Kinetic Modeling of Industrial Plastic Pyrolysis

A.E. Lechleitner^{1*}, T. Schubert¹, M. Lehner¹, W. Hofer²

 Chair for Process Technology and Industrial Environmental Protection, Montanuniversitaet Leoben, Franz-Josef-Str. 18, 8700 Leoben, Austria
OMV Refining & Marketing GmbH, Mannswoerther Straße 28, 2320 Schwechat, Austria *corresponding author, andreas.lechleitner@unileoben.ac.at

1. Introduction and Short Description:

Recycling of wastes is one environmental concern of the EU policy to reduce greenhouse gases and substitute raw materials. For this purpose, a co-pyrolysis of polyolefins has been developed in previous works. The process uses a high boiling by-product of the refinery as carrier medium to insert the plastic into pipe reactors for thermal cracking. To investigate the complex reaction scheme of the co-pyrolysis lumped kinetic modeling (LKM) is used. The model will be used to scale up an existing pilot plant to a demo plant.

2. Methodology, Results and Discussion

An integral laboratory plant provides the data for the kinetic model. The plant consists of two serial electrical heated tubular reactors variable in length. The maximum length is 25 meters each. The process temperature can reach up to 500°C and pressures up to 15 bars at flow rates about three kilograms per hour. The feed consists of different types of plastic, such

as low-density polyethylene (LDPE) or polypropylene (PP), mixed with at least 80 wt.% carrier medium. Details of the laboratory plant are described in (Schubert et al. 2019).

The description of the educts and products occurs in lumps. Lumping groups species with similar properties, such as boiling cuts, and thus the reaction system is simplified. A lumped model for the copyrolysis is shown in Fig. 1. It consists of four lumps. Plastic is classified in the "Residue" lump by definition and the carrier medium is integrated in the "Residue" and the "Spindle oil" lump. The temperature dependence of the six pseudo first order reactions are described by the Arrhenius equation. As a result, twelve reaction parameters must be determined. Additionally, collective a reaction enthalpy is introduced, so 13 parameters are unknown. The Four Lump System generates four mass balances and one heat balance. which have to be solved simultaneously. this То solve underdetermined equation system the optimization toolbox from Matlab is used.



Fig.1: Four lump system with six possible irreversible, monomolecular, first order reactions



Fig.2: Scheme of the generation process of suitable initial point via total lumping



Fig.3: Measured and modeled products and temperature trends over reaction length of an exemplary test run of the pilot plant with 20% PP and 80% carrier medium

To overcome inappropriate starting point at the nonlinear fitting procedure, a total lumping algorithm generates suitable initial values (Fig. 2). (Lechleitner et al. 2019)

Furthermore, the model uses flow patterns to describe the flow regime and the heat transfer. This is necessary because of the two-phase flow in the reactors, which induces different flow velocities and therefore the flow regime has a significant influence on residence times and kinetics. Additionally, determining the heat transfer at different flow patterns is needed to set up the heat balance and identify the reaction enthalpy.

Figs. 3 and 4 present results for the test series of 20% polypropylene and 80% carrier medium.



Fig.4: Measured and modeled temperatures (squares) and mass fractions (circles) at the reactor outlet of test runs with 20% PP. The ideal line is at a 45° angle and the ± 5 kg/kg or $\pm 5^{\circ}$ C deviation is marked with dashed lines

The standardized mean squared error between measured and modeled temperatures and mass fractions is 0.773%. Hence the fit converges well.

3. Conclusion and Outlook

The existing model can describe the reactors of a novel process at different mixtures of plastics and carrier medium. The kinetic data computed are comparable to literature and fit to observation of other pilot plants.

However, the model will be improved with molar balances, more accurate species data and more experimental data. At the end the model should be linked with a simulation tool, such as PetroSim or HYSYS, to simulate the whole industrial demo plant.

References

Lechleitner, Andreas; Schubert, Teresa; Lehner, Markus; Hofer, Wolfgang (2019): Kinetic modeling of pyrolysis within the scope of industrial plastic feedstock recycling. In: 10th International Symposium on Feedstock Recycling of Polymeric Materials. Budapest, 26-29.05.2019, S. 31–33.

Schubert, Teresa; Lehner, Markus; Karner, Thomas; Hofer, Wolfgang; Lechleitner, Andreas (2019): Influence of reaction pressure on co-pyrolysis of LDPE and a heavy petroleum fraction. In: Fuel Processing Technology 193, S. 204–211. DOI: 10.1016/j.fuproc.2019.05.016.