THE MATHEMATICAL MODELING OF THERMOCHEMICAL PROCESS IN THE PYROLYSIS ZONE OF A TWO-STAGE DOWNDRAFT GASIFICATION PROCESS

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ABSTRACT

This work developed a mathematical model to predict the temperature profile in pyrolysis zone, combustion temperature, feedstock feed rate and $\phi$ of the KU-KPS two-stage downdraft gasification process using wood chip as feedstock. Thermochemical concepts were applied to derive the energy and mass balance equations composed of chemical kinetic and three modes of heat transfer; conduction, convection and radiation. The feedstock was treated as a porous medium. The equations were solved by implicit finite difference method on the node of 200 and conversion criteria of $10^{-6}$. Experiments were also conducted to validate the model results. The validation results showed that the maximum temperature deviation between model and experiment was 62°C at the combustion temperature of 790°C while for the feedstock feed rate it had a deviation of 0.94 kg/h at the rate of 14.7kg/h. The experimental uncertainty was also analysed based on 95% level of confidence. The total experimental uncertainty of temperature and feedstock feed rate were 72°C and 0.95 kg/h, respectively.

Key words

Finite computation modeling of gasification process; Temperature profile along the pyrolysis zones of gasifier; Heat transfer in packed bed; Feedstock consumption prediction in two stage downdraft gasifier

INTRODUCTION

Greenhouse gas (GHG) emissions and fossil fuel oil price crisis are hot issues of the world today that we can say are very much interlinked. The use of fuel oil increases GHG emission which is harmful to our environment and contributes to global warming. In order to reduce this problem, renewable energy resources such as energy from solar, wind, hydro and biomass are being tapped. Biomass is considered as one of the best options to help overcome the shortage of fossil fuel and most conversion processes can use biomass as fuel for electricity generation. Moreover, using biomass results in zero net CO$_2$ emission that means reduced GHG emission (Jaojaruek, 2011; Ajay et al., 2010). Many researches forecast that the biomass will become sustainable energy resource in a near future (Battachaya and Salam, 2006). Biomass can be converted to combustible gas by using the gasification technology. The produced gas by gasification process is called producer gas and this gas can be used as fuel for internal combustion engine (ICE) or gas turbine depending on the produced gas quality.
An innovative high-performance two-stage downdraft gasification method was developed at Kasetsart University, Kamphaeng-Sean campus (KU-KPS). This two-stage gasifier use only air as gasification agent and can produce producer gas that has an HHV (higher heating value) and tar content as high as 6.7 MJ/nm$^3$ and 35 mg/nm$^3$, respectively. These values are at par with the requirements of fuel gas for direct-fed internal combustion engine (ICE) which also will not require complicated gas cleaning processes (Jaojaruek et al., 2011). To further study the developed downdraft gasifier, a mathematical model on the pyrolysis zone of the two-stage gasification process was also developed to predict the temperature profile, volatile gas generation profile and feedstock consume rate (Jaojaruek, 2011). The outputs from this model are very useful as important input parameters of many other models such as, gas composition prediction models in both pyrolysis and gasification by chemical equilibrium and kinetic methods, gas conversion capacity and thermal efficiency of gasification (Jarugthammachote, 2008; Jaojaruek and Kumar, 2009). The minimization of Gibbs free energy method has been used extensively to predict the gas composition, CO, H$_2$ and CO$_2$ of producer gas from gasification process. This method has results of good accuracy when compared with experimental data (Jarugthammachote, 2008). The feedstock supply rate is an important parameter for this method and can be obtained by pyrolysis model as mentioned by Jaojaruek (2011). However, the pyrolysis model in that study does not include the combustion in the gasification. The model would be more useful and realistic if combustion temperature can be predicted rather that measured from the experiments. This work developed and improved the original model by adding the combustion reaction zone into the model to enhance the model’s capability. The input parameter for the new model is air supply rate rather than combustion temperature as with the previous model. Thus, the combustion temperature in the reactor became the predicted value for the new model presented here. The outputs from new model will be very useful to enhance the ability of minimization of Gibbs free energy method because the equivalent ratio can be predicted rather than having to be measured from experiments. This new model can also serve as groundwork and can allow stacking of other important detailed calculations of gas composition product and/or profile taking place in the whole parts of gasification process whether in lump equilibrium or finite computation methods.

