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Numerical modeling of down draft gasification process using specified temperature profile

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Abstract. This paper introduces the one-dimensional CFD model for downdraft gasification by making use of temperature profile from the experiment. Thermal equilibrium between solid fuel and gas stream is assumed. The pyrolysis gas generation, char generation, homogeneous reaction rate and char heterogeneous combustion rate can be calculated following Arrhenius law and regarded as the source terms to transport equations of 8 gaseous species. Air flow rate was kept constant at 90 L/min. From the measured temperature profile, the reactor is divided into two distinctive zones which are 1.) Combustion zone and 2.) Reduction zone. Combustion zone is determined as heat release region as dominated by oxidation of the raw material, while reduction zone is depicted by endothermic mechanism. For simplicity, the process is assumed as one dimensional. With this alternative CFD procedure, non-linear coupling process from energy equation is ignored. Therefore, the computational effort is greatly reduced. Moreover, computational quality is improved with reduced residual as compared to conventional CFD procedure.

1. Introduction

Thailand is an agricultural producer. There are a lot of distributed biomass available in wide agricultural area. Biomass has the capability to perform thermal process for producing gaseous fuel. However, careful economical consideration should be thoroughly studied for each project. [1] had studied on thermal performance and economical point of the operation of Biomass fueled power generation and cogeneration project in USA. He concluded that the system thermal performance and local fuel management are the key factor for successful operation of the process.

Gasification is a complicate process. It involved a lot of detailed reaction mechanisms which are interact to each other. The process is strongly coupled and not easy to conduct modeling. Model developer need to deal with strongly non-linear term especially from energy equation which massive energy release during the combustion process. CFD modeling serve as an engineering tool to help engineer driving the improvement of the project. CFD modeling has an ability to predict the detailed process to help them understanding and pointing out performance improvement opportunity. CFD also working as a tool for project feasibility study to estimate the price to earnings ratio of the project. Since the system performance is the key for business success of the running project.

There are many engineering applications classified into continuum porous media category. For example, catalytic converter, submerged flame combustion in an inert porous media. The continuum porous media modeling had been employed for modeling of the fixed bed gasification [2]. The idea of continuum porous media modeling considers the occupied control volume consisting of solid and fluid pores region, as shown figure 1.

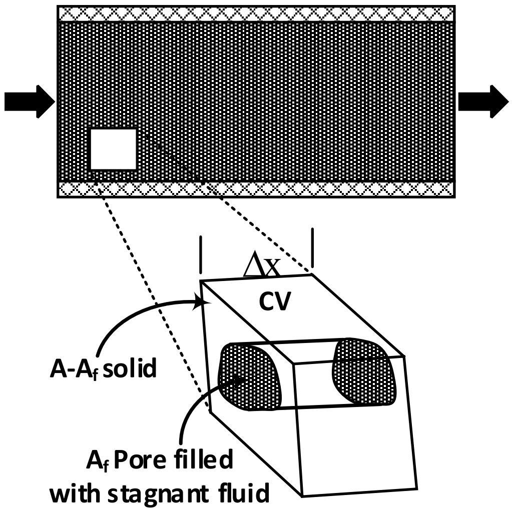

Figure 1. Continuum porous media concept.

Transport equation of the porous media could be written in the same form as the conventional form except that it has a porosity, a constant, being multiplied into each term. Transport of gaseous species through the finite control volume occurs only in the fluid space. The porosity reflects that the finite area and volume has the occupying solid constituent. Therefore, the convection, diffusion transport and source term is fractioned by porosity constant.

