Computational fluid dynamics modelling of biomass fast pyrolysis in fluidised bed reactors, focusing different kinetic schemes

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HIGHLIGHTS

• CFD model is developed for fast pyrolysis in 300 g/h fluidised bed reactor.
• Various kinetics schemes (simple, global and advanced) for fast pyrolysis process are tested.
• Model predictions are in good agreements with experiments.
• Biomass particle type and size and reactor temperature are also investigated.
• Developed models can be useful for the design of large-scale pyrolysis reactor.

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ABSTRACT

The present work concerns with CFD modelling of biomass fast pyrolysis in a fluidised bed reactor. Initially, a study was conducted to understand the hydrodynamics of the fluidised bed reactor by investigating the particle density and size, and gas velocity effect. With the basic understanding of hydrodynamics, the study was further extended to investigate the different kinetic schemes for biomass fast pyrolysis process. The Eulerian–Eulerian approach was used to model the complex multiphase flows in the reactor. The yield of the products from the simulation was compared with the experimental data. A good comparison was obtained between the literature results and CFD simulation. It is also found that CFD prediction with the advanced kinetic scheme is better when compared to other schemes. With the confidence obtained from the CFD models, a parametric study was carried out to study the effect of biomass particle type and size and temperature on the yield of the products.

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1. Introduction

Biomass fast pyrolysis offers a promising process for obtaining liquid fuels from the biomass feedstock, and the process involves thermal degradation of biomass in the absence of air or oxygen (Bridgwater, 1999). The product of biomass pyrolysis can be broadly categorised into three groups which include the condensable organic product (in the liquid state), char (solid) and non-condensable gases (CO, CO2, H2, CH4). Many studies have been carried out both on experimental and numerical aspects in the biomass fast pyrolysis, but the exact reaction mechanism and the kinetics involved in the pyrolysis reaction remain uncertain. Thus, several studies have been attempted for developing the kinetic model for biomass fast pyrolysis (Chan et al., 1985; Srivastava et al., 1996; Babu and Chaurasia, 2003). These studies assumed that three major products including gas, char, and organic liquid (tar) are obtained from the competitive pyrolysis reaction of a single component of biomass. The scheme of such a kinetic model is called as simple kinetic scheme. However, it has got limited application and is mainly useful for the qualitative prediction of the fast pyrolysis output. Multi-component multi-step kinetic mechanism was proposed by Miller and Bellan (1997) and Ranzi et al. (2008). In Miller and Bellan’s work, the kinetic model is based on the multistage and multicomponent scheme with cellulose, hemicellulose, and lignin as reference components. This scheme is called as global kinetic scheme. This can be considered as an improved version of the simple scheme. But the drawback of this scheme is that the interaction between the biomass components is not considered during the pyrolysis process. The global kinetic scheme can be further enhanced by the advanced kinetic scheme, which involves the feedstock characterisation in the form of cellulose, hemicellulose and different types of lignin which undergo a competitive reaction to produce a large number of representative
species (volatiles), char and gas. The pyrolysis reactions were
described by the superposition of different sub-mechanisms for
each biomass pseudo-component of cellulose, hemicellulose and
different types of lignin (Ranzi et al., 2008). In this model, tar pro-
duct of the primary reaction further undergoes a secondary reac-
tion which includes homogeneous and heterogeneous reactions.
Authors have included about 4500 secondary reactions in the gas
phase to account for a complete and thorough chemical kinetic
scheme.

For numerical modelling of biomass fast pyrolysis in a reactor-
scale, CFD, as an indispensable tool, has been used to understand
the underlying physics involved in the fast pyrolysis. For the sim-
ple kinetic scheme, many studies have already been reported in
the literature (Papadikis et al., 2009; Sharma et al., 2015).
Papadikis et al. (2009) have studied fast pyrolysis in a bubbling flu-
idised bed reactor using a Euler–Euler–Lagrangian approach.
Recently, Sharma et al. (2015) have studied the pyrolysis process
using the simple kinetic scheme in a fluidised bed reactor. CFD
study of biomass fast pyrolysis was carried out by Xue et al.
(2011) using the global kinetic scheme for biomass pyrolysis.
Xiong et al. (2013a,b, 2014a,b) have developed a generalised
numerical framework for biomass pyrolysis in a fluidised bed reac-
tor with interphase transport coefficients using global kinetic
scheme. Same authors have also investigated the different
devolatilization schemes including simple kinetic scheme with
only primary biomass decomposition, simple kinetic scheme and
global kinetic scheme for biomass pyrolysis (Xiong et al., 2014c).
They have found that the product yields from the global model
were best predictions. Recently, the same authors have studied
the impact of bed hydrodynamics on the yield prediction during
biomass pyrolysis (Xiong et al., 2016). Bruchmiller et al. (2012)
have studied the thermo-chemical decomposition of biomass using
a semi-global multicomponent mechanism by a discrete element
model (DEM) approach. They have also investigated a parametric
study of the fluidisation velocity, temperature and the moisture
content on the yield. For advanced kinetic scheme, recently,
Mellin et al. (2014) have studied the fast pyrolysis of biomass in
a pilot-scale fluidised bed based on multi-fluid Eulerian method.