METHODOLOGY

The mathematical model was developed and solved to predict feedstock consumption rate and the combustion temperature in the combustion zone, temperature profile along the height of pyrolysis zone. Experiments were also conducted to presents the actual data and validate the data from model.

Mathematical modelling

The governing equations were derived using the concepts of energy and mass conservation under steady state conditions and some assumptions (Jaojaruek and Kumar, 2009) are required as: heat loss at the reactor’s surface was considered to be negligible (the reactor is insulated); the packed bed in the considered zone was treated as fixed bed; the packed bed (solid fuel) inside the reactor was treated as porous media and was considered as heat transfer participant (Yang et al., 2004); the properties of materials/gas in the system were assumed to be constant at average temperature and the packed bed was assumed as a gray body; steady supply of the solid fuel with a sufficient quantity to replace the solid that is consumed in the
reactor was also assumed; and, the moisture in the solid fuel was also considered by including it as a drying load and it was assumed to be evenly distributed throughout the considered length. The premixed air and gas that was injected into the reactor at the pyrolysis nozzle are burned (complete combustion) and treated as heat source (Jaojaruek, 2011). The supplied O\textsubscript{2} in air at combustion nozzle has a reaction only with char (C) and heat release was treated as heat source.

**Figure 1: The considered control volume and computation domain.**

**Energy balance equations**

The reactor, fully filled with feedstock, has two nozzles located as shown in Fig. 1. One is located at combustion zone or combustion nozzle (z = L) and the other is located at pyrolysis zone or pyrolysis nozzle (z = L\textsubscript{g}). The air is supplied at combustion nozzles, and then the combustion takes place in this location. The premixed gas of air and producer gas is supplied into the reactor at the pyrolysis nozzle. This premixed gas is burned in the pyrolysis zone. The volatile matter converts to volatile gas in this pyrolysis zone and then flows downward to the gasification zone.

The energy balance was applied on each \( \Delta z \)-thick element located along the reactor length (z-axis). An illustration of the reactor showing the considered length is shown in Fig. 1. The heat balance equation was derived from heat transfer on the porous medium principle (Jaojaruek and Jugjai, 1999; Jugjai et al., 1998). For the gas phase at the considered pyrolysis zone \( 0 \leq z < L\textsubscript{g} \). The governing equation is as follow,

\[
\rho c_p \frac{dT}{dt} + \rho u c_p \frac{dT}{dz} = \lambda \frac{d^2T}{dz^2} + Hw + Q_{dry} - h_p n_p A_p (T - T_s)
\]  

(1)

The average gas velocity was related to feedstock feed rate using the equation below:

\[
\rho u A_c = v_f \hat{m}_f Y_L
\]  

(2)
The gas velocity $u$ over porous medium (feedstock) can be represented by face velocity based on the reactor’s cross sectional area $A_c$ (Jaojaruek and Jugjai, 1999; Jugjai and Phothiya, 2007). The drying load was evaluated as:

$$Q_{\text{dry}} = \frac{w_i \dot{m}_f h_{fg,w}}{L_g A_c} \quad (3)$$

Heat was added into the reactor at the pyrolysis zone from the burned premixed gas supply at $z = L_g$. So, the equation at this location becomes:

$$\begin{align*}
\rho c_p \frac{dT}{dt} + \rho uc_p \frac{dT}{dz} &= \lambda \frac{d^2T}{dz^2} + H_w + H_v \dot{m}_g - h_p n_p A_p (T - T_s)
\end{align*} \quad (4)$$

$H_v$ is high heating value of premixed gas per specific heat source volume and $\dot{m}_g$ is mass flow rate of premixed gas that was conducted to be burned into the pyrolysis zone. So, the additional term $H_v \dot{m}_g$ is the generated heat per specific heat source volume of supplied premixed gas. For $L_g < z < L$ the equation therefore becomes:

$$\begin{align*}
\rho c_p \frac{dT}{dt} + \rho uc_p \frac{dT}{dz} &= \lambda \frac{d^2T}{dz^2} + H_w - h_p n_p A_p (T - T_s)
\end{align*} \quad (5)$$

