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Full Length Article

# Numerical simulations on the effect of potassium on the biomass fast pyrolysis in fluidized bed reactor

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## HIGHLIGHTS

- CFD model developed for fast pyrolysis of cellulose with potassium.
- Effect of potassium on the products yield and composition has been studied and analyzed.
- Effect of reactor temperature has been analyzed.
- Effect of unstable flow on the products yield has been studied.

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## ABSTRACT

In this study, the effect of potassium on the cellulose fast pyrolysis in a fluidized bed reactor has been studied using Computational Fluid Dynamics (CFD). A multiphase pyrolysis model of cellulose has been implemented by integrating the hydrodynamics of the fluidized bed with an adjusted cellulose pyrolysis mechanism that accounts for the effect of potassium. The model has been validated with the reported experimental data. The simulation results show that potassium concentration and reactor temperature have a significant effect on the yield and component of cellulose pyrolysis products. The product yields fluctuate is caused by the unstable flow in the fluidized bed. The result shows that the increased potassium concentration in the cellulose causes a significant increase of the gas and char yields and reduction in the bio-oil. Also, the dramatic composition variations in bio-oil and gas were observed due to the inhibition of fragmentation, and the depolymerization reaction of activated cellulose, and the catalysis of the depolymerization reaction of cellulose. It is also found that the increase in reactor temperature greatly enhances the endothermic pyrolysis reaction, which leads to the significant changes in the yield and composition of cellulose pyrolysis products.


## 1. Introduction

Fast pyrolysis is one of the most promising technologies for producing bio-oil, gas and char from biomass [1–3]. Fluidized bed reactor is widely used in biomass fast pyrolysis, as they have good temperature control and high heat transfer rates [3,4]. The thermochemical conversion of biomass in fluidized beds has been extensively investigated using both experimental and numerical methods in the literature [5–8].

Biomass usually contains considerable amounts of alkali and alkaline earth metallic species (AAEMs) such as sodium, potassium, calcium, etc. Many studies have reported that AAEMs play an important role in biomass pyrolysis reactions [9–15]. Shimada et al. [9] studied the effect of AAEMs on cellulose pyrolysis and found that potassium chloride and sodium chloride caused a reduced levoglucosan yield and increased the yield of water, carbon monoxide, and char. Patwardhan et al. [10] found that potassium chloride and sodium chloride led to a significant increase in the yield of low molecular weight species, while there was a severe reduction of the levoglucosan yield. Rutkowski [11] investigated the effects of potassium carbonate on cellulose pyrolysis. The results indicate that potassium carbonate influenced the decomposition temperature of cellulose and the composition of a pyrolysis product significantly. Hu et al. [12] investigated the effects of the inherent AAEMs on biomass pyrolysis. The results indicate that inherent AAEMs can enhance the production of carbon dioxide

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and hydrogen, and the decomposition of levoglucosan significantly.

Computational Fluid Dynamics (CFD) has been widely used for modeling of the hydrodynamics, heat transfer and chemical reactions inside the fluidized bed, and various CFD models for biomass pyrolysis process in fluidized bed have been developed that can be categorized into Euler–Lagrangian and Euler–Euler models. The Euler–Euler model could simulate the biomass pyrolysis in a fluidized bed reactor effectively. It includes the space-time evolution of pyrolysis products in a fluidized bed, the interaction between the sand, biomass and gases, and the effects of operating conditions on the yield and composition of pyrolysis products [16–23]. The Euler-Lagrangian model could simulate the pyrolysis of discrete biomass particle in a fluidized bed reactor accurately, but it needs huge computational cost [24–27].

There are several experimental studies on the effect of potassium on the cellulose fast pyrolysis. However, a numerical study has not been conducted and published so far. In this work, a model of cellulose fast pyrolysis in a fluidized bed based on the Eulerian multiphase flow framework has been developed. The spatial-temporal evolutions of products from cellulose fast pyrolysis in a fluidized bed are studied using CFD. The effects of potassium concentration and reactor temperature on the composition and yield of cellulose fast pyrolysis products are intensively investigated.

## 2. Model description

The sketch of the numerically simulated 300 g/h fluidized bed reactor of Aston University is shown in Fig. 1, and the specifications of the computational domain can be seen in Table 1 [28]. 2-D simulations are performed in the present work. The fluidization gas is preheated pure nitrogen, which flows from the bottom of the reactor at a velocity of 0.744 m/s. The biomass is injected from the beginning of the simulation at the side of the reactor. A constant biomass particle diameter of 0.6 mm is used in all simulations. The initial biomass is cellulose with potassium concentration varied from 0.0 wt.% to 1.0 wt.%.

