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A parallel reaction kinetic model based on probability density functions and its application in various biomass pyrolysis

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Publication date:
2019

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Citation for published version (APA):

Gu, T., & Yin, C. (2019). *A parallel reaction kinetic model based on probability density functions and its application in various biomass pyrolysis*. Poster presented at The 2nd International Symposium on Biomass/Wastes Energy and Environment (BEE2019), Tianjin, China.

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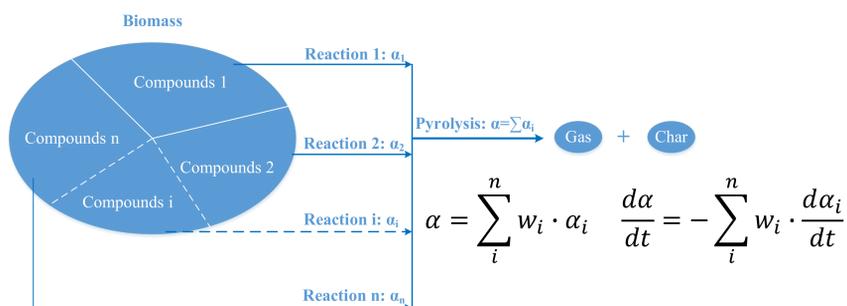


INTRODUCTION

- Pyrolysis, as the key stage of biomass thermochemical conversion technologies, plays a dominant role in bio-production.^[1]
- Developing a kinetic model of biomass decomposition or bio-production is crucial for optimization and reactor design.
- Recently Weibull distribution has been successfully utilized in the description of biomass pyrolysis, such as DAEM and Weibull mixture model.^[2]
- In this study, a novel kinetic model using Weibull distribution is developed with the assumption of several parallel reactions during biomass pyrolysis.
- The model is applied into various biomass: alpha cellulose, cardboard, and whitepaper, it provides another view of modeling biomass pyrolysis process.

MODELING DESCRIPTION

- The parallel reaction kinetic model assumes the pyrolysis progress of biomass is made up by several parallel reactions, each reaction corresponding to the decomposition of one compound, and all the reactions are independent of each other.^[3]



Where α is the overall conversion degree, w denotes the mass fraction, subscript i refers to the i -th reaction.

- The conversion degree of each reaction can be described via Weibull distribution:

$$\alpha_i = 1 - \exp\left[-\left(\frac{T - T_0}{\xi \eta_i}\right)^{\beta_i}\right] \quad \frac{d\alpha_i}{dt} = \frac{\beta_i}{\xi \eta_i} \left(\frac{T - T_0}{\xi \eta_i}\right)^{\beta_i - 1} \exp\left[-\left(\frac{T - T_0}{\xi \eta_i}\right)^{\beta_i}\right]$$

Where β , η are the shape, scalar parameters of Weibull distribution, T_0 and ξ are initial temperature and heating rate respectively, n indicates the number of the reactions.

- An improved differential evolution (DE) algorithm with constraint is implemented to estimate the Weibull parameters, the objective function to and the constraints are summarized below.

$$\text{Min: } \text{O.F} = \sum_{j=1}^N \left\{ [\alpha^{sim} - \alpha^{exp}]^2 + \lambda \times \left[\left(\frac{d\alpha}{dt}\right)^{sim} - \left(\frac{d\alpha}{dt}\right)^{exp} \right]^2 \right\}$$

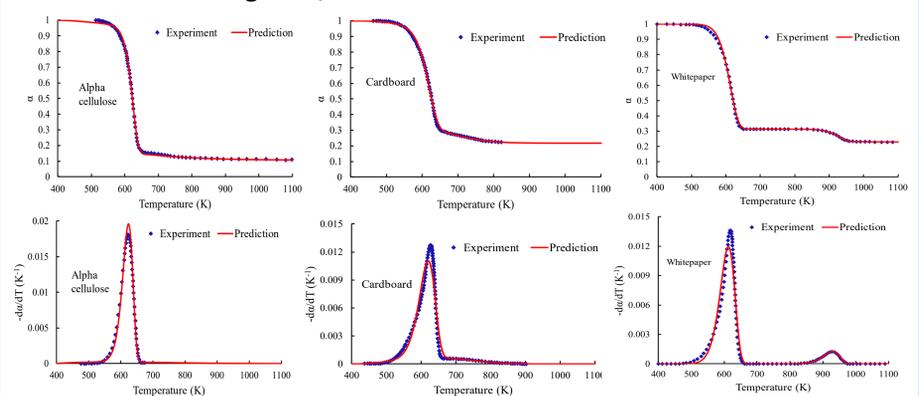
$$\text{s.t: } \begin{cases} 0 < w_i < 1, i = 1, 2, \dots, n \\ \sum_{i=1}^n w_i = 1 \end{cases}$$

Where λ is the scale coefficient, j refers to the experimental data points used, N is the total number of the used data points.

The improved DE algorithm is coded in MATLAB 2018b, with the assumption of 3 parallel reactions of biomass pyrolysis.

RESULTS & DISCUSSION

- The materials used are different type of lignocellulosic biomass: alpha cellulose, cardboard, and white paper.
- A simultaneous thermal analyzer (TA Instruments SDT Q600) was used to characterize the pyrolysis behavior of each of three biomass samples (3-7 mg per sample).
- In each experiment, the sample was heated from the initial temperature 323 K to the final temperature 1273 K with the constant heating 10 K/min. ^[4]



The prediction of the new model shows good agreements with TGA data of different types of biomass, all the Weibull parameters in the model are estimated out which represented in the table.

| Weibull parameters | Biomass samples | | | |
|--------------------|-----------------|-----------|------------|--------|
| | Cellulose | Cardboard | Whitepaper | |
| Reaction 1 | w | 0.09 | 0.17 | 0.08 |
| | η | 28.68 | 27.64 | 53.10 |
| Reaction 2 | β | 1.67 | 2.81 | 22.42 |
| | w | 0.80 | 0.61 | 0.69 |
| Reaction 3 | η | 22.48 | 22.22 | 21.50 |
| | β | 14.71 | 10.19 | 10.12 |
| | w | 0.11 | 0.22 | 0.23 |
| | η | 208.76 | 252.21 | 261.62 |
| | β | 12.79 | 28.31 | 3.51 |

- The DTG of alpha cellulose shows only one significant peak at ~ 620 K, corresponding to the only dominated reaction.
- The DTG curve of cardboard also shows one sharp peak at ~ 620 K, probably due to the high cellulosic content, another peak at ~ 620 K is not observed resulting from the lower weight fraction and the smaller scale parameter than those of the dominant reaction.
- While, whitepaper shows 2 peaks in the DTG curve at the temperature of ~ 620 K and ~ 930 K, respectively. The second peak is probably due to the higher lignin content or other additives in the whitepaper.
- The parameters of Reaction 3 are nothing but demonstrating the residue inside the biomass, as the significant shape parameters indicate the reaction rate to be zero.

CONCLUSION

- A novel kinetic model based on Weibull distribution has been developed with the assumption of parallel reactions scheme during pyrolysis.
- The predicted results are validated by experimental TGA data of the different types of biomass.
- The model shows another way for the description of biomass pyrolysis using Weibull distribution.

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