At $z = L$, the combustion was taken place of between $O_2$ in air and char (C). The heat from combustion is treated as heat source per specific volume, $Q_{\text{com}}$. The equation in this range is:

$$\begin{align*}
\rho c_p \frac{dT}{dt} + \rho uc_p \frac{dT}{dz} + Q_{\text{com}} &= \lambda \frac{d^2T}{dz^2} + H_w - h_p n_p A_p (T - T_s)
\end{align*} \quad (6)$$

and the combustion heat $Q_{\text{com}}$ can be calculated by:

$$Q_{\text{com}} = \frac{H_c \times \dot{m}_c}{2 \times b_c \times A_c} \quad (7)$$

$H_c$ is higher heating value of char (C) and $\dot{m}_c$ is a mass rate of char that was burned completely with air at stoichiometric condition. Thus, the $\dot{m}_c$ can be obtained when air supply is known.

On the other hand, the heat balance equations for the solid phase that was treated as fixed bed at the considered pyrolysis zone $0 \leq z \leq L$ was defined as:

$$\begin{align*}
\rho_s c_{ps} \frac{dT_s}{dt} &= \lambda_s \frac{d^2T_s}{dz^2} - \frac{dq_s}{dz} + h_p n_p A_p (T - T_s)
\end{align*} \quad (8)$$
The radiation heat flux ($q_r^+$ and $q_r^-$) and divergence of heat flux ($\frac{dq_r}{dz}$) were taken from Jugjai et al. (1998), Echigo et al. (1987), Yoshizawa et al. (1988) as follows:

$$
q_r^+(\tau) = 2\pi \left[ I_b E_3(\tau) + \int_0^\tau I_b(\tau')E_2(\tau'-\tau)d\tau' \right]
$$

(9)

$$
q_r^-(\tau) = -2\pi \left[ I_b E_3(\tau_c-\tau) + \int_{\tau_c}^\tau I_b(\tau')E_2(\tau'-\tau)d\tau' \right]
$$

(10)

and,

$$
\frac{dq_r}{dz} = -2\pi \kappa \left[ I_b E_2(\tau) + I_c E_2(\tau_c-\tau) - 2I_b(\tau) + \int_0^\tau I_b(\tau')E_2(\tau'-\tau)d\tau' \right]
$$

(11)

here, $I_b(\tau) = \frac{\sigma T^4}{\pi}$, $\tau$ = optical thickness and $E_n(\tau)$ = exponential integral function of $n^{th}$ order was taken from Ozisik (1985):

$$
E_n(\tau) = \int_0^1 \tilde{\mu}^{n-2} \exp(-\tau / \tilde{\mu})d\tilde{\mu}
$$

(12)

**Mass balance equations**

The concept of mass conservation was applied only for the gas phase because the solid phase was treated as a fixed bed. Additionally, the gas phase in this model refers to the volatile gas. The model presents the development of volatile gas through the volatile gas fraction ($Y$) which is defined as the ratio between generated volatile gas and available volatile gas (volatile matter) residing in the biomass bed. The analysis was performed on each $\Delta z$-thick element at $z$ location along the reactor length of the pyrolysis zone up to combustion nozzle as shown in Fig. 1.

