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 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.

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.
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]:

\[ R_{\text{exp}} = A_{h} h_{s} (C_{w,s} - C_{w,b}) T_{s} < 100^\circ C \]  
(1)

or \[ R_{\text{exp}} = \frac{Q_{C}}{h_{w}} T_{s} = 100^\circ C \]  
(2)

\[ Q_{C} = A_{t} (h_{i} (T_{g} - T_{s}) + \epsilon \delta (T_{s} - T_{g}^{2})) \]  
(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].

\[ R_{g} = -\rho_{b} \frac{dV}{dt} = \rho_{b} Y_{g} A_{v} n_{g} \exp \left( \frac{E_{g}}{RT_{g}} \right) \]  
(4)

\[ A_{v} = 3.63 \times 10^{3} \frac{1}{1/s} \cdot \frac{E_{v}}{R} = 9340 \]  

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]:

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

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

\[ A = 150 \frac{D_{w}(1 - \phi)^{1/3}}{d_{p} \phi} + 1.75 \frac{V_{w}(1 - \phi)^{1/3}}{d_{p} \phi} \]  
(6a)

\[ B = \min \left( \frac{C_{\text{fuel}}}{S_{\text{fuel}}}, \frac{C_{\text{char}}}{S_{\text{char}}} \right) \]  
(6b)

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

\[ R_{CH} = 59.8 T_{g}^{0.6} \exp \left( \frac{-12,200}{T_{g}} \right) \]  
(7)

\[ R_{CO} = 1.3 \times 10^{11} \exp \left( \frac{-62,700}{T_{g}} \right) \]  
(8)

\[ R_{H_{2}} = 3.9 \times 10^{17} \exp \left( \frac{-20,500}{T_{g}} \right) \]  
(9)

\[ R_{CO} = 2.78 \exp \left( \frac{-12600}{R T_{g}} \right) \left( C_{CO} C_{H_{2}} - 0.0265 \exp (65000/R T_{g}) \right) \]  
(10)

\[ R_{C} = 0.3 \times 10^{9} \exp \left( \frac{-125400}{R T_{g}} \right) \]  
(11)

4. Combustion

\[ C + a O_{2} \rightarrow (1-a)CO + (2a-1)CO_{2} \]

\[ a = \frac{CO}{CO_{2}} = 2500 \exp \left( \frac{-6420}{T} \right) \]  
(12)

For temperatures between 730 and 1170 K

\[ R_{c} = \frac{P_{o_{2}}}{K_{c} + K_{r}} \]  
(13)

\[ K_{c} = 5.06 \times 10^{-7} \left( \frac{T + T_{s}}{2} \right)^{0.75} \]  
(14)

\[ K_{r} = A_{c} T_{e} \exp \left( \frac{E_{r}}{RT_{e}} \right) \]  
(15)

\[ A_{c} = 3 \text{ kg/m}^{3} \text{s kPa and } E_{r}/R = 10300 \text{ K} \]

B. Transport Equations for Gas and Solid Phases

1. Continuity Equation

Gas Phase:

\[ \frac{\partial (\rho_{\phi} u_{\phi})}{\partial t} + \nabla \cdot (\rho_{\phi} u_{\phi} u_{b}) = S_{gb} \]  
(16)

Solid Phase:

\[ \frac{\partial ((1 - \phi) \rho_{s})}{\partial t} + \nabla \cdot (\rho_{s} u_{b}) = -S_{gb} \]  
(17)

\[ S_{gb} = R_{\text{exp}} + R_{v} + R_{c} \]  
(18)

2. Momentum Equation

Gas Phase:

\[ \frac{\partial (\rho_{\phi} u_{\phi})}{\partial t} + \nabla \cdot (\rho_{\phi} u_{\phi} u_{b}) = -\phi \nabla p_{g} + \phi \rho_{g} g - \beta (u_{g} - u_{s}) + \nabla \phi \tau_{g} \]  
(19)
The gas–solid inter-phase drag coefficient, $\beta$, is calculated as follows [20, 21]:

$$\beta = 150 \frac{(1 - \phi)^2 \mu_T}{\phi d_p^2} + 1.75 \frac{\rho_s(1 - \phi)}{d_p} \left| U_g - U_s \right|$$  (20)

The gas phase stress tensor is expressed as:

$$\tau_g = \mu_g \left[ \nabla u_g + \nabla u_g^T \right] - \frac{2}{3} \mu_g \nabla \left( \nabla \cdot u_g \right)$$  (21)

$$\mu_T = \mu_g + \mu_s$$  (22)

$$\mu_s = \rho_g C_v \frac{k^2}{\varepsilon}$$  (23)

$C_v$ is the constant, which is set as 0.09.

