A Numerical Model Simulation for an Updraft Gasifier Using High Temperature Steam

T. M. Ismail, M. Abd El-Salam

Abstract—A mathematical model study was carried out to investigate gasification of biomass fuels using high temperature air and steam as a gasifying agent using high-temperature air up to 1000°C. In this study, a 2D computational fluid dynamics model was developed to study the gasification process in an updraft gasifier, considering drying, pyrolysis, combustion, and gasification reactions. The gas and solid phases were resolved using a Euler–Euler multiphase approach, with exchange terms for the momentum, mass, and energy. The standard k–ε turbulence model was used in the gas phase, and the particle phase was modeled using the kinetic theory of granular flow. The results show that the present model giving a promise way in its capability and sensitivity for the parameter affects that influence the gasification process.

Keywords—Computational fluid dynamics, gasification, biomass fuel, fixed bed gasifier.

I. INTRODUCTION

The conversion of biomass materials has the precise objective to transform a carbonaceous solid material, which is originally difficult to handle, bulky and low energy concentration, into higher energy density fuels that permit easy storage and transfer through conventional pumping and transport systems [1]. Gasification is a chemical conversion process of any carbonaceous into a process or fuel gases with a useable heating value. The term ‘fuel gases’ represent gases that are destined for combustion purposes and their heat of combustion is of great importance, whereas ‘process gases’ are produced in chemical synthesis processes [2].

The gasification process requires some gasifying agent that provides oxygen for the formation of CO from solid carbon in the fuel. The gasifying agents include air, oxygen, steam, and CO2. The most common agent is air because of its extensive availability at no cost [3]. Steam is another alternative. The key advantage is that it increases the hydrogen content of the product gas. Furthermore, the production of tars is minimized, in particular at high steam temperatures. The presence of steam is important to further catalytic upgrading of the product syngas [4].

Numerical simulations have become popular in recognizing the complex gas–solid flow behaviors as in [5] and chemical reactions [6], which can offer the detailed information about the gasification processes and bridge the gap effectively between large-scale commercialized beds and small scale testing models. For gas–solid flow, two different calculation models can be used to describe the complex gas–solid flow behaviors. They are the trajectory model and the continuum description model [6]. As a most popular trajectory model, discrete element method (DEM) offers a more natural way to simulate gas–solid flow [7], but it becomes more and more computational expensive (CPU and memory resource requirements) as the number of particles increases. Eulerian approach is the other popular method for describing gas–solid flow due to little CPU and memory resource requirements [8]. In most recent continuum models constitutive equations according to the kinetic theory of granular flow (KTGF) are incorporated [9]. Benyahia et al. [10] and Zhong et al. [11] also applied KTGF to study the dense gas–solid flow characteristics of circulating fluidized bed and spout-fluid bed, respectively. Although numerical calculation has been widely used to simulate the gas–solid flow in fluidized beds, there has been little study on the simulation of gas–solid flow coupling with chemical reactions in updraft and downdraft gasifiers. Two methods could couple gas–solid flow with chemical reactions based on DEM and Eulerian approaches, respectively. For DEM-based simulation, the natural framework for the implementation of the physical models is offered. But it is computationally expensive, especially when the chemical reactions are added [12]. The other method, Eulerian-based simulation, has been used by Yu et al. [13] to simulate coal gasification in a bubbling fluidized bed gasifier.

The mathematical model of the gasifier in the present work will be simulated using a new development code, namely COMMENT-Code (Combustion Mathematics and Energy Transport) [14] to simulate the processes rate and combustion process within the bed. The model will be divided into two parts; firstly the process rate models and then the transport equation model for gas and solid phases. Validation of the code developed in the current study is conducted through experimental results for the HTAG process of biomass fuels [15].

II. EXPERIMENTAL SETUP

Fig. 1 shows the HTAG test facility that has been built at KTH-Royal Institute of Technology. This system has been described in a previous publication [16], [17]. The height of the gasifier is 3200mm with an internal diameter of 400mm. The produced gas flows out of the reactor at the top.

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III. COMPUTATIONAL FLUID DYNAMICS SIMULATION

The developed model presented in the current work to solve the governing equations of mass, momentum and energy, by means of a multi-fluid Eulerian model incorporating the Kinetic Theory of Granular Flow (KTGF), taking under consideration the process rates.