In the present study, a numerical model is developed for the
biomass fast pyrolysis process using sand as the bed material.
The main objective of the present work is to focus on the various
kinetic schemes and its accuracy in the prediction of the fast pyro-
lysis yield of products. It is a comparative study of yield prediction
between the simple, global and advanced kinetic schemes. A sys-
tematic study was carried out with a primary focus on hydrody-
namic characteristics of a fluidised bed reactor; later the study
was extended to study the chemical reactions during fast pyrolysis.
Numerical results were compared with the experimental data from
the literature. The work was further extended to study the effects
of biomass particle type and size and the operating temperature on
the yield formation.

2. Methodology

2.1. Hydrodynamic modelling

The main process that occurs during the fast pyrolysis is heat
and momentum transfer between the reacting biomass particle,
sand, and the fluidising gas. Also, the mass transfer from the bio-
mass reactants as they undergo a chemical reaction in the presence
of high temperature fluidising gas occurs in this process. This study
involves two solid phases (biomass and sand) and one gaseous
phase (fluidising gas of N₂). The Eulerian method was used for
the multiphase flow model. In this method the governing
equations of the continuity, momentum and energy are solved
separately for each phase. Coupling between the phases is achieved
through the interphase exchange coefficients. For interphase
momentum transfer, the drag force by Gidaspow et al. (1992)
was used. For interphase heat transfer, the heat transfer exchange
coefficient between the sand and the gas mixture by Gunn (1978)
and between the biomass and the gas mixture by Ranz and
Marshall (1952a,b) were chosen. A kinetic theory of granular flow
was used to describe particle flows in the reactor. In this approach,
granular bulk viscosity for the sand particle is calculated based on
Lun et al. (1984), and granular viscosity is calculated based on the

2.2. Biomass pyrolysis kinetic modelling

Biomass feedstock consists of the basic components of cellulose,
hemicellulose, and lignin, with some percentage of water (~10%) and
little ash content. The devolatilisation of biomass involves dif-
ferent reactions within the biomass component itself leading to
different species at a different temperature. Initially, the decom-
position of hemicellulose occurs in the temperature range of about
450–550 K. Breakdown of cellulose occurs at a temperature of
about 500–620 K, and pyrolysis of lignin occurs over a wider tem-
perature range of 500–770 K. Up to this temperature range, char
yield increases and tends to remain constant with increasing tem-
perature. Several feedstocks can be used in the fast pyrolysis pro-
cess including Beechwood, Pinewood, rice husk, sugarcane
bagasse, spruce, etc. In the present work, Beechwood, Pinewood,
and sugarcane bagasse are used. To get reliable numerical results
of the fast pyrolysis process from the CFD simulation, the kinetic
model used in the analysis has to be very accurate. In this work,
a study was conducted to compare different kinetic schemes; they
are (a) simple kinetic scheme (Di Blasi, 1996); (b) global kinetic
scheme (Miller and Bellan, 1997); and (c) advanced kinetic scheme
(Ranzi et al., 2008).

2.2.1. Simple kinetic scheme

The simple kinetic scheme proposed by Di Blasi (1996) was
used in this study. The kinetic parameters such as the pre-
exponential factor and the activation energy used were given by
Di Blasi (1996). In this scheme, a reaction model is considered by
having biomass as a single component of reagent that undergoes
the primary reaction for giving three main products of non-
condensable gas, tar (high molecular weight organic liquid) and
char. Based on the literature, these reactions are found to be first
order in nature (Chan et al., 1985; Di Blasi, 1996). The tar or the pri-
mary tar, in general, is a mixture of oxygenated hydrocarbon com-
 pounds which further undergo a chemical reaction at higher
temperature leading to the formation of gaseous components and
secondary tar. The secondary tar undergoes heterogeneous reac-
tion to produce the char at a higher temperature. This secondary
tar reaction also depends on factors such as the residence time of
both gas and the catalyst. In general, the presence of char in the
reaction can act as a catalyst for the decomposition of tar product.

