



Numerical investigation of the heterogeneous combustion processes of solid fuels



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HIGHLIGHTS

- Heterogeneous combustion processes of biomass in solid carbon phase are investigated.
- Combustion of pulverized coal in an axisymmetric burner is studied by an Euler–Lagrange approach.
- Combustion process is affected by the particulate size of solid fuels.
- Optimised parametric results are found for the chemical kinetic of NO_x prediction.
- Numerical predicted results show very good agreement with experiment.

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ABSTRACT

Two-phase computational modelling based on the Euler–Euler was developed to investigate the heterogeneous combustion processes of biomass, in the solid carbon phase, inside a newly designed combustion chamber (Model 1). A transient simulation was carried out for a small amount of carbon powder situated in a cup which was located at the centre of the combustion chamber. A heat source was provided to initiate the combustion with the air supplied by three injection nozzles. The results show that the combustion is sustained in the chamber, as evidenced by the flame temperature. An axisymmetric combustion model (Model 2) based on the Euler–Lagrange approach was formulated to model the combustion of pulverized coal. Three cases with three different char oxidation models are presented. The predicted results have good agreement with the available experimental data and showed that the combustion inside the reactor was affected by the particulate size. A number of simulations were carried out to find the best values of parameters suitable for predicting NO_x pollutants.

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1. Introduction

There is a gradual transition globally to carbon-neutral fuels to potentially reduce global warming and at the same time, dependency on traditional carbon-based fuels such as coal, oil and natural gases which are facing the risk of depletion. The supply of energy has been dominated by fossil fuels for decades and currently, almost 80% of the world's energy is produced from fossil based fuels [1]. Coal and biomass are widely used for producing energy among the solid fuels and pulverized combustion is one of the common combustion technologies which utilise them.

While coal is causing serious environmental pollution and carbon dioxide emissions, it is still one of the important resources meeting the demand for power generation and about 45% of the

global energy demands was met by coal in the past decade [2]. On the other hand, biomass is environmental friendly and renewable for its carbon dioxide neutrality when it is utilised for energy production. Only about 10% of the world's current energy consumption is met by biomass [1], but this is considered to be one of the vital renewable sources of energy along with others such as wind, solar, hydro and geothermal. The interest, however, in using of biomass fuels for energy production across the world has been growing rapidly and it is potentially one of the options to replace fossil fuels causing emissions of greenhouse gases [3]. Particularly, the interest in using biomass within the European Union (EU) has strongly increased with a target to produce at least 20% of energy from renewable sources by 2020 [4].

Chemical compositions and molecular structures in any carbonaceous fuel, such as coal or biomass, are very complex. The main elements present in biomass, determined by ultimate analyses, are usually carbon (C), hydrogen (H), oxygen (O) and nitrogen (N).

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Other elements also found include sulphur, chloride and other impurities.

Despite the general similarities between the pulverised combustion of coal and that of biomass, there is a difference between their chemical compositions. Biomass has significantly lower fractions of carbon, while its oxygen content exceeds that of coal. The hydrogen fraction is also somewhat higher than that of coal. The typical weight percentages for C, H and O, respectively are 30–60%, 5–6% and 30–45% [1]. For coal, the typical compositions (mass percentages) include 65–95% C, 2–7% H, up to 25% O and 1–2% N [5]. Moreover, there is also a difference between biomass and coal regarding their devolatilization. Compared to coal, biomass has a much higher amount of volatile matter leading to a dominating role of devolatilization in the overall conversion process of biomass particles. The volatiles fraction in biomass is usually 70–80%, whereas the fraction in coal is 10–50%. The high level of volatiles makes biomass a combustible fuel which means that it is easier to ignite even at low temperature. However, it has lower energy content due to the higher O/C and H/C atomic ratios when compared to coal. With anthracite less than 10% and bituminous from 5% to 6%, biomass fuels can lose up to 90% of their masses during the process of devolatilization [1]. The devolatilization of biomass and coal has been extensively investigated in [6–9].

In numerical simulations, most researchers for simplicity considered the combustion of solid fuels occurring in two individual steps. The first one is the combustion of volatiles and the second one is the combustion of char, neglecting the interaction between the two steps. But, for any two-phase flow, such as pulverized coal combustion, the interactions between the gaseous and solid phases needs to be taken into account because such a type of flow is characterised by non-linear coupling between the two phases such as gas turbulence influencing both the particle motion and heat up. This requires an accurate description of both the continuous gas phase and the dispersed particle phase. This may be studied by using the Euler–Lagrange or Euler–Euler modelling approaches and it is crucial for practical application of prediction of solid fuels combustion for different technologies.