Transport equation for continuum porous media could be re-written as the equation below.

$$div(\rho u \varepsilon \phi)v = div(\tau \varepsilon grad \phi) + S\varepsilon \tag{1}$$

In terms of modeling, fixed bed gasification process modeling is resemble to the combustion in an inert porous media except that the solid matrix in fixed bed gasification is not inert. On the contrary, it has pyrolysis kinetic taking place in the solid volume matrix. Moreover, it has heterogeneous char combustion at the surface of the solid matrix. Pyrolysis is the biomass thermal decomposition process, in which the rate is defined by Arrhenius form. It generates several gas, solid char and tar vapor. The pyrolysis equation can be written below.

$$\text{Biomass} \rightarrow \text{a}Char + \text{b}Tar + \text{c}Gas \tag{2}$$

In CFD modeling, the gas composition is directly prescribed into the model as the mass percentage of the total gas generated from pyrolysis process. Pyrolysis gas composition can be obtained from either the experimental pyrolysis test rig [3] or available data from other reference works.

Several homogeneous combustion kinetic are taking place in fluid pores space in parallel with the combustible gas generation from pyrolysis. Tar cracking kinetic also occur in homogeneous form with water gas shift and CO combustion. Tar and steam condensation can be added into the model by estimating the saturation temperature of tar vapor and heat transfer rate between hot gas and cold solid porous fuel matrix.

In this paper, alternative CFD procedure of down draft gasification process is proposed. The measurement of temperature profile from Kasemsil O. et.al. [3] was adopted. Various homogeneous and heterogeneous kinetics are calculated based on pervailing temperature profile. Transport equations of 8 gas species together with biomass and char transport were solved by TDMA algorithm. Iteration coupling between kinetic rate, source term and transport equation were performed until convergence was achieved.

2. Exerimental setup

The experimental set up case is refer to Kasemsil O.and team [3]. The air input rate was 90 litre/minute.

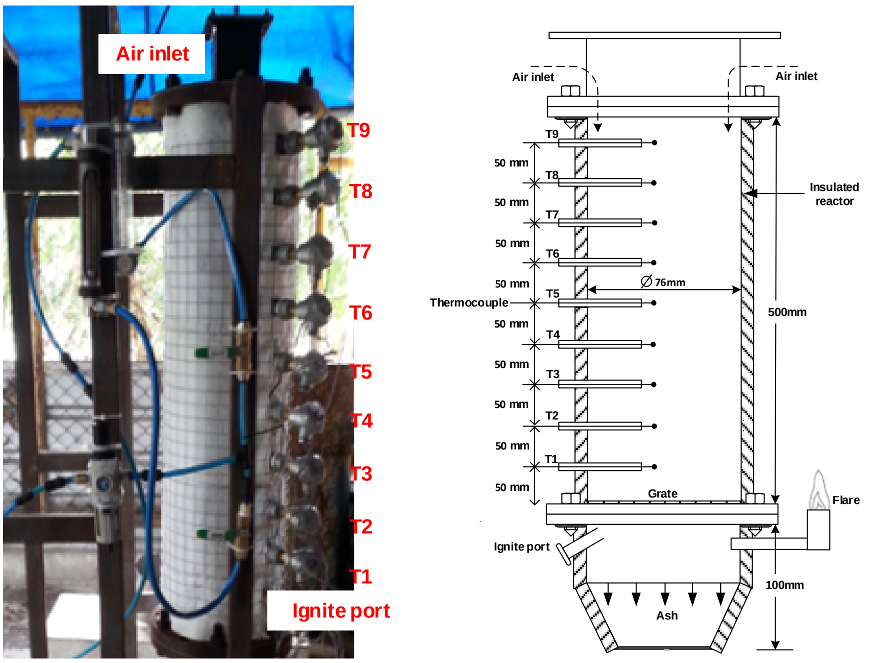

Figure 2. (a) Air inlet and thermocouple arrangement in the reactor. (b) Thermocouple arrangement in the reactor.

Temperature profile for mathematical modelling was simplified from the measured profile. The first temperature rising rate, slope1, is obtained by identifying the distance between the location of maximum temperature and the location at the interface of preheat zone and the reaction zone. Slope 2 indicates the recession rate due to endothermic reaction. This second slope is obtained from linear approximation of temperature profile from the location of maximum measured temperature and the location at the interface of reduction and extinction zones, as seen in figure 4.