A. Process Rate Equations

1. Drying

The rate of moisture release from solids can be expressed as [18]:

\[ R_{\text{exp}} = A_h(T_s - 100^\circ C) \quad \text{T}_s < 100^\circ C \]  
(1)

or \[ R_{\text{exp}} = \frac{\rho_a}{R_{\text{exp}}} \text{T}_s = 100^\circ C \]  
(2)

\[ Q_{cr} = A^* \left( h_i^* \left( T_g - T_s \right) + \epsilon \left( T_g^* - T_s^* \right) \right) \]  
(3)

2. Pyrolysis

The pyrolysis is very important in updraft gasifier, where the volatilization of the biomass is assumed to give rise to volatile species and char [19].

\[ R_v = -\rho_a \frac{\partial \phi_v}{\partial t} = \rho_a Y_v A_v \rho \exp \left( \frac{E_v}{R_T} \right) \]  
(4)

\[ A_v = 3.63 \times 10^4 \frac{1}{J \cdot F} \cdot \frac{E_v}{R_T} = 9340 \]  

3. Gasification

The gaseous fuels released from the pyrolysis process have first to mix with the surrounding gasification agent before their chemical reaction can occur. In this model, the actual reaction rates of volatile species are taken as [14]:

\[ R = \min \left[ R_{\text{kin}}, R_{\text{mix}} \right] \]  
(5)

\[ R_{\text{mix}} = C_{\text{mix}} \rho_g \times A \times B \]  
(6)

\[ A = 150 \frac{D_y (1 - \phi)^{1/3}}{d_p \phi} + 1.75 \frac{V_y (1 - \phi)^{1/3}}{d_p \phi} \]  
\[ B = \min \left\{ \frac{C_{\text{mol}} \rho}{S_{\text{mol}} S_{\phi}} \right\} \]  
(6a)

The rate for each species is given by the following expressions;

\[ R_{\text{CH}_4} = 59.8 \frac{R_T}{T_g} \rho_{\text{CH}_4} \exp \left( \frac{-12200}{T_g} \right) \]  
\[ C_{\text{CO}} \frac{T_g}{2} \rho_{\text{CO}} \exp \left( \frac{-62700}{T_g} \right) \]  
\[ R_{\text{H}_2} = 3.9 \times 10^{17} \exp \left( \frac{-205000}{T_g} \right) \]  
\[ \left( \frac{C_{\text{H}_2}^{125} C_{\text{H}_2}^{25} C_{\text{H}_2}^{25}}{\text{RT}_g} \right) \]  
\[ R_{\text{H}_2} = 2.78 \exp \left( \frac{-12600}{R_T \rho} \right) \left( \frac{C_{\text{H}_2} C_{\text{H}_2}^{25}}{0.0265 \exp (65800/R_T)} \right) \]  
\[ R_{\text{H}_2} = 0.3 \times 10^9 \exp \left( \frac{-125400}{R_T \rho} \right) \]  
\[ C_{\text{CO}} \frac{C_{\text{H}_2} C_{\text{H}_2}^{25}}{0.0265 \exp (65800/R_T)} \]  
\[ R_{\text{H}_2} = 0.3 \times 10^9 \exp \left( \frac{-125400}{R_T \rho} \right) \]  
\[ C_{\text{CO}} \frac{C_{\text{H}_2} C_{\text{H}_2}^{25}}{0.0265 \exp (65800/R_T)} \]  
(7)

1. Continuity Equation

Gas Phase:

\[ \frac{\partial \phi_g}{\partial t} + \nabla \left( \phi_g \rho_g u_g \right) = S_{\phi_g} \]  
(16)

Solid Phase:

\[ \frac{\partial \left( 1 - \phi \right) \rho_s}{\partial t} + \nabla \left( (1 - \phi) \rho_s u_s \right) = -S_{\phi_g} \]  
(17)

\[ S_{\phi_g} = R_{\text{exp}} + R_v + R_c \]  
(18)

2. Momentum Equation

Gas Phase:

\[ \frac{\partial \left( \phi_g \rho_g u_g \right)}{\partial t} + \nabla \left( \phi_g \rho_g u_g \right) = -\nabla P_g + \phi_g g - \beta \left( u_g - u_s \right) + \nabla \left( \rho_g \right) \]  
(19)
The gas–solid inter-phase drag coefficient, $\beta$, is calculated as follows [20], [21];

$$\beta = 150 \left(1 - \phi\right)^2 \frac{\mu_T}{\phi \rho_p} + 1.75 \frac{\rho_b}{\phi} \left[U_g - U_s\right] \frac{d_p}{\rho_p}$$  \hspace{1cm} (20)