At the considered pyrolysis zone, $0 \leq z \leq L$ :

$$
\rho \frac{dY}{dt} + \rho u \frac{dY}{dz} = D\rho \frac{dY^2}{dz^2} + w
$$

(13)

where, $w$ is the volatile gas generation rate which can be evaluated by treating the volatile matter conversion as first order single step reaction in Arrhenius’s form (Turns, 1996):

$$
w = \rho Ae^{-\frac{k}{RT}}(1-Y)
$$

(14)

**Numerical procedure**

Fig. 1 also illustrates the computation domain for the numerical analysis. The governing equations were rearranged into different equation forms and were solved by implicit finite
difference method on the node number of 200 throughout the length of 40 cm. of the considered range up to combustion nozzle \((Z = L)\). The reactor diameter was taken as 20 cm. The unknowns were solid and gas temperature profiles, combustion temperature, feedstock feed rate and equivalent ratio. Volatile gas generation is also an output of the model. The calculation convergence criteria were set at \(10^{-6}\). The calculation was done by a program that was coded by Fortran Power Station 4.0 on a Windows XP platform. The input parameters consisted of feedstock initial temperature, thermodynamic properties, heat transfer properties, physical properties and chemical kinetic properties of the feedstock. The varying input parameter for this study is the flow rate of premixed gas at pyrolysis nozzle and air supply at the combustion nozzle. The outputs/results of the model are the temperature profile include combustion temperature, volatile fraction profile, feedstock feed rate and equivalent ratio. The feedstock properties were referred to eucalyptus wood chip. The feedstock was sampled for its properties testing by proximate analysis following the standard procedure described in ASTM E871–82, ASTM E872–82 and ASTM E1534-93. The CHON compositions were evaluated by ultimate analysis. The ultimate analysis was done with ThermoFinnigan (FlashEA™ 1112) to find the composition percentage of C, H, O and N. The results were C = 47.12%, H = 4.62%, O = 48.26% and N = 0.0%. The results of the proximate analysis showed that %volatile mater, %fixed carbon, %humidity and %ash were 70%, 16%, 10% and 4%, respectively and bulk density was found to be 259 kg/m³. The wood chip cubical size is 2.0 cm. The kinetic parameters of wood is averaged from the values that were adopted from a previous work by Koufopanos et al. (1989).

**Experiment apparatus and measurement system**

The experiment apparatus and measurement system is illustrated in Fig. 2. The mechanical apparatus consisted of gasification reactor (gasifier), cyclone, suction blower, piping and it’s associated devices such as valves and fittings. The measuring system consisted of several instruments, data acquisition (DAQ), communication devices and computer. The installed

![Figure 2: Overall schematic of experiment apparatus and instrument setup.](image-url)
instruments were composed of air flow meter (rotameter), gas flow transmitter, level transmitter, gas flow counter and temperature sensor (type J thermocouple).

The gasifier is constructed from steel. It has a cylindrical shape of 25 cm diameter and 120 cm high. The top of reactor is feedstock hopper (conical shape). The span between pyrolysis nozzle and combustion nozzle is 13 cm, and gas-out nozzle location is 10 cm from bottom as shown in Fig. 2. Inside of the reactor is insulated with 1-inch thick reectory cement (1200 °C grade). This made the reactor inside diameter become 20 cm. The air supply rate at combustion and pyrolysis nozzles is measured by rotameters 1 and 2. The 8 thermocouples (type-J) were installed to measured the temperature profile along the height of the reactor as shown in Fig. 2. The gas flow transmitter F1 was used to measure the quantity of bypass gas required to mix with air at stoichiometric ratio and this premixed air/gas is supplied into the reactor at pyrolysis nozzle. The level transmitter L1 was installed to evaluate the feedstock feed rate. The measuring instruments for temperature, gas flow rate and feedstock level were connected to DAQ (Hilogger-1775, Hioki) and the data was sent to computer. The data were recorded and some calculations were provided to display the measured values online. The screen interface or human machine interface (HMI) as shown in Figure 2 is programmed by LabView 6.0a. The data presented on the screen were graphs, tables and sever styles of dial gauge.

RESULT AND DISCUSSION

The temperature profile along the height of reactor was plotted and shown in Fig 3. An air supply of 100 LPM was supplied into the combustion zone through the combustion nozzle. The producer gas at the outlet nozzle was branched to mix with air at stoichiometric ratio. The premixed combustible gas was supplied into the reactor at the pyrolysis zone through the pyrolysis nozzles (at 13 cm above the combustion nozzles) at a rate of 100 LPM. This created two locations of combustion as can be seen in Fig 3. The temperatures at 20 cm and 33 cm are around 734°C and 581°C, respectively. The supply of premixed air and gas allows easier burning of the feedstock at the pyrolysis zone and this method can therefore help control the flame location and temperature better than by only supplying air for a more effective gasification process.