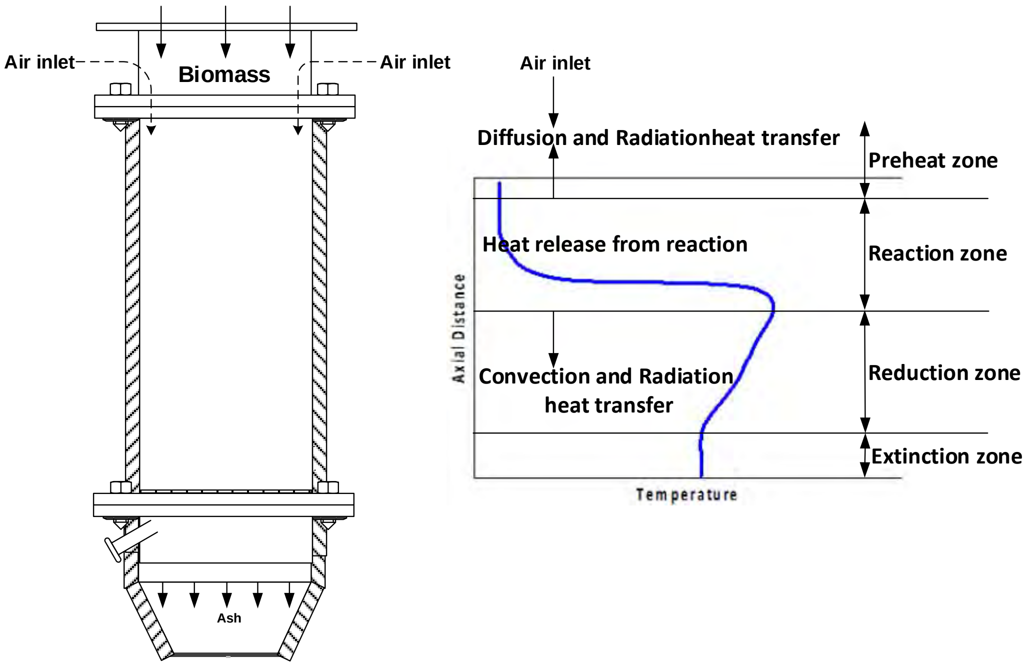

Figure 3. Temperature distribution in the reactor.