The gas phase stress tensor as follows;

$$\tau_g = \mu_b \left[ \nabla U_g + \nabla U_g^T \right] - \frac{2}{3} \mu_r \nabla (\nabla U_g)$$  \hspace{1cm} (21)

$$\mu_r = \mu_b + \mu_t$$  \hspace{1cm} (22)

$$\mu_t = \rho g C_t \frac{k^2}{\varepsilon}$$  \hspace{1cm} (23)

The stress tensor of the solid phase is expressed as

$$\tau_s = \mu_b \nabla u_s + \nabla (\mu_b \nabla u_s + u_s^2)$$  \hspace{1cm} (26)

where the stress tensor of the solid phase is expressed as follows;

$$\tau_s = \left( \mu_b - \frac{2}{3} \mu_s \right) \nabla u_s + \mu_s (\nabla u_s + u_s^2)$$  \hspace{1cm} (28)

The equation of the solid shear viscosity, $\mu_s$, is derived from [23] as follows;

$$\mu_s = \frac{4}{3} \left(1 - \phi\right) \rho_b \Delta_g$$  \hspace{1cm} (29)

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$$\mu_s = \frac{4}{3} \left(1 - \phi\right) \rho_b \Delta_g$$  \hspace{1cm} (29)

The solution process $P_s$ is as follows;

$$P_s = \left(1 - \phi\right) \rho_b \Theta_s + 2(1 + e)(1 - \phi)^2 g_0 \rho_b \Theta_s$$  \hspace{1cm} (31)

where $\Theta_s$ is granular temperature; $e$ is the coefficient of restitution for particle collisions; $g_0$ is the radial distribution function. For the restitution coefficient, the different values were presented, from 0.18 to 0.4. In the present work, a restitution coefficient value of 0.2 was used from [24]. For the radial distribution function of solid phase, $g_\phi$ is expressed as [25];

$$g_\phi = \frac{3}{5} \left[ 1 - \left( \frac{1 - \phi}{(1 - \phi)_{\text{max}}} \right)^2 \right]^{-1}$$  \hspace{1cm} (32)

The granular temperature $\Theta_s$ is a pseudo-temperature, which can be defined as:

$$\frac{3}{2} \Theta_s = \frac{1}{2} (u_s^2 + \Delta g)$$  \hspace{1cm} (33)

where $\zeta$ is a random number that obeys the Gauss distribution, $0 \leq \zeta \leq 1$.

3. Energy Equation

Gas Phase:

$$\frac{\partial}{\partial t} \left( \rho u_T \right) = \partial (\rho u_T v_T) + \rho_f (v_T \cdot \nabla) u_T$$  \hspace{1cm} (34)

Solid Phase:

$$\frac{\partial}{\partial t} \left( \rho \phi T \right) = \partial (\rho \phi T v_T) + \rho_f (v_T \cdot \nabla) T + \rho (\varepsilon_T - T)$$  \hspace{1cm} (35)

The radiative flux density is given by Rosseland (1936) [26] as follows;

$$\nabla q_r = -16T^2 - \frac{K}{3R} \left( \nabla T \right)^2 + 16T^3 - \frac{K}{3R} \left( \nabla T \right)^2$$  \hspace{1cm} (36)

The thermal dispersion coefficient $\lambda_g$ can be expressed as:

$$\lambda_g = k_{\text{eff,0}} + 0.5 \times d_p \times U_g \times \rho_g \times C_{pg}$$  \hspace{1cm} (37)

$$k_{\text{eff,0}} = \phi (k_f + h_s \Delta l) + \frac{\left(1 - \phi\right) \Delta l}{1/(\gamma - 1) + h_s / h_s}$$  \hspace{1cm} (38)

where $d_p = \frac{2d_p}{3}$, $k_f$ is the thermal conductivity of the pure solid, $h_s$, $h_s$, and $\Delta l$ are written as follows:

$$l = 0.1519 \times 12 \left( \frac{k_f}{k_{\text{eff}}} \right)$$  \hspace{1cm} (39)

$$h_s = 0.1952 \left( 1 + \frac{\phi (1 - e)}{2(1 - \phi) e} \right)^{-1} \frac{T_{\text{eff}}}{1000}$$  \hspace{1cm} (40)

$$h_s = 0.1952 \times d_p \left( \frac{e}{2} \right) \left( \frac{T_{\text{eff}}}{1000} \right)$$  \hspace{1cm} (41)

$$\Delta l = 0.96795 \times d_p \left( 1 - \phi \right)^{-1/3}$$  \hspace{1cm} (42)
The mass of charge was constant and equal to 20 kg. The temperature of the feed gas varied from 350 up to 900 °C whereas its flow rate was slightly varied from 50 to 56 Nm³/h. Molar fraction of the steam of the feed gas was varied from 0% up to 83%. All cases the gasification process starts as soon as the feedstock is charged into the gasifier.

