SINGLE EVENT MICROKINETIC MODELING OF LIGNIN FAST PYROLYSIS: A STUDY ON ANISOLE AS MODEL COMPOUND

Sri Bala Gurugantu, Ruben De Bruycker, Hans-Heinrich Carstensen, Kevin M. Van Geem*, Guy B. Marin
Laboratory for Chemical Technology
Technologiepark 914, 9052 Ghent, Belgium
http://www.ict.UGent.be E-mail: Kevin.VanGeem@UGent.be

INTRODUCTION

Lignin pyrolysis chemistry: complicated due to its structure
- Involves formation of char, permanent gases and tars
- Tars produced from lignin can be classified:
  1. Primary: oxygenated aromatics
  2. Secondary: monosyclic aromatic hydrocarbons
  3. Tertiary: Polycyclic aromatic hydrocarbons

MECHANISM

In this study two mechanisms were adopted:
1. Nowakowska et al. formation of intermediates during anisole pyrolysis
   - Experiments: in a jet stirred reactor at 2s residence time and 0.01 mole% anisole in N₂
   - Consists of 1922 reactions and 303 species
   - Rate parameters derived using ab-initio, GA method and literature sources

EXPERIMENTAL DETAILS

- Experimental conditions:
  - Temperature: 525-675 °C
  - Residence time: 1s
  - Pressure: 1.3 bar
  - Anisole was fed at 20 mole % in N₂ atmosphere

- Experimental results show significant formation of PAHs.
- Phenol, benzene cresols and benzaldehyde were detected as the major products.
- Polycyclic aromatics like benzo[1,2-c:4,5-c]dibenzofuran, dibenzofuran and biphenyl with oxygenated side chains were also found in abundance.
- Formation of PAHs like Dibenzo furan is not predicted by the model of Nowakowska et al. while the mechanism by Ranzi et al. over predicts them.

RESULTS

- GC×GC at 575 °C
- GC×GC at 675 °C
- GC-GC-TID chromatogram of the anisole pyrolysis effluent for a residence time of 1s and isothermal operation at a temperature of 575 °C (top) and 675 °C (bottom)

- Reaction path analysis of anisole pyrolysis mechanism proposed by Nowakowska et al. (left) and Ranzi et al. (right) at 600 °C, 1.3 bar pressure and a residence time of 2s.

CONCLUSION

- New anisole pyrolysis data is obtained in flow reactor at low dilution conditions to focus on its bimolecular chemistry
- High yields of phenol, benzaldehyde and benzene observed, while cresol yields are surprisingly low.
- Anisole decomposition profiles were reasonably well predicted, however, more insights into the formation of cresols, benzene, PAHs are needed.

FUTURE WORK

- Repeat anisole pyrolysis in a quartz reactor
- Evaluation of potential wall effects
- Develop a detailed elementary-step kinetic model to improve predictions.

REFERENCES