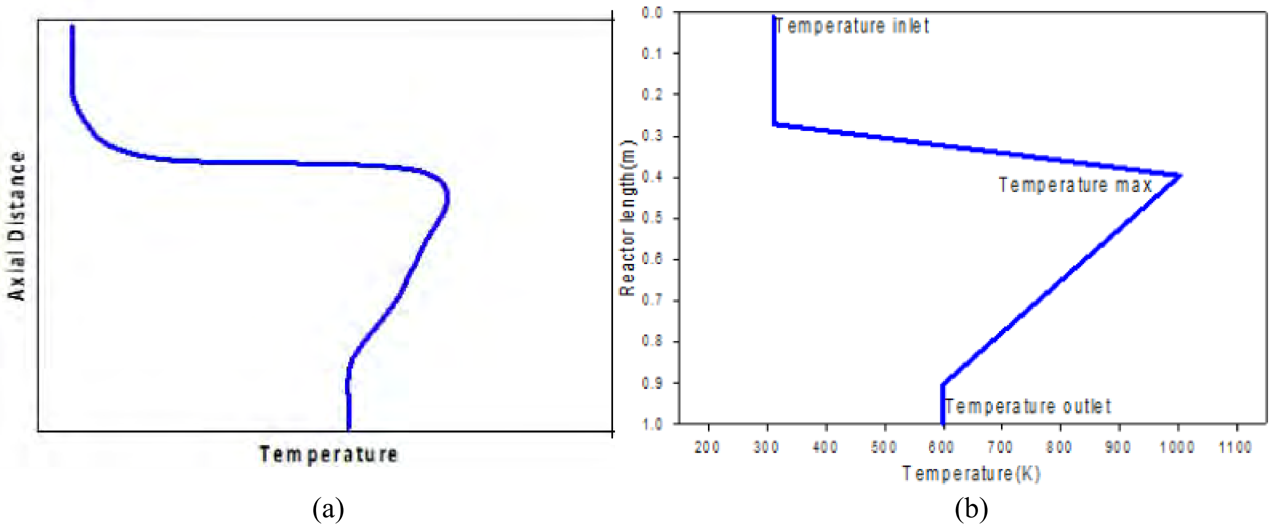

Figure 4. Temperature distribution in the reactor a) Experimental data b) Simplified temperature profile for mathematical modelling

Kasemsil O. et.al. [3], has perform experimental study of stratified downdraft process of biomass. He concluded that the process consisted of 2 distinct thickness in the reactor comprised of 1.) Combustion zone and 2.) Reduction zone as shown in figure 3. All zones propagated in counter direction with supply air flux. The propagation speed depended on gas mixture and thermal energy transport within the reactor. There have been many research into the propagation front in a packed bed. [4-8] has studied on the thermal propagation speed in downdraft gasification configuration with different supply air mass flux. He found that the propagation speed was dominated by convection and radiation heat transfer at the combustion front layer.

The flame propagation rate is calculated by knowing the distance between two consecutive thermocouples and the time required to reach a particular temperature between those thermocouples. The distance between two consecutive thermocouples is 5 cm. The time required to reach the reference temperature between two consecutive thermocouples is calculated by using the temperature profiles between two consecutive time steps. The flame propagation rate is calculated by using the following relation Eq.(1) [5]

$$\text{Propagation rate(cm/min)} = \frac{\text{Distance between thermocouples(cm)}}{\text{Time required to reach the particular temperature(min)}} \tag{3}$$

3. Numerical modeling

Estimated temperature profile and propagation speed is prescribed for CFD modeling. The problem is assumed to be quasi-steady. Instead of treating flame propagation moving, all reaction zones are kept stationery with an influx of biomass into the calculation domain with the velocity equal to the flame speed.

Transport equation of 8 gas species are treated as continuum porous media with predefined porosity.

$$div(\rho u\varepsilon\phi)v = div(\tau\varepsilon grad\phi) + S\varepsilon \tag{4}$$

Solid biomass and solid char transport equations are written in the same form as gas transport equation except that it has no mass diffusion transport term. It can be written as below.

$$div(\rho u\varepsilon\phi)v = S\varepsilon \tag{5}$$

While molecular weight of mixture can be calculated as.

$$MW_{mix} = \frac{1}{\sum_i Yi / MWi} \tag{6}$$

Various reaction rates are calculated by Arrhenius form with the input of defined temperature field. Each reaction rate will then link to particular mass generation and finally total mass generation of spcific species will transfer to source term of the transport eqution during coupling process. Conversion between concentration rate to mass rate can be written as below.

$$PMW_{mix}\phi / RU(T)(MW\phi) \tag{7}$$

Gas phase combustion kinetic employed in the modeling are as follow

$$(tar)CH_{1.522}O_{0.0228} + 0.86O_2 \xrightarrow{Kc1} CO + 0.76H_2O \tag{8}$$

$$CH_4 + 1.5O_2 \xrightarrow{Kc2} CO + 2H_2O \tag{9}$$

$$2CH + O_2 \xrightarrow{Kc3} 2CO_2 \tag{10}$$

$$H_2 \xrightarrow{Kc4} 2H_2O \tag{11}$$

$$R_j = A_j \exp\left(-\frac{E_j}{RT_g}\right) T_g C_i^{0.5} C_{O2}, j = c1, c2, i = T, CH_4 \tag{12}$$

$$R_{C3} = A_{C3} \exp\left(-\frac{E_{C3}}{RT_g}\right) C_{CO} C_{O_2}^{0.25} C_{H_2O} \tag{13}$$

$$R_{C4} = A_{C4} \exp\left(-\frac{E_{C4}}{RT_g}\right) C_{H_2} C_{O_2} \tag{14}$$