<table>
<thead>
<tr>
<th>Case number (-)</th>
<th>Temperature of feed gas (°C)</th>
<th>Total flow of feed gas (Nm³/h)</th>
<th>Molar fraction of steam in feed gas (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C₁</td>
<td>350</td>
<td>50</td>
<td>0</td>
</tr>
<tr>
<td>C₂</td>
<td>700</td>
<td>50</td>
<td>0</td>
</tr>
<tr>
<td>C₃</td>
<td>830</td>
<td>53</td>
<td>25</td>
</tr>
<tr>
<td>C₄</td>
<td>900</td>
<td>53</td>
<td>52</td>
</tr>
<tr>
<td>C₅</td>
<td>900</td>
<td>56</td>
<td>83</td>
</tr>
</tbody>
</table>

V. RESULTS AND DISCUSSION

The geometry of the gasifier is approximately symmetrical in the width direction; therefore, the longitudinal section of the gasifier can be used as a 2D geometry. The fuel gas was assumed to leave from the gasifier top. The total number of mesh cells is 100,000. The time step is 10⁻² s and the gasification time of the biomass were resolved by 480000 time steps. The computational grid was adapted in each time step to the height of the gasifier. The staggered grid was utilized, which set vectors at the boundaries of cells and scalars at the center. The partial differential equations were discretized by the finite volume method (FVM) using the Upwind Difference Scheme.

Table I present operation conditions of 5 selected gasification runs of wood pellets (sized 12mm in diameter).
gasification is applied. The results show that the gasification temperature response to the change of the feed gas composition and temperature of the feed gas.

Results of Computational model and experiments conducted in a high-temperature air/steam fixed bed updraft gasifier presented in Figs. 4, 5 show the capability of this technology of maximizing the gaseous product yield as a result of the high heating rates involved and the efficient tar reduction. Increase of the feed gas temperature reduces production of tars, soot and char residue as well as increases the heating value of the dry fuel gas produced.

**Fig. 4** Effect of steam on molar fraction of H\textsubscript{2} (%) for various gasification processes (cases in Table I) gasification of 20 kg of wood pellets 12 mm; (a) H\textsubscript{2} 0%steam, (b) H\textsubscript{2} 25%steam, (c) H\textsubscript{2} 52%steam, (d) H\textsubscript{2} 83%steam

**Fig. 5** Effect of steam on molar fraction of CO\textsubscript{2} (%) for various gasification processes (cases in Table I) gasification of 20 kg of wood pellets 12 mm; (a) CO\textsubscript{2} 0%steam, (b) CO\textsubscript{2} 25%steam, (c) CO\textsubscript{2} 52%steam, (d) CO\textsubscript{2} 83%steam

A validation for the present model by the experimental setup is used in this study in order to allow a direct comparison with experimental measurements, to validate the presented model to be applicable with different cases for the gasification process in this experiment, the biomass types used for the investigation were Black pellets and Gray pellets. Black pellets are based on the 75% softwood and 25% hardwood, pretreated with a steam explosion. Gray pellets are normal
pellets without pretreatment. Fuel properties and characteristics are given in [16]. The prediction of the composition of the producer gas was in good agreement as shown in Fig. 6, probably caused by the complicated description of pyrolysis model inserted in the present model and also for the sufficient data for the pyrolysis of biomass obtained from experimental works by KTH [29].

Fig.6 Simulated and experimental effect of steam on syngases composition

VI. CONCLUSION

A Eulerian-Eulerian CFD model incorporating the kinetic theory of granular flow was applied, by developing a novel mathematical model in the form of COMMENT code applicable for predicting combustion and gasification processes of biomass fuel using high air/steam temperature, giving a promise way in its capability and sensitivity for the parameter effects that influence the gasification process.