The governing transport equations for $k$ and $\varepsilon$ respectively are:

$$\frac{\partial}{\partial t} (\phi \rho_k u_k) + \nabla \cdot (\phi \rho_k \nabla u_k) = \nabla \cdot (\phi \rho_k \mu_T \nabla u_k) + \phi g_k - \phi \rho_k \varepsilon$$  (24)

$$\frac{\partial}{\partial t} (\phi \rho_{\varepsilon} \varepsilon) + \nabla \cdot (\phi \rho_{\varepsilon} \varepsilon \nabla \varepsilon) = \phi C_f \varepsilon - C_d \rho_{\varepsilon} e^C \varepsilon$$  (25)

In the above equations $G_k$ represents the generation of turbulence kinetic energy due to the mean velocity gradients and is expressed as follows:

$$G_k = \mu_k \nabla u_k \cdot \nabla u_k - \frac{2}{3} \mu_k \nabla(\nabla \cdot u_k) + \rho_g k$$  (26)

$C_{c1} = 1.44$ and $C_{c2} = 1.92$, the turbulent Prandtl numbers of $k$ and $\varepsilon$ are $C_{c1} = 1$ and $C_{c2} = 1.3$, respectively [22].

Solid Phase:

$$\frac{\partial}{\partial t} (\phi \rho_{\varepsilon} \varepsilon) + \nabla \cdot (\phi \rho_{\varepsilon} \varepsilon \nabla \varepsilon) = \nabla \cdot (\phi \rho_{\varepsilon} \mu_s \nabla \varepsilon) + A_\varepsilon \left( \nabla \cdot \nabla \varepsilon \right) + S_{\varepsilon}$$  (27)

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

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

In the above equation represents the bulk viscosity, which may be obtained as follows:

$$\mu_s = \frac{4}{3} (1 - \phi) \rho_s d_g g_s$$  (29)

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

$$\mu_s = \frac{2}{3} \left( 1 - \phi \right) \rho_s g_s \left( 1 + e \right)^2 \left[ 1 + \frac{10}{12} \left( \nabla \cdot u_s \right)^2 \right] \left[ 1 + \frac{3}{2} \rho_s (1 - \phi)(1 + e) \right]^2$$  (30)

The solid pressure $P_s$ is as follows:

$$P_s = (1 - \phi) \rho_s g_s \Theta_s + 2(1 + e)(1 - \phi)^2 g_s \rho_s \Theta_s$$  (31)

where $\Theta_s$ is granular temperature; $e$ is the coefficient of restitution for particle collisions; $g_s$ 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, $g_s$ is expressed as [25]:

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

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

$$\frac{3}{2} \Theta_s = \frac{1}{2} \left( \frac{u_s^2}{c_s^2} \right)$$  (33)

$u_s^2$ is the fluctuating velocity of the particles and can be determined by turbulence kinetic energy as follows:

$$u_s^2 = \zeta \left( \frac{2k}{3} \right)^{0.5}$$

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

3. Energy Equation

Gas Phase:

$$\frac{\partial (\phi \rho \varepsilon)}{\partial t} + \nabla \cdot (\phi \rho \varepsilon \nabla \varepsilon) = \nabla \cdot (\phi \rho \mu_T \nabla \varepsilon) + A_{\varepsilon} \varepsilon + S_{\varepsilon}$$  (34)

Solid Phase:

$$\frac{\partial (\phi \rho_{\varepsilon} \varepsilon)}{\partial t} + \nabla \cdot (\phi \rho_{\varepsilon} \varepsilon \nabla \varepsilon) = \nabla \cdot (\phi \rho_{\varepsilon} \varepsilon \nabla \varepsilon) + A_{\varepsilon} \varepsilon + S_{\varepsilon}$$  (35)

The radiative flux density is given by Rosseland (1936) as follows:

$$\nabla q_r = -16\sigma T^4 (\nabla T)^2 + 16\sigma T^3 (\nabla^2 T)$$  (36)

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

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

$$k_{eff,0} = \phi (k_t + h_{rs} \Delta l) + \frac{(1 - \phi) \Delta l}{(l_{T_s} + h_{rs} + l_{T_s})}$$  (38)

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

$$l_{T_s} = 0.151912 \left( \frac{k_t}{k_{al}} \right)$$  (39)

$$h_{rs} = 0.1952 \left( \frac{1 + \phi(1 - e)}{2(1 - \phi) e} \right) \left( \frac{T_s}{100} \right)^n$$  (40)

$$h_{rs} = 0.1952 \times d_p \left( \frac{c_s}{2} \right) \left( \frac{T_s}{100} \right)^n$$  (41)

$$\Delta l = 0.96795 \times d_p (1 - \phi)^{-1/3}$$

k_{air} is the air thermal conductivity,
\[ k_{air}(T_g) = 5.66 \times 10^{-5}T_g + 1.1 \times 10^{-2} \]  
(42)

\( n \) is an empirical parameter related to the fuel packing conditions. In this model,
\[ n = 1.93 + 0.67 \exp \left( -\frac{(m_p-0.39)}{0.054} \right) \]  
(43)

Source term of the energy equation for both gas and solid is calculated as follows:
\[ S_{T_g} = -R_{exp} \times h_{f,CO} \]  
\[ S_{T_s} = -R_{exp} \times \frac{M_{CO}}{M_{CO}} \times [h_{f,CO2} - h_{f,CO}] \times \left( \frac{Y_{CO}}{2} - 1 \right) \]  
(45)