2.2.2. Global kinetic scheme

A global kinetic scheme based on the three components of bio-
mass (cellulose, hemicellulose and lignin) involves multicompo-
ent, multistage scheme for predicting biomass fast pyrolysis
process. In this scheme, individual biomass components are trea-
ted as a lumped one that undergoes the pyrolysis resulting the pro-
duct of tar, char and the non-condensable gases. The kinetic
parameter of the pre-exponential factor and the activation energy
by Miller and Bellan (1997) were used in this study. It differs from
the simple kinetic scheme by considering the biomass components
namely cellulose, hemicellulose and lignin as lumped components
2.2.3. Advanced kinetic model

The lack of details in both simple kinetic and global kinetic schemes is compensated by having a large number of intermediate reactions to simulate the real physics involved in the biomass fast pyrolysis process. In this scheme, the biomass characterisation plays a significant role in determining the product of the reaction. Therefore, it is necessary to have accurate information about the composition (cellulose, hemicellulose and lignin) of biomass. The reaction mechanism used in this numerical study was proposed by Ranzi et al. (2008). They have presented detailed kinetic schemes for each component of biomass based on the reported schemes in the literature. These kinetic schemes were validated by comparing mass loss profiles between the experimental and model predictions. There are 16 reactions (main species) considered in this scheme. The reaction details are shown in Table 1. In this work, the primary reactions only were considered because the secondary reactions were not found to be significant for fast pyrolysis as reported in the literature (Trendewicz et al., 2014). It has been reported in the literature that this scheme has the capability for the prediction of fast pyrolysis process (Mellin et al., 2014). However, the interactions between biomass components are not considered in this model.

2.3. Simulation methodology

The sketch of fluidised bed reactor used for the present study is shown in Fig. 1. The reactor geometry for the biomass fast pyrolysis process is based on 300 g/h fluidised bed reactor available at Aston University (Kalgo, 2011). Nitrogen was used as a fluidising gas and sand was used as an inert bed material which has a density of 2670 kg/m³ with the size of 0.725 mm. Biomass feedstock was introduced into the reactor from the side of the reactor. Boundary conditions used in this study are shown in Table 2. An initial study was carried out to understand the effects on the hydrodynamic mixing behaviour for different particles like sand, Beta-Mo₂C/Al₂O₃, and ground bagasse pellet with different particle diameter. Physical properties of biomass and bed materials are shown in Table 3.

Two-dimensional fluidised bed reactor was taken for the simulation study. A commercial solver code, ANSYS Fluent v.14.0 was used for solving the governing equations for heat, mass and momentum transfers (ANSYS Fluent v.14.0, 2014). Finite volume method was used for the domain discretisation. High resolution

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### Table 1

Kinetic parameter for the advanced kinetics scheme (Ranzi et al., 2008).