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NOMENCLATURE

\begin{itemize}
  \item \(A\): pre-exponent factor, particle surface area \(1/s, \text{m}^2\)
  \item \(C_p\): specific heat capacity \(\text{J/kg K}\)
  \item \(C_{mix}\): mixing rate constant
  \item \(C_{w,g}\): moisture concentration in the gas phase \(\text{kg/m}^3\)
  \item \(C_{w,s}\): moisture concentration at the solid phase \(\text{kg/m}^3\)
  \item \(D_g\): mass diffusion coefficient of gas \(\text{m}^2/\text{s}\)
  \item \(D_m\): mass diffusion coefficient of oxygen \(\text{m}^2/\text{s}\)
  \item \(d_p\): particle diameter \(\text{m}\)
  \item \(E\): activation energy \(\text{kJ/mol}\)
  \item \(H_{evp}\): evaporation heat of the solid material \(\text{J/kg}\)
  \item \(h_{r,s}\): radiation heat transfer coefficient \(\text{W/m}^2\)
  \item \(h_{r,v}\): effective radiation heat transfer coefficient of the voids \(\text{W/m}^2\)
  \item \(h_c\): convective mass transfer coefficient
  \item \(h_v\): convection heat transfer coefficient \(\text{W/m}^2\)
  \item \(I\): radiative intensity \(\text{W}\)
  \item \(K\): extinction coefficient
  \item \(K_d\): turbulent kinetic energy \(\text{m}^2/\text{s}^2\)
  \item \(k_d\): diffusion rates \(\text{kg/\text{atm m}^2}\)
  \item \(k_t\): thermal conductivity of the fluid \(\text{W/mK}\)
  \item \(k_s\): thermal conductivity of the pure \(\text{W/mK}\)
  \item \(k_p\): absorption coefficient
  \item \(k_{eff}\): effective thermal conductivity \(\text{W/mK}\)
  \item \(k_{eff,0}\): thermal conductivity for no fluid flow \(\text{W/mK}\)
  \item \(l_s\): equivalent thickness a layer of solid \(\text{m}\)
  \item \(M\): molecular weight \(\text{kg/kmol}\)
  \item \(Q_{cr}\): heat absorbed by the solid \(\text{W}\)
  \item \(q_r\): radiative flux density \(\text{W}\)
  \item \(R\): gas universal constant \(\text{J/kmol K}\)
  \item \(R_{evp}\): moisture evaporation rate \(\text{kg/s}\)
  \item \(R_c\): char consumption rate \(\text{kg/s}\)
  \item \(R_{sr}\): steam reform reaction \(\text{kg/s}\)
  \item \(R_v\): volatile matter in solid rate \(\text{kg/s}\)
  \item \(R_{wg}\): water gas shift reaction \(\text{kg/s}\)
  \item \(S_{\Phi}\): Source term
  \item \(T_{env}\): environment temperature \(\text{K}\)
  \item \(T_g\): gas temperature \(\text{K}\)
  \item \(T_s\): solid temperature \(\text{K}\)
  \item \(X\): species generation
  \item \(Y\): mass fraction of volatile matter
  \item \(U\): velocity component \(\text{m/s}\)
\end{itemize}

Greek Letters

\begin{itemize}
  \item \(\alpha\): absorption coefficient
  \item \(\beta\): drag coefficient
  \item \(\mu\): dynamic viscosity \(\text{kg/m s}\)
  \item \(\Phi\): void fraction in bed
  \item \(\epsilon\): dissipation rate of turbulent kinetic energy \(\text{m}^2/\text{s}^3\)
  \item \(\varepsilon\): Emissivity
  \item \(\sigma_p\): scattering coefficient
  \item \(\Sigma\): Stephan-Boltzmann constant \(\text{W/m}^2\text{K}^4\)
  \item \(P\): density \(\text{kg/m}^3\)
  \item \(\lambda_{th}\): thermal dispersion coefficient
  \item \(\lambda_{mix}\): effective dispersion coefficient
  \item \(\Phi\): dependent variable
  \item \(\tau_s\): stress tensor \(\text{Pa}\)
\end{itemize}

Subscripts

\begin{itemize}
  \item \(b\): Bulk
  \item \(C\): char burnout
eff Effective
  \item \(f\): Fluid
  \item \(g\): Gas
  \item \(p\): Particle
  \item \(s\): Solid
  \item \(sg\): solid to gas
\end{itemize}

REFERENCES