4. Species Equation

**Gas Phase:**
\[ \frac{\partial (\rho \phi Y_i)}{\partial t} + \nabla \left( \rho \phi_i u_j Y_i \right) = \nabla \left( D_i \nabla (\rho \phi_i Y_i) \right) + S_i \]  
(46)

**Solid Phase:**
\[ \frac{\partial ((1-\phi) \rho_i Y_i)}{\partial t} + \nabla \left( (1-\phi) \rho_i u_j Y_i \right) = S_i \]  
(47)

**IV. NUMERICAL METHOD AND BOUNDARY CONDITIONS**

The transport equations described earlier form a set of nonlinear parabolic partial differential equations can be solved numerically, by using the SIMPLE algorithm. Transport equations are generalized into a standard form;
\[ a_{ij}\Phi_{i,j} + a_{i,j-1}\Phi_{i,j-1} + a_{i,j+1}\Phi_{i,j+1} + a_{i-1,j}\Phi_{i-1,j} + a_{i+1,j}\Phi_{i+1,j} = S_{ij} \]  
(48)

The whole geometrical domain of the bed is divided into a number of small cells and (48) is discretized over each cell and solved numerically using SIMPLE algorithm [27, 28].

The feedstock used for the present model was wood pellets. The fuel has a composition (ultimate analysis) of C, 50.4%; H, 6.2%; O, 42.8%. Other properties were ash, 0.4%; total moisture, 8.22%; fixed C, 15.7%; volatiles, 83.9%; LHV, 17.1MJ/kg.

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^{-5} 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 presents operation conditions of 5 selected gasification runs of wood pellets (sized 12mm in diameter).

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 I: Operation Conditions for Run Cases

<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**

Figs. 2, 3 show that the higher the molar fractions of steam in the feed gas, the higher the content of hydrogen in the produced gas. Comparing the effect of the feed gas (air and steam) it could be seen that increase of the lower heating value was due to the increases in the molar fraction of the combustible gases (H₂, and CO₂) caused by the pyrolysis process and cracking of hydrocarbons when high-temperature
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 H₂ (%) for various gasification processes (cases in Table I) gasification of 20 kg of wood pellets 12 mm; (a) H₂ 0%steam, (b) H₂ 25%steam, (c) H₂ 52%steam, (d) H₂ 83%steam

Fig. 5 Effect of steam on molar fraction of CO₂(%) for various gasification processes (cases in Table I) gasification of 20 kg of wood pellets 12 mm; (a) CO₂ 0%steam, (b) CO₂ 25%steam, (c) CO₂ 52%steam, (d) CO₂ 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 world Academy of Science, Engineering and Technology.

International Scholarly and Scientific Research & Innovation 8(5) 2014 scholar.waset.org/1999.8/9998128
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].

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.

ACKNOWLEDGMENT

Many thanks to Associate Professor Weihong Yang at Royal Institute of Technology (KTH) for his continuous support, supervision and the fruitful discussion. Special thanks are directed towards Yueshi Wu for technical supervision in this work during the experimental and theoretical work. We also would like to express our gratitude to all the collaborators from the Royal Institute of Technology.

NOMENCLATURE

Greek Letters

A absorption coefficient
B drag coefficient
M dynamic viscosity kg/m s
Φ dependent variable
ε dissipation rate of turbulent kinetic energy m²/s³
σp scattering coefficient
Σ Stephan-Boltzmann constant W/m² K⁴
P density kg/m³
λd thermal dispersion coefficient
λmix effective dispersion coefficient

Subscripts

A pre-exponent factor, particle surface area 1/s, m²
Cp specific heat capacity J/kg K
Cmix mixing rate constant
Cw,g moisture concentration at the gas phase kg/m³
Cw,s moisture concentration at the solid phase kg/m³
Dmix mass diffusion coefficient of gas m²/s
dp particle diameter m
E activation energy K/mol
Hevaporation heat of the solid material J/kg
h incalpy of formation J/kg
hr,s radiation heat transfer coefficient m/s
hr,v effective radiation heat transfer coefficient of the voids m/s
hc convective mass transfer coefficient
hc convection heat transfer coefficient W/m² K
I radiative intensity W
K extinction coefficient
K turbulent kinetic energy m²/s²
kd diffusion rates kg/atm m² s
kr thermal conductivity of the fluid W/mK
ks thermal conductivity of the pure W/mK
kp absorption coefficient
koff effective thermal conductivity W/mK
koff,0 thermal conductivity for no fluid flow W/mK
ls equivalent thickness a layer of solid m
M molecular weight kg/kmol
Qs heat absorbed by the solid W
qr radiative flux density W
R gas universal constant J/kmol K
Recp moisture evaporation rate kg/s
Re char consumption rate kg/s
Rv steam reform reaction kg/s
Rv volatile matter in solid rate kg/s
Rwg water shift reaction kg/s
SΦ Source term
Tenv environment temperature K
Tg gas temperature K
Ts solid temperature K
X species generation
Yv mass fraction of volatile matter
U velocity component m/s

REFERENCES