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Investigation on the quality of bio-oil produced through fast pyrolysis of biomass-polymer waste mixture

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Abstract. A high-impact poly-styrene (HIPS) was mixed with dried and ground coconut shell (CS) at equal weight percentage. Fast pyrolysis was carried out on the mixture in a fixed bed reactor over a temperature range of 573 K to 1073 K, and a nitrogen (N_2) linear velocity range of $7.8x10^{-5}$ m/s to $6.7x10^{-2}$ m/s to produce bio-oil. Heat transfer and fluid dynamics of the pyrolysis process inside the reactor was visualised by using Computational Fluid Dynamics (CFD). The CFD modelling was validated by experimental results and they both indicated that at temperature of 923 K and N_2 linear velocity of $7.8x10^{-5}$ m/s, the maximum bio-oil yield of 52.02 wt% is achieved.

1. Introduction

Although the major source of global energy today is fossil fuels, based on its finite amounts, fluctuating prices, associated emission of carbon dioxide (CO_2) to the atmosphere, new energy sources especially renewable ones are being investigated by scientists [1]. The emphasis on renewable sources is ever more important considering the growing worldwide population and hence energy demand. Biomass is one of the important energy sources as it can be directly converted into liquid biofuel through pyrolysis, and can reduce CO_2 footprint. The liquid fuel out of pyrolysis is called bio-oil, and it has not only the highest energy concentration compared to other pyrolysis by-products, but also it is more user friendly in terms of transportation, storage and applications [2–3].

Increasing usage of plastic materials in all industries has becomes a concern since plastic waste mainly stay in the environment forever. Reusing it as a fuel can help in reducing waste as well as producing new energy source. Thus, the feedstock of interest in this project is a mixture of biomass (coconut shell, CS) and plastic (high-impact poly-styrene, HIPS).

The effect of pyrolysis parameters such as reaction temperature and N_2 velocity on final products can be investigated through experiments, but it is important to visualise the dynamics and heat transfer processes so that further improvement can be implemented to the process. The heat transfer and fluid

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dynamics play important roles in pyrolysis as the parameters will be affected directly when the biomass-plastic waste is gaining heat inside the reactor. One of the tools is numerical approach such as computational fluid dynamics (CFD) modelling that can simulate the dynamics of the flow inside of the reactor while similar experimental input parameters are being used. Till now, to the best knowledge of the authors, by using CFD modelling, the effect of wall conduction of a fixed bed reactor tube [4], the convective heat transfer at low and high pressure in a fixed bed reactor [5] and the fluid dynamics as well as the heat and momentum transfer during pyrolysis in a fluidised bed [6] have been investigated. In contrast, this study focuses on CFD modelling for a rapid heating fast pyrolysis fixed bed reactor to investigate the effect of reaction temperature and N_2 velocity on the yield of bio-oil produced from a mixture of coconut shell and HIPS. The results were validated by experimental data taken from the existing bio-oil production rig that was modelled.

2. Methodology

2.1. Experimental

Coconut Shell (CS) powder was produced by using the method detailed in [7]. CS powder and recycled HIPS that was supplied by Wespack Waste Management Sdn Bhd in Malaysia and was ground into granules (<2 mm) using a Retsch SM100 Comfort grinder machine were mixed with equal weight. This mixture was pyrolysed in the rapid heating fast pyrolysis rig described in [7], over the same range of reaction temperature and N_2 velocity matrix that was used in [8].

2.2. Computational Fluid Dynamics

Simulations were run by Academic CFD software package, ANSYS version 15.0 on a desktop computer that is configured with Intel® CoreTM i7-3770 @ 3.40 GHz Processor with 8 GB RAM. The pressure was assumed as atmospheric pressure and the pyrolysed materials were assumed to be spherical wood and polystyrene from the material list available in the software. The heating process was assumed to be in steady state condition, and radiation was neglected due to stainless steel wall of the reactor. The geometry for the present work was created by Design-Modeller with a three-dimensional domain for CFD simulation. The fixed bed reactor was modelled as a cylindrical hollow tube and the spherical pyrolysed material positioned in the middle section of the reactor according to the parameters listed in Table 1. The mesh cells for this geometry domain were generated by using ANSYS-Meshing in tetrahedral format. Three boundary surfaces which are inlet, reactor wall and outlet were defined and the details of all the boundary conditions are tabulated in Table 2.