Pulverized combustion is characterised by small volume fraction of the dispersed particle phase and as a result, in this study, the former approach was used to model the pulverized coal combustion in Model 2, whereas the latter one was applied in Model 1.

Several models adopted Lagrangian approach in treating the particle phase when modelling pulverized coal combustion [10–12]. Concerning the biomass combustion, the Lagrangian approach was used by Fletcher et al. [13] to simulate the flow and reactions inside an entrained biomass gasifier and the numerical results showed the capability of the Lagrangian model to optimise the design of such gasifiers. Another study regarding the modelling of pulverized wood combustion was carried out in which the Lagrangian manner was also adopted [14]. Additionally, several recent studies successfully used the Euler–Euler approach in modelling wood gasification in a fluidised bed reactor [15], dispersed two-phase flow in pulverized coal combustion [16] and coal gasification in a fluidized bed reactor [17].

Furthermore, combustion of solid fuels such as coal and biomass influences the environment mainly through emissions of nitrogen oxides (NO_x) to atmosphere. These emissions are associated with a variety of environmental concerns such as the formation of acid rain and photochemical smog in urban air. In a combustion system, including pulverized combustion, the formation and destruction of NO_x emissions are influenced by several factors such as fuel properties and, combustion conditions e.g. temperature of reaction and the fuel–air ratio [18]. Nitrogen from combustion of solid fuels with air is then converted to pollutants: nitric oxide (NO), nitrogen dioxide (NO_2), nitrous oxide (N_2O), ammonia (NH_3) and hydrocyanide (HCN). NO_x oxides include

mostly NO and much lower concentration of NO_2 and N_2O . So, NO_x modelling is particularly focussed on the prediction of NO concentration in the reactive field of interest. However, in combustion systems of solid fuels without considering the nitrogen contained in fuels (fuel-N), NO_x emissions formed at high temperatures from nitrogen of the combustion air, can be limited by combustion engineering measures to allowable values. On the other hand, when using nitrogenous fuels and low combustion temperatures, the formation of NO_x is mainly due to the conversion of fuel-N, partially or totally into nitrogen oxides [19].

The overall aim of this study is to provide a deeper understanding on the process of heterogeneous combustion of solid fuels by applying computational fluid dynamics techniques. In particular, the objectives include the following:

- To study the interactions between the gas and solid phases of fuels during the combustion process.
- To develop a combustion model that takes into account the different gas–solid behaviours, heat transfer and thermal conversion processes, by using multiphase modelling.
- To investigate the formation of nitric oxide (NO) during combustion.

2. Combustion mechanisms and heterogeneous reactions

Four well-defined steps are usually involved in the chemical processes of solid fuel combustion: drying, devolatilization, volatile combustion and char oxidation. Once solid fuels are injected into a combustion chamber, they are heated up and the drying process (the release of moisture) occurs immediately, followed by the rapid devolatilization process (the release of volatiles) which occurs due to high temperatures. Char produced through the volatilization process is consumed by heterogeneous processes of combustion and gasification and its combustion yields carbon monoxide (CO) and carbon dioxide (CO_2) according to the following reactions:



Reactions (R1) and (R2) are exothermic and will occur very rapidly but reaction (R3) is endothermic. In general, a dominating heterogeneous reaction is related to whether the char combustion rate is limited by either the diffusion of oxygen through the boundary layer surrounding particles or the kinetic rate of carbon oxidation reactions. Heterogeneous reactions can also include the following endothermic reaction:



where the carbon monoxide (CO) and hydrogen (H_2) resulting from reactions (R3)–(R5) are incorporated to the gas phase and oxidised to CO_2 and H_2O according to the following homogeneous reactions:



However, for the Eulerian–Eulerian simulation (Model 1), the only reaction included is (R1). The combustion rate of char is assumed to be limited by the chemical kinetics because the only reactive species that is included in the gas phase is O_2 . Then, the reaction rate r_a ($\text{kmol/m}^3 \text{ s}$) is defined as

$$r_a = k_a \cdot C_{\text{C(s)}} \cdot C_{\text{O}_2} \quad (1)$$

where $C_{\text{C(s)}}$ and C_{O_2} (kmol/m^3) are the concentrations of carbon and oxygen respectively; and k_a is the reaction rate constant given by the Arrhenius type relation:

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