed reactor by integrating neural network-inspired kinetics, particle scale model, and coarse-grained DEM-CFD simulations. The validated model was applied for the analysis of particle mixing and segregation, axial distribution and residence time, Lacey mixing index, and pyrolysis products. This study provides experimental and theoretical foundations for designing multiphase fluidized bed reactors for HDPE thermochemical conversion.

In the second work, a kinetic model of secondary cracking of plastics at high temperatures was developed using a neural network-based method. A series of pyrolysis experiments of HDPE in a fluidized bed at different temperatures were also carried out. The kinetics obtained were coupled with CFD to develop a multiscale model in the open-source MFiX software, which was validated by segmented pressure drop, gas and liquid product yields. The simulations and experiments provided mutual confirmation that the yields of gas and C_5-C_{10} in HDPE pyrolysis increased with increasing temperature, while the yields of other products decreased. The simulation results were used to analyze the axial distribution and degree of mixing of particles inside the reactor. Relevant findings in this study provide important guidance for the development and optimization of HDPE pyrolysis reactors.