Fig. 4 shows the simulation results from the mathematical model developed for the pyrolysis and combustion zones. This figure is for the case of 100 LPM air supply and premixed gas supply of 75 LPM. The temperature profile started to elevate at distance 25 cm from air supply location (combustion nozzle) from around 40°C at the feedstock entering temperature to 479°C at the premixed gas supply location. Combustion also took place on this zone but temperature sagged a little bit due to the heat flow effects of heat transfer. After that the temperature was increased due to influence of higher temperature at the combustion zone and temperature was continually elevated until it reached the highest temperature of 718°C at the main combustion zone. Moreover, the volatile gas fraction that represents the development of volatile gas along the pyrolysis zone was also displayed on this figure. The volatile gas was converted from volatile matter and its conversion started at the temperature of around 280°C or at the distance of 12 cm. on figure. This conversion rate grew very fast and became completely volatile gas at the temperature of around 420°C or at the location 10 cm approximately. The conversion temperature range then is between 280 – 420°C that is consistent with the results of Koufopanos et al., 1989 and Jaojaruek et al, 2011.
Figure 3: Temperature profile from experiment.

Figure 4: Temperature profile from model.

Figure 5: Temperature against varied gas supply.

Figure 6: Feedstock consumption versus gas supply.

Figure 7: Equivalent ratio (φ) versus gas supply.

Figure 8: Temperature profile validation.
Fig. 5 shows the three cases of model results for the air supply of 100 LPM at distance 40 cm. (combustion nozzle) for the mixed gas supply of 75, 100, 125 and 150 LPM, respectively, at distance 27 cm (pyrolysis nozzle). The temperature profile and combustion temperature at combustion nozzle location of higher premixed gas supply was higher because more premixed gas supply means more heat input to help increase the temperature. The higher heat input also resulted to increased devolatilization rate, which consequently resulted to an increased feedstock feed rate as seen in Fig. 6. The reaction equivalent ratio (φ) against varied gas supply rate at fixed 100 LPM air supply was plotted as shown in Fig. 7. The φ is decreased as gas supply increased, because of the effect of increasing rate of feedstock consumption is more than that increasing rate of air supply.

The model validation of feedstock consumption rate, φ and temperature profile (at air supply 100 LPM and premixed gas supply 150 LPM) were also done and shown in Figs. 6, 7 and 8, respectively. The consumption rate from the model is higher than the values from the experiment because the model treated the system as an adiabatic process. While in reality some heat loss occurred. The other significant factor is that the O₂ is not only burned with char. Some portion of it is also burned with the volatile gas which has a lower HHV. This made lower heat inputs and results in lower consumption rate and lower combustion temperature. The combustion temperature from model was around 790°C. While the data from experiment was 728 ± 72°C. The experiments uncertainty bands based on the confidence level of 95% were also plotted on the graphs. It can be observed that the models deviation from experiments are still within the experiments uncertainty bands.

CONCLUSION

This study shows that the developed model, which used the chemical kinetic and heat transfer approach, can predict the temperature profile, feedstock feed rate, and generated volatile gas fraction well. Additionally, in lump analysis such as the minimization of Gibbs free energy method (a very popular method used to predict the gas composition percentage of producer gas), φ is required as a parameter in the input. Since φ is an output of the mathematical model developed in this study, then this study can serve and fulfil a weakness of the Gibbs free energy method. Finally, if a similar approach will be applied to the other zones, then future studies on integration of all individual zone models will be very useful and can provide a more realistic and sturdy overall mathematical model for a two-stage downdraft gasification.

NOMENCLATURE

<table>
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<tr>
<th>Symbol</th>
<th>Definition</th>
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<td>$A$</td>
<td>pre-exponential factor or collision factor, sec⁻¹</td>
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<td>$m_c$</td>
<td>mass of air in combustion, kg</td>
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**REFERENCES**


