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A numerical approach for displaying molecular composition profiles of species occurred during lignin devolatilization upon heating

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A numerical approach [1] is presented for displaying molecular compositions of primary products obtained from rapid pyrolysis of three types of lignin (enzymatic hydrolysis lignin, EHL; organic extracted lignin, OEL; and Klason lignin, KL) in an originally designed two-stage tubular reactor (TS-TR) at 773–1223 K. The heating rate of lignin particle in the TS-TR was estimated by solving the heat transfer equation. As show in Fig.1, the pyrolytic behavior of lignin and the formation of products during heating were computed using a detailed kinetic model consisting of over 90 species and around 400 reactions proposed by Hough et al. [2]. The computational yields of primary products were compared with experimental data for the critical evaluation. The predicted yields were generally in good agreement with the experimental results. The model also reproduced the varying product distributions among the three types of lignin, the char yield increased in the order of EHL < OEL < KL, whereas the tar yield decreased.

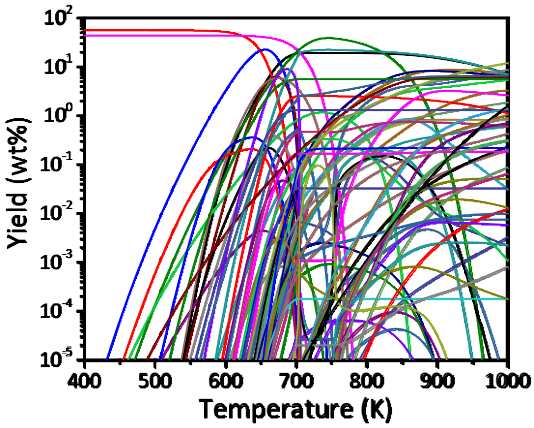

Fig. 1 All species profiles during the pyrolysis of a lignin at a heating rate of 1000 K/s computed by the detailed chemical kinetic model.

References

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