Part-Load Simulations and Experiments of a Small Coal Gasifier

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ABSTRACT

An oxygen-blown, coal powder-feed, entrained-flow demonstration gasifier was constructed and operated by the Industrial Technology Research Institute (ITRI) in Taiwan. Specific tests have been conducted to investigate the gasifier's performance and gain operation experience under part-load conditions either caused by reduced load demands or maintenance needs. Water spray near the exit of the gasifier was employed to test its feasibility in tuning H$_2$ content or controlling gas exit temperature. To help understand the gasifying characteristics of various part-load conditions, computational simulation was conducted using the commercial CFD solver FLUENT. The 3-D Navier-Stokes equations and seven species transport equations were solved with eddy-dissipation combustion model.

The simulation results provide the velocity, temperature, and species distributions inside the gasifier. The results indicate that water spray injection cools down the gas and increases H$_2$ mole fraction at the cost of the reduction of CO and increased production of CO$_2$. It is recommended that a better way to produce H$_2$ is to inject steam near the feedstock injection ports where plenty carbon is available and temperature is high and favorable to produce H$_2$ more efficiently via the gasification reaction without producing CO$_2$. The simulated results were compared with the experimental data including situations when two of the three fuel injectors were under maintenance. Employing fuel injection through a single injector unexpectedly performs better than applying three injectors. The results indicate the injection velocity speed and momentum strength of each injector, rather than the total injection momentum, are more influential in affecting the gasification efficiency. The results of this study can be used to improve prediction of future part load performance.

1.0 INTRODUCTION

The Energy and Resources Laboratories of the Industrial Technology Research Institute (ITRI) constructed a demonstration gasifier [Hsu, et. al., 2003] in the Southern Taiwan city of Kaohsiung. The gasifier, shown in Fig. 1, is designed for a maximum load of two tons of coal per day. The gasifier is operated with oxygen-blown scheme. Coal powder is transported by nitrogen and is fed from the bottom. The produced hot gas flows upwards and exits from the top. A water spray device is installed on the top of the gasifier to adjust the H$_2$ or CO content of the syngas. If necessary, the water spray device is also used to control the exit gas temperature. Slag that forms on the inside wall flows to the bottom and is quenched in a water bath.

This facility is designed to convert pulverized coal and petroleum cokes into syngas at a pressure below 15 bar. The designed coal gasification efficiency under full-load operation is approximately 75%, and carbon conversion exceeds 90%. The experimental system includes the following major sections: solids handling, solids feeding, gas feeding, gasification, syngas cooling, slag discharge, fines removal.

The solids feed materials include pulverized coal, petroleum cokes, and fluxing agents such as limestone. The feed materials are pulverized to a size distribution of greater than 70% by weight by passing through 200 mesh. The feed solids are discharged by the hoppers via rotary feeders and a screw conveyor, and then transferred to the three feed injection vessels. The feed solids are discharged from the injection vessels by variable speed metering screws located at the bottom of the injection vessels. These screws are used to control the rate that the solids are fed into the pipes of gasifier. The feed solids are mixed with oxygen and steam and injected into the gasifier through three feed nozzles by a dense-phase pneumatic conveying system using high-pressure nitrogen.

The gasifier consists of a gasification section and a slag quench section. The gasification section is a single-stage, refractory-lined, entrained-flow reactor where the feed solids react with oxidants and steam to be converted into syngas. The molten slag generated from the gasification section falls into the slag quench section for water quenching. Hot syngas leaving the top of the gasifier is subjected to an optional water spray for tuning H$_2$ content or controlling gas temperature.

The solidified fly slag and unreacted coal, upon leaving the gas cooler, enters a cyclone separator, where the entrained fines are removed from the cooled syngas stream. The fines fall into a fines lockhopper, which is periodically isolated and depressurized. Syngas leaving the cyclone separator is partially depressurized by the gasifier.
backpressure valve and then routed to the flare. The cleanup system will be installed to remove H₂S and fine particles from syngas to meet the requirements for power generation.