Gas-phase water gas shift.

$$CO + H_2O \overset{K_{wg}}{\Leftrightarrow} CO_2 + H_2 \tag{15}$$

$$R_{wg} = \varepsilon k_{wg} \left(C_{CO} C_{H_2O} - \frac{C_{CO_2} C_{H_2}}{K_E} \right) \tag{16}$$

$$K_{wg} = A_{wg} \exp\left(-\frac{E_{wg}}{RT_g}\right)_{wg} \quad K_E = A_E \exp\left(\frac{E_E}{RT_g}\right) \tag{17}$$

$$K_E = A_E \exp\left(\frac{E_E}{RT_g}\right) \tag{18}$$

Heterogeneous char surface combustion is calculated by one film model [9]. The thermal equilibrium between solid fuel matrix and fluid is assumed. Char surface temperature was assumed equal to measured gas temperature. There was a research on computational work proving that the temperature inequilibrium occurred around the combustion zone for combustion within inert porous media [10] which drive additional heat recirculation to the flame zone. However, if solid fuel particle is very small this assumption would be acceptable.

3.1 Mesh generation

Mesh generation is in one dimensional for 90 centimeters long. The domain was divided into 100,000 equally control volumes, as shown in Figure 5. The code was tested by employing the material property and boundary condition as shown in Table 1.

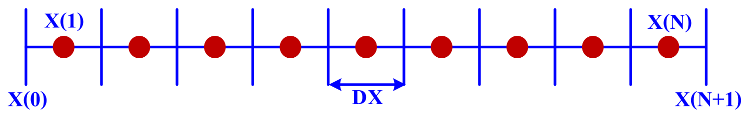

Figure 5. Mesh generation in calculation domain

Table 1. Boundary condition

Boundary condition	
Mixture inlet velocity	0.30 m/s
Mixture Inlet temperature	310 K
Oxygen mass fraction	0.40
Nitrogen mass fraction	0.60
Biomass relative velocity	0.001 m/s

Table 2. Material property

Material property	
Porous void fraction	0.5
Mixture binary diffusivity	0.0008 m2/s
Pressure	101325N/m2
Biomass density	100 kg/m2

All transport equation are discretized into finite volume according to figure 1. In order to calculate convection term, face property was estimate by first order upwind scheme. All transport equations are written in system of algebraic equations. The volume at boundary was treated separately according to assigned boundary condition. All of the system of algebraic equations were solved by TDMA algorithm. The equation of state is calculated based on previous round of solved property field. All of the system of algebraic equation is then updated. The process is repeated until the convergence is achieved.

4. Result and Discussion

The custom made CFD code for biomass gasification is during the development stage. Code structure is divided into various subroutines. Every subroutine is tested individually whether they are capable to perform the desired task. Then the subroutine will be integrated into the programing loop in coupling procedure. The coupling test started from few variables until all variables are coupled and under controlled.

The solid biomass transport and decomposition testing result is demonstrated in this paper. This is the test of coupling between biomass transport subroutine and pyrolysis subroutine. These two subroutines need to be coupled in order to correctly define biomass density distribution along the reactor.

Figure 6 shows solid biomass density distribution along the reactor after the convergence of two subroutines coupling is achieved. This shows that major biomass decomposition process occur at the reactor length of 0.5 to 0.7 meter, because the temperature in this region is high. The decomposition rate is determined by Arrhenius rate, with the parameter for biomass decomposition from [2]. The biomass decomposition only 30% from the initial value which is considerable smaller than the experimental result from the author's test rig [3].

Figure 7 shows the rate of biomass decomposition versus temperature while the biomass density is kept constant at 100kg/m3. It was demonstrated that the kinetics start around 800 Kelvin. It exponentially increases with the increasing temperature. This Arrhenius rate parameter is likely to be slower than the experimental result. Rice husk start to emit smoke or undergoing pyrolysis process at temperature much lower than 800K. The Arrhenius parameter will need to be revised whether it is suitable to describe rice husk decomposition rate.