Table 1. Parameters of the geometry.

Parameter	Unit	Quantity
Inner diameter of the reactor	mm	48.7
Outer diameter of the reactor	mm	50.7
Total length of the reactor	mm	200.0
Radius of each biomass powder	mm	2.0

Table 2. Details of boundary conditions.

Boundary zone	Pressure (kPa)	Velocity (m/s)	Temperature (K)
Inlet	101.33	5 combinations[a]	298
Outlet	101.33	Not fixed	Not fixed
Wall	101.33	0	5 combinations[a]

[a] Same points as mentioned in [8]

After confirming by manual calculation of the Reynolds number, laminar flow modelling was considered. For the solver, pressure-based solver was selected by the SIMPLE algorithm for pressure-velocity coupling and the Second Order Upwind for momentum and energy equations. The solutions were implemented 25 times for 5 different N_2 linear velocities and 5 different temperatures based on experiments that were conducted in [8].

3. Results and discussion

From the CFD results, it was found out that the surface temperature of the pyrolysed grains (which is visualised over the 10 cm heating zone of axial length of the reactor and shown in Figure 1 for wall temperature of 1073 K and N_2 velocity of 6.7×10^{-2} m/s) decreases linearly with increase in the distance of the grains from the reactor wall. This characteristic of the temperature distribution is due to the one direction laminar flow of N_2 that mentioned in [9], which is dominated by direct conduction of the heat. This phenomenon can be described based on the existence of conduction heat transfer from inner wall of the reactor to the grains and from each grain to the next neighbour grain toward the centre. As maximum temperature is at the wall, the surface temperature of the grains, which are closer to the wall are higher than grains closer to the centre line of the cylinder as can be seen in Figure 1. With the existence of temperature gradient between materials, the heat transfer will then occur as the higher temperature from the inner reactor wall transferred heat to the lower temperature of grains until equilibrium is reached and steady state condition of heat transfer is reached.

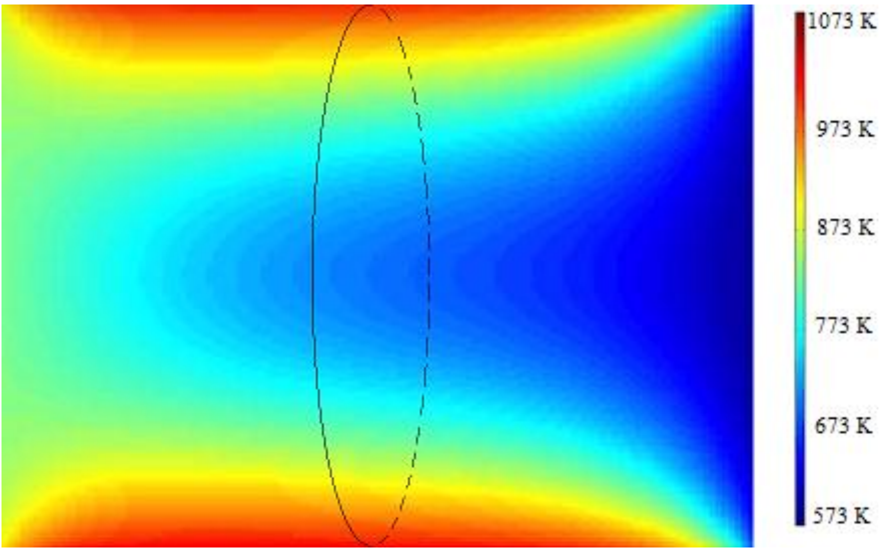

Figure 1. Heat distribution inside the reactor over heating zone for the wall temperature of 1073 K and N_2 velocity of 6.7×10^{-2} m/s

