Modelling and Simulation of the HDPE Pyrolysis Process

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Abstract

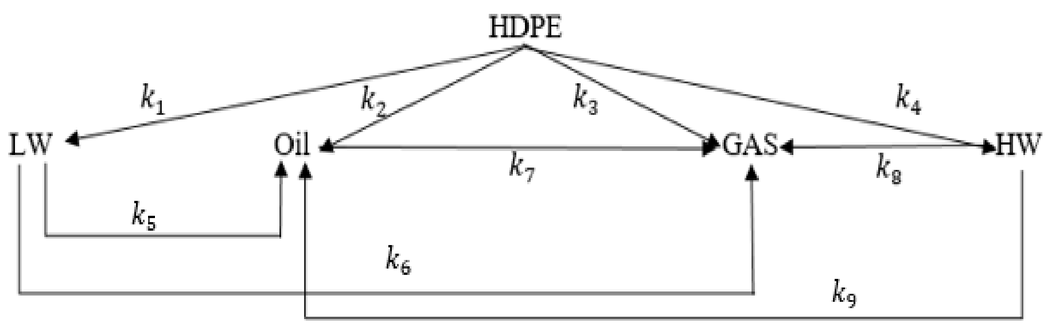
Pyrolysis is a thermochemical decomposition of organic compounds such as High-density polyethylene (HDPE) plastics. The product of the HDPE pyrolysis is usually diesel with other wastes (such as carbon black, etc.). A pyrolysis reaction is essentially a decomposition reaction performed at elevated temperatures in the absence of oxygen.

This work aims to describe some of the primary driving reactions in pyrolysis and to model and simulate the process . In pyrolysis, on a molecular level, there are many complex reactions taking place. To define all the reactions and include them in a model is a very expensive and time-consuming.

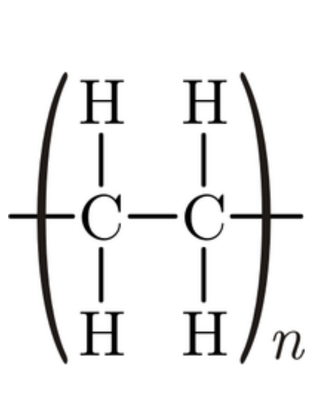
In this work, the reactions considered are limited to: $\beta-$scission, hydrogen abstraction and chain fission. To be able to simulate a chemical reaction, reaction equations are needed. These set of equations are available in the literature. We have solved them in MATLAB® using the in-built ordinary differential equation (ODE) solver. The solution represents the rate of the reaction and the product yield. The key to the solution are the reaction constants.

Overview of HDPE Pyrolysis

HDPE pellets into chamber → Add heat, pyrolysis starts → Outputs are oil, gas and carbon black



High-Density Polyethylene (HDPE)



Chemical formula

Molecular model

Branching structure

Pyrolysis Reaction Governing Equations

$$\frac{dP}{dt} = -k_1P - k_2P - k_3P - k_4P \quad (1)$$

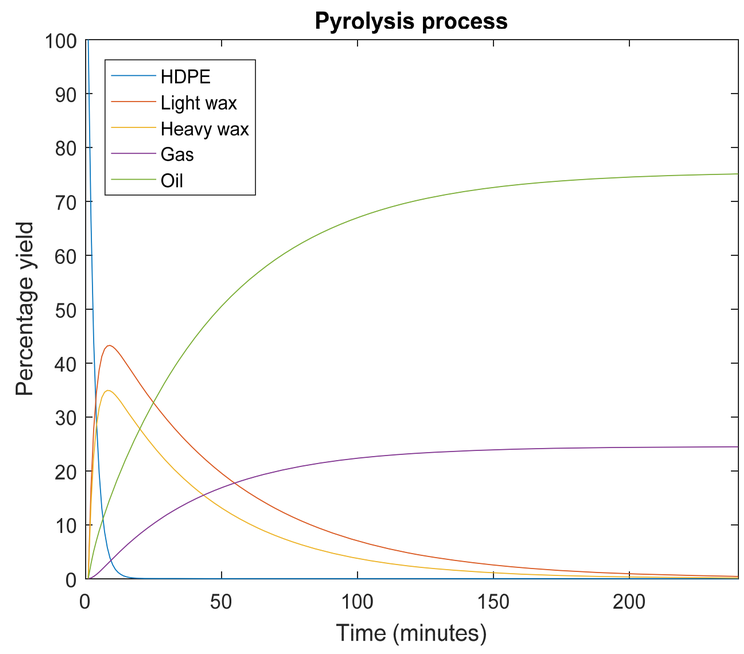
$$\frac{dHw}{dt} = k_4P - k_8Hw - k_9Hw \quad (2)$$

$$\frac{dLw}{dt} = k_1P - k_6Lw - k_5Lw \quad (3)$$

$$\frac{dOil}{dt} = k_2P + k_5Lw + k_9Hw - k_7Oil \quad (4)$$

$$\frac{dGas}{dt} = k_3\ P + k_6Lw + k_7Oil + k_8Hw \quad (5)$$

HDPE Pyrolysis Yield at 420°C



Conclusion

This obtained results obtained were found in good agreement with the literature. A key to model are the reaction constants $(k_1, k_2, \dots, k_8, k_9)$ which can be obtained by solving the pyrolysis reaction governing equations using MATLAB® ODE solver.

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