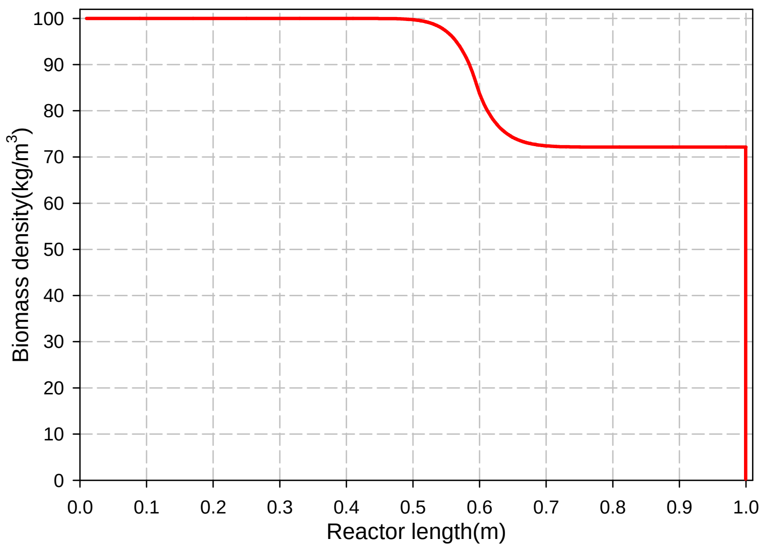

Figure 6. Solid biomass density distribution along the reactor

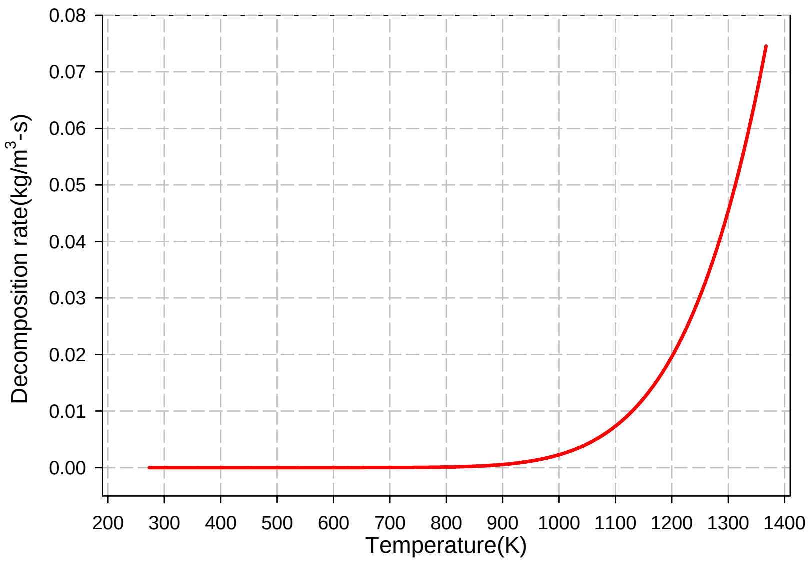

Figure 7. The rate of biomass decomposition versus temperature

5. Conclusion

The CFD code development is demonstrated in this paper. Since the biomass gasification is very complex process. All individual physics need to be modelled and programmed in separate subroutine and finally coupled until convergence was achieved. The couple between multi-physics is started from few variable then tested and calibrate with the experimental test whether it can properly describe the real process. Moreover, coupled stability also monitor at this stage. The couple between pyrolysis and solid biomass transport equation was demonstrated in this paper. It shows that coupling process is stable and reach convergence. However, the result of biomass decomposition is much slower than the experimental case. The Arrhenius rate parameter shows that the pyrolysis start at 800K which is considerable higher ignition temperature than in the experimental result. The parameter need to be revised whether it is appropriate description for rice husk decomposition rate.

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