<table>
<thead>
<tr>
<th>Reaction</th>
<th>A (s⁻¹)</th>
<th>E (kJ mol⁻¹)</th>
<th>ΔH (kJ kg⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Cell → Cell A</td>
<td>8 × 10⁻³⁸</td>
<td>192.5</td>
<td>447.7</td>
</tr>
<tr>
<td>2 Cell → 5 H₂O + 6 Char</td>
<td>8 × 10⁻⁶</td>
<td>125.5</td>
<td>-1087.8</td>
</tr>
<tr>
<td>3 Cell A → LVG</td>
<td>8 × 10⁻⁷</td>
<td>41.8</td>
<td>732.2</td>
</tr>
<tr>
<td>4 Cell A + 0.25 Glyoxal + 0.25 Acetaldehyde + 0.25 HMFU + 0.2 Acetone + 0.16 CO₂ + 0.23 CO + 0.9 H₂O + 0.1 CH₄ + 0.61 Char</td>
<td>1 × 10⁻⁴⁸</td>
<td>133.9</td>
<td>859.6</td>
</tr>
<tr>
<td>5 HCell → 0.4 HCell 1 + 0.6 HCell 2</td>
<td>1 × 10⁻¹⁵</td>
<td>129.7</td>
<td>548.1</td>
</tr>
<tr>
<td>6 HCell 1 → 0.75 H₂ + 0.8 CO₂ + 1.4 CO + 0.5 Formaldehyde</td>
<td>3 × 10⁻⁰⁵</td>
<td>113.0</td>
<td>447.7</td>
</tr>
<tr>
<td>7 HCell 1 → Xylan</td>
<td>3 × 10⁻⁷</td>
<td>46.0</td>
<td>707.1</td>
</tr>
<tr>
<td>8 HCell 2 → CO₂ + 0.25 CH₄ + 0.25 C₂H₄ + 0.8 CO + 0.8 H₂ + 0.7 Formaldehyde + 0.25 Methanol + 0.125 Ethanol + 0.125 H₂O + Char</td>
<td>1 × 10⁻¹⁰</td>
<td>138.1</td>
<td>259.4</td>
</tr>
<tr>
<td>9 LignC → 0.35 LignCC + 0.1 pCoumaryl + 0.08 Phenol + 0.41 C₂H₄ + H₂O + 0.495 CH₄ + 0.32 CO + CO + H₂ + 5.35 Char</td>
<td>4 × 10⁻⁵</td>
<td>202.9</td>
<td>602.5</td>
</tr>
<tr>
<td>10 LignH → LignOH + Acetone</td>
<td>2 × 10⁻¹³</td>
<td>156.9</td>
<td>523.0</td>
</tr>
<tr>
<td>11 LignO → LignOH + CO₂</td>
<td>1 × 10⁻⁰⁶</td>
<td>106.7</td>
<td>510.4</td>
</tr>
<tr>
<td>12 LignCC → 0.3 pCoumaryl + 0.2 Phenol + 0.35 Acrylic-acid + 0.7 H₂O + 0.65 C₂H₄ + 0.6 C₂H₆ + 1.8 CO + H₂ + 6.4 Char</td>
<td>5 × 10⁻⁴</td>
<td>131.8</td>
<td>288.7</td>
</tr>
<tr>
<td>13 LignOH → Lign + H₂O + Methanol + 0.45 CH₄ + 0.2 C₂H₄ + 2 CO + 0.7 H₂ + 4.15 Char</td>
<td>3 × 10⁻¹⁰</td>
<td>125.5</td>
<td>100.4</td>
</tr>
<tr>
<td>14 Lign → Lumped-phenol</td>
<td>8 × 10⁻⁰⁸</td>
<td>50.2</td>
<td>577.4</td>
</tr>
<tr>
<td>15 Lign → H₂O + 2 CO + 0.2 Formaldehyde + 0.4 Methanol + 0.2 Acetaldehyde + 0.2 Acetone + 0.6 CH₄ + 0.65 C₂H₆ + 0.5 H₂ + 5.5 Char</td>
<td>1.2 × 10⁻⁰⁶</td>
<td>125.5</td>
<td>-209.2</td>
</tr>
<tr>
<td>16 H₂O (l) → H₂O (g)</td>
<td>5.3 × 10⁻¹⁴</td>
<td>88</td>
<td>2260.0</td>
</tr>
</tbody>
</table>

---

### Table 2

Boundary conditions used in this study.

<table>
<thead>
<tr>
<th>Boundary condition</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Biomass</td>
<td>Mass flow inlet (kg/s)</td>
</tr>
<tr>
<td>Fluidising gas</td>
<td>Velocity inlet (m/s)</td>
</tr>
<tr>
<td>Mixture</td>
<td>Pressure outlet (pa)</td>
</tr>
</tbody>
</table>
structured mesh was used with 50 nodes along the width and 380 nodes along the height. Time derivative in the governing equation was discretised with the second order implicit scheme with a time step size of about 10^{-4} s. Momentum equations were resolved with the second order accurate upwind scheme. Volume fraction equations were solved using QUICK scheme. The governing equations were solved using phase coupled SIMPLE algorithm. Standard k–ε turbulence model was used for predicting the turbulence flow in the reactor. The heterogeneous reactions of biomass pyrolysis were implemented along with stiff heterogeneous chemistry in the ANSYS Fluent v.14.0. Since the present models use the Eulerian approach, the heat of reaction was calculated by the difference in standard state enthalpy of products versus reactants.