In addition, the above metioned grain temperature distribution is lower when the velocity of the nitrogen gas is lower. This phenomenon is due to the effect of N_2 velocity on the convection that is developing inside the reactor. It means the centrifugal body forces are stronger and the flow was more affected by the natural convection at low Reynolds number [10]. Furthermore, heat loss through the N_2 will be occurred more in higher Reynold numbers [11]. Also it has been observed that the velocity of the N_2 was affected by reaction temperature. The increasing of the velocity is due to the heat that was transferred to the N_2 from the heating sources, hence the kinetic energy of the N_2 increases [4]. The lower the N_2 velocity is, the higher it is affected by reaction temperature and this characteristic can have significant effect on pyrolysis process by having more concentrate high temperature zone in the reactor. The results of the above observation are tabulated in Table 3.

Table 3. Variation of the N_2 velocity

Initial N_2 velocity(m/s)	Maximum N_2 velocity (m/s)	Increment (m/s)	Increment (%)
0.000078	0.00016	0.000082	105.13
0.007000	0.01098	0.003980	56.86
0.013922	0.01940	0.005478	39.35
0.037000	0.04400	0.007000	18.92
0.067000	0.07755	0.010550	15.75

In order to validate the simulated results, the bio-oil production weight percentages were estimated and compared to the experiment results. The estimated bio-oil yield in constant N_2 velocity was calculated according to the developed empirical correlation that generalised version is shown as Equation (1), where T is the reaction temperature.

$$\text{Yield} = \sum (\text{fraction of T} \times \text{estimated bio-oil yield fraction from experiment}) + \sum \text{previous yield} \qquad (1)$$

From the simulated results, the yield of bio-oil was measured and the results of both experimental (three experiments were run for repeatability test and shown by using error bars) and CFD simulation are plotted in Figure 2. As can be observed maximum yield of 52.02 wt% with the percentage error of less than 5% can be achieved at a temperature of 923 K and N_2 velocity of 7.8×10^{-5} m/s. As the results have a maximum percentage error of below 5%, the validated simulation can be used for further investigation of the pyrolysis process in other input parameters of other materials.

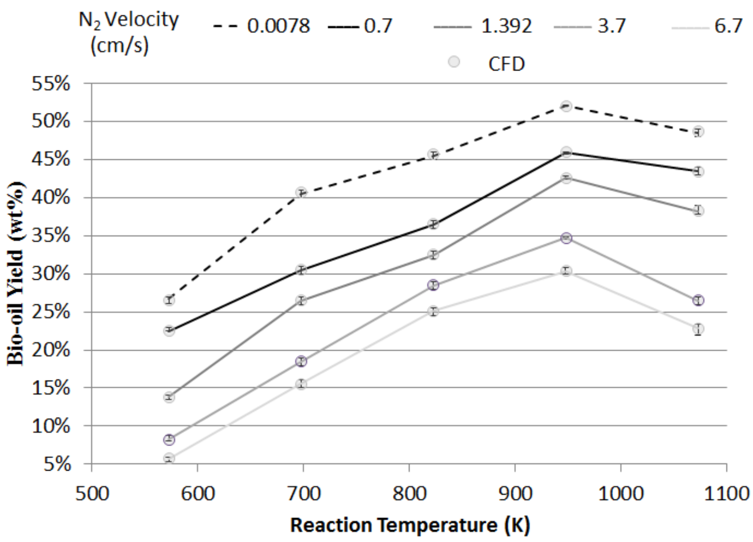

Figure 2. Bio-oil yield in all testing points

4. Conclusions

The optimum conditions to obtain maximum bio-oil yield of 52.02% wt% from the equal weight mixture of ground CS and HIPS are at reaction temperature of 923 K and N_2 linear velocity of 7.8×10^{-5} m/s. The results from CFD simulations and experiments have less than 5% difference at all 25 testing points. As the CFD model has been validated, it can be used in further investigations for other testing points or even other pyrolysed materials such as different plastics.

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