## 3. Computational model

In order to accurately simulate the biomass pyrolysis in a fluidized bed reactor, the gas-solid flows are modeled using an Euler–Euler multiphase model, and the cellulose pyrolysis reactions are simulated using a detailed chemical kinetic model. These models were solved using the CFD software ANSYS Fluent 15.0.

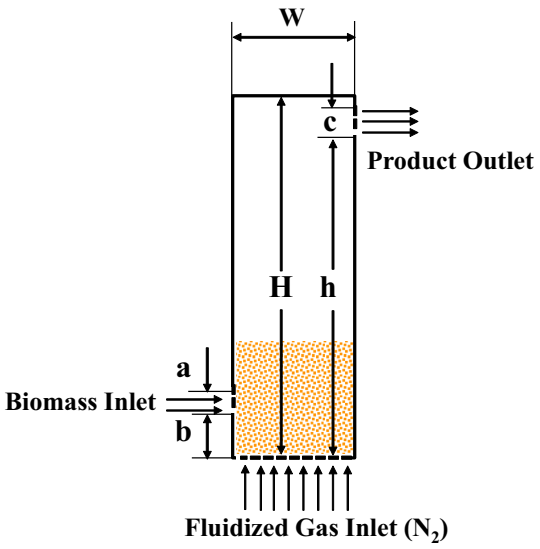


**Fig. 1.** Schematic diagram of the 2-D fluidized bed reactor.

**Table 1**
Specifications of the computational domain [28].

| | | | |
|---|---|---|---|
| Reactor height, H | 257 mm | Reactor width, W | 41 mm |
| Biomass inlet diameter, a | 14 mm | Biomass inlet height, b | 16 mm |
| Product outlet diameter, c | 7 mm | Product outlet height, h | 244 mm |

### 3.1. Multiphase flow governing equations

There are three phases in the fluidized bed reactor, i.e., gas phase, biomass particles and sand. The gas phase includes nitrogen as a fluidization gas and gas products from biomass fast pyrolysis. The biomass particle includes unreacted cellulose, activated cellulose which is an intermediate product of cellulose pyrolysis and char produced from biomass pyrolysis. In the Euler–Euler multiphase model, all the three phases are treated as interpenetrating continua. The gas phase is the primary phase and the solid phases, i.e., biomass particles and sand, are considered as secondary phases.

#### 3.1.1. Gas phase

The continuity equation for the gas phase is

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g) = \dot{m}_g \tag{1}$$

where $\vec{v}_g$ and $\rho_g$ are the velocity and density of gas, respectively, $\dot{m}_g$ is the mass transfer between phases and $\alpha_g$ is the gas volume fraction [29].

The species transport equation is

$$\frac{\partial}{\partial t}(\alpha_g \rho_g Y_k) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g Y_k) = \sum_{m=1}^{M} \dot{m}_{s_m,gk} \tag{2}$$

where $Y_k$ is the mass fraction of $k$th species, $\dot{m}_{s_m,gk}$ is the net mass exchange between the gas phase component $k$ and the solid phase $m$, and $M$ is the total number of solid phases [29].

The conservation of momentum for the gas phase is

$$\frac{\partial}{\partial t}(\alpha_g \rho_g \vec{v}_g) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g \vec{v}_g) = -\alpha_g \nabla p + \alpha_g \rho_g \vec{g} + \nabla \cdot \bar{\bar{\tau}}_g + \sum_{m=1}^{M} (K_{s_m g}(\vec{v}_{s_m} - \vec{v}_g) + \dot{m}_{s_m g} \vec{v}_{s_m}) \tag{3}$$

where $p$ is the pressure, $\vec{g}$ is the acceleration of gravity, $\bar{\bar{\tau}}_g$ is the gas phase stress-strain tensor, and $K_{s_m g}$ is the interphase momentum exchange coefficient between $m$th solid phase and gas phase.

Gas-solid exchange coefficient is given by Gidaspow [30]. Although Gidaspow drag model does not work well in the freeboard region of fluidized bed reactor, according to the previous studies reported in the literature [8,18], this model is suitable for simulating the biomass pyrolysis in the bubbling fluidized bed. The model equations are

when $\alpha_g > 0.8$, the exchange coefficient $K_{sg}$ is

$$K_{sg} = \frac{3}{4} C_D \frac{\alpha_s \alpha_g \rho_g |\vec{v}_s - \vec{v}_g|}{d_s} \alpha_g^{-2.65} \tag{4}$$

where

$$C_D = \frac{24}{\alpha_l Re_s}\left[1 + 0.15(\alpha_g Re_s)^{0.687}\right] \tag{5}$$