### 3. Results and discussion

#### 3.1. Hydrodynamic study

First, a hydrodynamic study was carried out to analyse the mixing behaviour in the fluidised bed reactor. A mixing medium in the form of quartz sand was used as an inert bed in the reactor that helps in mixing and for improving the heat transfer rate. Different parameters that decide the mixing characteristics of the reactor are the particle diameter and density, and fluidising gas velocity. On the numerical side, it depends on the parameters such as drag coefficient, viscosity models (granular and bulk viscosity). Different bed particles based on the type (sand, Beta-Mo2C/Al2O3, and bagasse) were considered for this study. The details of the particles are shown in Table 3.

For the hydrodynamic study, the superficial gas velocity was held constant at 0.507 m/s. Fig. 2(a–d) show the volume fraction of the different bed material at various times at 1 s, 5 s, 10 s, and 20 s. It can be seen from the figures that the bed height increases with time due to the raising gas in the reactor and at higher times the bed height almost remains the same, indicating that the fluidisation has reached a steady state. It is also seen that the different behaviours of mixing between the fluidising gas and bed material occur until it reaches the steady state. In the case of the sand bed, the mixing takes a longer time to get a good fluidising behaviour in the reactor. This may be because the density of sand is higher compared to other particles used in this study. Also, the formations of bubbles are not prominent at the initial period for the high-density particle. This may be because the density of sand is higher compared to other particles used in this study. Also, the formations of bubbles are not prominent at the initial period for the high-density particle which leads to the delay for the formation of bubble coalescence by the fluidising gas flowing from the bottom of the fluidised bed reactor which is already shown in Fig. 2. This bubble motion in the reactor helps to have a good mixing inside the reactor. However, when the fluidising gas velocity goes to the higher range, the bed changes from the bubbling regime to the transport regime.

![Image](image_url)

**Table 3**

<table>
<thead>
<tr>
<th>Particle</th>
<th>Diameter (mm)</th>
<th>$V_g$ (m/s)</th>
<th>Density (kg/m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sand</td>
<td>0.6</td>
<td>0.507</td>
<td>1638.3</td>
</tr>
<tr>
<td>Sand</td>
<td>0.6</td>
<td>0.744</td>
<td>1638.3</td>
</tr>
<tr>
<td>Beta-Mo2C/Al2O3</td>
<td>0.6</td>
<td>0.507</td>
<td>638.03</td>
</tr>
<tr>
<td>Ground Bagasse pellets</td>
<td>0.6</td>
<td>0.507</td>
<td>1086.1</td>
</tr>
<tr>
<td>Ground Bagasse pellets</td>
<td>0.1</td>
<td>0.507</td>
<td>1086.1</td>
</tr>
</tbody>
</table>

The time-averaged volume fraction of solid for the three different particles is shown in the same figure. It is found that the bed expansion height is higher for the Beta-Mo2C/Al2O3 particle. Expansion ratio ($H/H_0$) is lower for the sand particle. It follows from the fact that the bed expansion ratio depends on the density of the bed particle and the drag force acting on the particle. Higher the particle density results in smaller bed expansion ratio, which is about 1.44 for the sand particle. The sand particle experiences low drag due to its high density. The other two particles subject to large drag force that results in moving the bed particle to the higher column length. This shows the higher expansion ratio of 2.06 and 1.8 for Beta-Mo2C/Al2O3 and bagasse respectively. This is also confirmed by the plot shown in Fig. 3a which shows the mean particle volume of fraction along the length of the reactor for different particles. Mean axial particle velocity plot is shown in Fig. 3b at two different locations in the reactor. This plot shows the different trend for different particles. For a high-density particle, the velocity at the centre of the reactor is higher and near the wall where the restriction is more in the form of shear stress, the velocity is low. Therefore, the raised particle due to the upward flowing gas in the centre tries to come down along the side of the reactor and thus negative velocity is observed near the wall of the reactor. For low-density particles, it shows the negative velocity in the centre region of the reactor whereas near the wall region, the same behaviour is observed as a high-density particle.

A mixing study is also carried out for biomass particle along with inert bed material without considering any chemical reactions. Biomass particle undergoes a severe mixing due to the formation of bubble coalescence by the fluidising gas flowing from the bottom of the fluidised bed reactor which is already shown in Fig. 2. This bubble motion in the reactor helps to have a good mixing inside the reactor. However, when the fluidising gas velocity goes to the higher range, the bed changes from the bubbling regime to the transport regime.

