Change in size and apparent density of charcoal particles during heterogeneous reactions

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Highlights

- The model describes changes in size and density during char gasification
- Simple and predictive model is the main target of the model development
- Model validation by image analyses of single particle conversion in a flat flame burner

1. Introduction

Heterogeneous reactions with O_2, CO_2, and/or H_2O take place at the last stage of combustion and gasification of solid fuels. Due to the consumption of carbon, the particles decrease their apparent density and size, which in turn affect the apparent reactivity and the motion of the particles. Two extreme models, overall reactions and shrinking core models, do not represent the realistic conditions in industrial reactors, i.e. simultaneous change in size and density. Although it is possible to solve the phenomena numerically, high computational load is unfavorable for implementation in reactor models. Therefore, the effectiveness factor was modified to consider the change in particle size using threshold values for char conversion by Umeki et al. [1]. The model was successfully validated by experimental results with respect to conversion rate albeit with the help of fitting parameters. In this work, the model will be extended to predict the changes in size and apparent density of charcoal during heterogeneous reactions. The model will be validated by the change in the size of charcoal particle during the reaction in a flat flame burner (FFB).

2. Methods

2.1 Experimental method

Charcoal was prepared from pyrolysis of birch in a tubular reactor. A single particle of birch around 20-30 mm was heated from room temperature to 500 ˚C at the heating rate of 3 K min^{-1} under the flow of N_2. The char sample was then shaped to be a sphere with diameter of 1-3 mm. Gasification experiment of the char was conducted in a FFB represented in Figure 1a. During the test, premixed flame of CH_4/O_2-CO_2 mixture was fed to create well defined gas composition at the temperature of 1300-1700 K. A charcoal particle was inserted to high temperature zone and particle images were recorded by a CCD camera at 30 Hz. The particle temperature could be calculated based on the pyrometry principle. An example of particle images captured by the CCD camera is shown in Figure 1b.

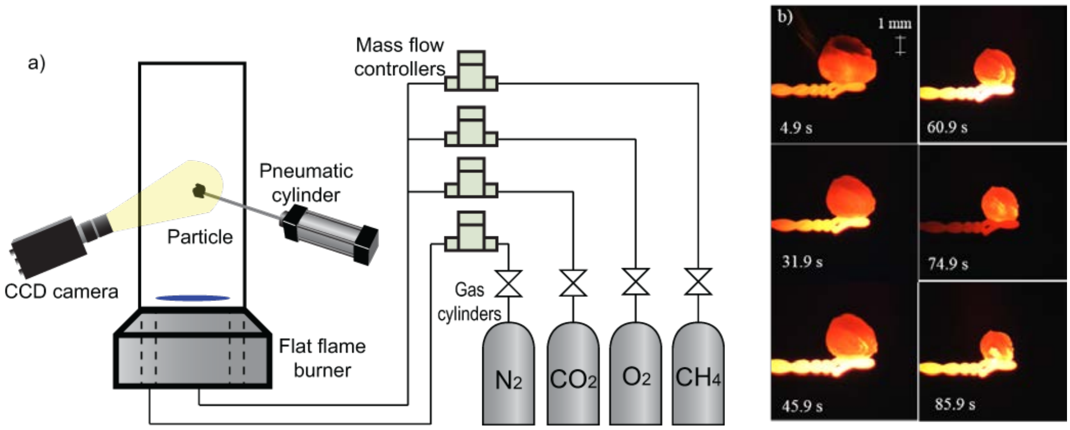

Figure 1. Experimental method a) Schematic diagram of the gasification experiment in FFB b) Example of particle images during conversion of birch char particle

2.2 Model development

The model was extended from the expression by Umeki et al. [1], which divided char conversion into 3 stages. First, the density of particles changes by uniform conversion without shrinking. When the overall conversion reaches to a certain value (X_1), the particle starts shrinking without density changes. After the overall conversion reaches to a certain value (X_2), particle density reduces uniformly with constant particle size until the end of reaction. The particle radius becomes a function of charcoal conversion as:

$$R_p = \begin{cases} R_{p,0} & (0 < X < X_1) \\ R_{p,0}\left(1 - \frac{X - X_1}{1 - X_1}\right)^{1/3} & (0 < X < X_1) \\ R_{p,0}\left(1 - \frac{X_2 - X_1}{1 - X_1}\right)^{1/3} & (0 < X < X_1) \end{cases} \quad (1)$$

Apparent density can also be expressed as a function of charcoal conversion:

$$\rho_p = \begin{cases} \rho_{p,0}\,(1 - X) & (0 < X < X_1) \\ \rho_{p,0}\,(1 - X_1) & (0 < X < X_1) \\ \rho_{p,f}\left(1 - \frac{1-X}{1-X_2}\right) + \rho_{p,0}\,(1 - X_1)\left(\frac{1-X}{1-X_2}\right) & (0 < X < X_1) \end{cases} \quad (2)$$

where subscription 0 and f are initial stage and final state, respectively.

3. Results and discussion

Preliminary results of the model are shown in Figure 2 with comparison to the numerical model from Haugen et al.[2]. Two models showed negligible difference during stage 1. During the stage 2, the current model showed faster reduction in radius than the numerical simulation. Density decreased in the numerical model during stage 2 while it was kept constant in the simple model. To adjust the deviation in size and density, the current model requires the 3rd stage. Further model development will focus on (1) simultaneous change in size and density during the stage 2, and (2) a method to predict threshold conversion, X_1, based on the effectiveness factor, with the help of information from numerical simulation.

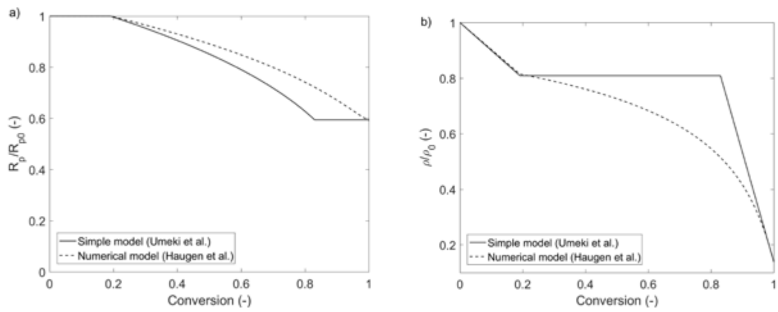

Figure 2. Comparison of the models for a) particle radius and b) apparent density. The model was calculated for the initial particle diameter of 30 µm and the reaction temperature of 1300 K.

4. Conclusions

A simple, predictive model describes the variation in particle size and apparent density of charcoal during gasification. From the preliminary results, the simple model behaved differently from the numerical model due to the model simplification. Furthermore, two fitting parameters are required. Therefore, the simple model will be further developed to be more accurate and predictive. In addition, experimental validation will be conducted with the size change of single particle in a flat flame burner.

References

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Keywords: Biomass gasification, apparent reaction rate