#### 3.2. Biomass fast pyrolysis

The hydrodynamic study was further extended to study the biomass fast pyrolysis process with different chemical kinetic schemes discussed in the last section. In this work, various type of biomass like Beechwood, Pinewood and sugarcane bagasse were used to study for fast pyrolysis process in the fluidised bed reactor. The composition of biomass used in the numerical modelling is shown in Table 4. Various products formed during fast pyrolysis are evaluated regarding three main components including condensable gas, char, and non-condensable gas by calculating the formation rate of the products. The products rate was obtained by a volume integration of these products in the reactor. The total amount of condensable gas, char and non-condensable gas formed in the reactor for various cases investigated in this study (see Table 5) was calculated as follows.

$$m_{\text{condensable gas}} = \int_{V \text{reactor}} \left( \text{density of the gas} \times \text{volume fraction of the gas} \times \text{total mass fraction of condensable gas} \right) dv$$

$$m_{\text{char}} = \int_{V \text{reactor}} \left( \text{density of the gas} \times \text{volume fraction of the gas} \times \text{total mass fraction of char} \right) dv$$

$$m_{\text{non-condensable gas}} = \int_{V \text{reactor}} \left( \text{density of the gas} \times \text{volume fraction of the gas} \times \text{total mass fraction of non-condensable gas} \right) dv$$

where $V$ is the reactor volume.
Fig. 2. Instantaneous volume fraction of solid particles in fluidised bed reactor for various time at superficial gas velocity of 0.507 m/s.
The yield of condensable gas, char and non-condensable gas was calculated as

\[ Y_{\text{condensable gas}} = \frac{m_{\text{condensable gas}}}{m_{\text{condensable gas}} + m_{\text{non-condensable gas}} + m_{\text{char}}} \]

\[ Y_{\text{non-condensable gas}} = \frac{m_{\text{non-condensable gas}}}{m_{\text{condensable gas}} + m_{\text{non-condensable gas}} + m_{\text{char}}} \]

\[ Y_{\text{char}} = \frac{m_{\text{char}}}{m_{\text{condensable gas}} + m_{\text{non-condensable gas}} + m_{\text{char}}} \]

### 3.2.1. Comparison of products yields for the different kinetic scheme

A study was carried out to understand the CFD prediction of products yield from biomass fast pyrolysis using different kinetic schemes including (i) simple kinetic scheme; (ii) global kinetic scheme; and (iii) advanced kinetic scheme. The process parameters used in this case were as follows: temperature: 773 K; Beechwood particle size: 0.625 mm; inert bed material: sand (density: 2670 kg/m³; size: 0.725 mm) and gas superficial velocity: 0.6366 m/s. The results were compared with the experimental values from the literature (Kalgo, 2011). The yield of condensable gas, char, and non-condensable gas compared for the three kinetic schemes is shown in Table 6.

It can be seen from the table that the results from the advanced kinetic scheme show a better prediction with reported experimental data. The reason may be because the advanced kinetic scheme involves multiple reactions between the products of the reaction. The improvement in prediction was attained because of the improvement in the modelling of various reactions. It is also observed in this study that the yield of condensable gas for the simple kinetic scheme is high when compared to the other models. The reason for the higher prediction of condensable gas in the simple kinetic scheme may be because the primary reaction starts at the biomass inlet and produces condensable gases quickly. This trend is consistent with the previous work of Sharma et al. (2015) who used a simple kinetic scheme and found the higher condensable gas yield. In the case of global kinetic mechanism, the yield of non-condensable gas is over predicted. This may be because the secondary reaction of primary tar results in the further production of non-condensable gas. A similar trend is also reported by Xiong et al. (2013). In the advanced kinetic mechanism, detailed
kinetic schemes for each component of biomass account a large number of representative species of volatiles which are closely related to the actual pyrolysis process, it is thus possible to obtain satisfactory results. The prediction of char yield from simple and global kinetic schemes is low. Since the advanced scheme involves the intermediate reactions which lead to the formation of char, the char yield is slightly higher and can be comparable to the experimental data. It is also worth noting that the computational cost for advanced scheme compared to other schemes is higher as it involves a lot of reactions to computing.

The contour plot of reactor temperature for the three different kinetic schemes is shown in Fig. 4. The temperature profile is similar to the global and advanced scheme while it is different for the simple scheme. It is more realistic for both the global and the advanced scheme as the biomass enters the reactor the particle tries to move towards the lower part of the bed due to gravity. As it falls under gravity, it is carried away by the fluidising inert gas towards the freeboard region. So the temperature gradient is clearly seen in the lower bed portion and is mainly due to the heat transfer from the sand particle. Also, the biomass spread is more in the lower bed region for both global and the advanced schemes. Since the change in temperature with time for the gas and sand phases are almost the same, it is shown here only for the biomass phase. As the temperature of the biomass inlet is about 300 K, the significant change in temperature from 300 K to the reactor temperature of 773 K for the biomass phase is clearly seen from the contour. The convective heat transfer between the fluidising gas and the biomass particle and conductive and convective heat transfer from sand and the gas phases towards the biomass particle cause temperature changes in the reactor.

With the above general analysis and comparison between the kinetic scheme, the study was further studied with the parametric study about the biomass particle type and diameter, and reactor temperature using advanced kinetic scheme.

3.2.2. Effect of biomass particle type
A comparative study was performed on different biomass particles of Beechwood, Pinewood and sugarcane bagasse. The yields of condensable gas, char, and non-condensable gas are shown in Fig. 5. The composition of biomass tested in the numerical modelling is shown in Table 4. It is found that the yield of condensable gas is almost the same at about 65% for all the three biomass particles tested whereas the non-condensable gas yield is higher (20%), and the char formation is lower (15%) for the case of sugarcane bagasse when compared to the yield of other biomass. The higher char prediction for both Beechwood and Pinewood is found. This may be due to higher lignin content in both biomass particles. Also, it is found that a similar trend in the yields for both Beechwood and Pinewood. This is mainly because the biomass components of cellulose, hemicellulose and lignin contents in both Beechwood and Pinewood are more or less similar.

<table>
<thead>
<tr>
<th>Products Yield</th>
<th>%Yield Simple scheme</th>
<th>%Yield Global scheme</th>
<th>%Yield Advanced scheme</th>
<th>Experimental data (Kalgo, 2011)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Condensable gas</td>
<td>78.63</td>
<td>65.97</td>
<td>58.98</td>
<td>63.15</td>
</tr>
<tr>
<td>Non-condensable Gas</td>
<td>14.98</td>
<td>31.06</td>
<td>15.36</td>
<td>13.56</td>
</tr>
<tr>
<td>Char</td>
<td>6.39</td>
<td>2.97</td>
<td>25.67</td>
<td>23.29</td>
</tr>
</tbody>
</table>

3.2.3. Effect of particle diameter

Effect of biomass particle size on the yields is shown in Fig. 6a. The superficial gas velocity of 0.6366 m/s and the reactor temperature of 773 K with various particle sizes in the range of 0.427–1.05 mm were used in this case study. It is found that with an increase in the particle diameter the percentage yield of non-condensable gas decreases which is matching with experimental observation whereas condensable gas yield increases and char yield decreases which are not matched with experimental findings. The increase in condensable gas yield with an increase in particle size may be explained because the particle resides the longer time in the bed for higher particle size due to the higher particle Reynolds number which in turn large number of biomass particles can be converted into the condensable gas through the primary reactions. A similar trend was also reported by Xiong et al.
who found that the increase in the particle size increases the yield of tar.

3.2.4. Effect of temperature

The operating temperature in the reactor was varied to study the temperature effect on the product yields. The temperatures were varied in the range of 673–873 K and other process parameters used in this case were Beechwood particle size of 0.65 mm and superficial gas velocity of 0.6366 m/s. Fig. 6b shows the yields of the different products used in this case. The char and non-condensable gas at different temperatures. It is observed from the figure that with the increase in the yield of the condensable gas decreases. This may be due to the occurrence of thermal cracking of condensable gas during the pyrolysis process. Due to the thermal cracking of condensable gas from the primary reaction gets converted to the secondary product and the final product may polymerise to form char. This is clearly observed from the figure that the char yield is higher at a higher temperature.

4. Conclusions

In the present study, CFD modelling of biomass fast pyrolysis in fluidised bed reactor was reported using Eulerian–Eulerian approach. First, a hydrodynamic study was studied for understanding the mixing behaviour; later the work was extended to investigate the different kinetic schemes for the biomass fast pyrolysis process. The advanced kinetic scheme results in the improved prediction of the yield of products. Further, the effect of biomass particle type and diameter, and operating temperature on the yield of products was conducted. This study can be further investigated for residence time distribution of gas and particle phases in fast pyrolysis process.

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