![Figure 1](image)

Figure 1 (a) Actual facility and (b) schematic of the ITRI Gasifier. The computational domain is highlighted red.

During the experiments, the system has not been able to maintain the full-load operation for an extended time. Various operational issues and maintenance calls have frequently affected the operation to be undertaken under part-load conditions. Therefore, it is desired to obtain some educated knowledge of the gasifier performance under various part-load conditions. To this end, specific tests are conducted to investigate the gasifier's performance and to gain operation experience under part-load conditions. In addition, computational simulations are conducted to help understand the gasifying characteristics of various part-load conditions. The ultimate goal is to compare the simulated and experimental results to improve the simulation model. The improved model is expected to be used for providing guidance for selecting appropriate approaches for future part-load and off-design operations.

### 1.1 Gasification Process

The global chemical reactions of coal gasification [Smoot and Smith, 1985] can be generalized as below:

**Heterogeneous (solid and gas) phase**

\[
\begin{align*}
C(s) + \frac{1}{2} O_2 & \rightarrow CO, \quad \Delta H^{°}_R = -110.5 \text{ MJ/kmol} \quad \text{(R1.1)} \\
C(s) + CO_2 & \rightarrow 2CO, \quad \Delta H^{°}_R = +172.0 \text{ MJ/kmol} \quad \text{(R1.2)} \\
C(s) + H_2O(g) & \rightarrow CO + H_2, \quad \Delta H^{°}_R* = +131.4 \text{ MJ/kmol} \quad \text{(R1.3)} \\
\end{align*}
\]

Gasification, Boudouard reaction

**Homogenous gas phase**

\[
\begin{align*}
CO + \frac{1}{2} O_2 & \rightarrow CO_2, \quad \Delta H^{°}_R = -283.1 \text{ MJ/kmol} \quad \text{(R1.4)} \\
CO + H_2O(g) & \rightarrow CO_2 + H_2, \quad \Delta H^{°}_R = -41.0 \text{ MJ/kmol} \quad \text{(R1.5)} \\
CO + 3H_2 & \rightarrow CH_4 + H_2O, \quad \Delta H^{°}_R = -205.7 \text{ MJ/kmol} \quad \text{(Methanation)} \\
C + 2H_2 & \rightarrow CH_4, \quad \Delta H^{°}_R = -87.4 \text{ MJ/kmol} \quad \text{(Direct methanation)} \\
\end{align*}
\]

Reactions given in R1.1 and R1.4 are two exothermic reactions that provide the complete energy for the gasification. Based on these global reactions, approximately 22% of the stoichiometric oxygen is required to provide sufficient energy for gasification reactions. In real applications, 25~30% of the
stoichiometric oxygen is provided to ensure high-efficient carbon conversion. Methanation (R1.6 and R1.7) is assumed to be negligible in this study, so it is not included in the computational model in this study.

Partial combustion occurs when the coal mixes with oxygen (R1.1). The energy released from (R1.1) also heats up any coal that has not burned. When the coal is heated without oxygen, it undergoes pyrolysis during which phenols and hydrocarbon gases are released. At the same time, char gasification (R1.2) takes place and releases CO. If a significant amount of steam exists, gasification (R1.3) and water shift reaction (R1.5) occur and release H₂.

2.0 COMPUTATIONAL MODEL

The schematic of the ITRI gasifier is shown in Fig. 1. The area highlighted by the red bold line is the computational domain considered for this study. The detailed computational model and associated equations have been documented in detail by Silaen and Wang [2005 and 2006]. Only the major procedures are outlined in this paper.

2.1 Physical Characteristics of the Model and Assumptions

The physical characteristics of the model are:

1. Three-dimensional
2. Buoyancy force and radiation are considered
3. Varying fluid properties
4. Impermeable walls

The following general assumptions are made in this study:

1. The flow is steady.
2. No-slip condition (zero velocity) is imposed on wall surfaces.
3. Chemical reaction is faster than the time scale of the turbulence eddies: eddy dissipation model is adopted.
4. Walls are insulated (i.e. adiabatic).
5. Slagging is not considered.

2.2 Governing Equations

The equations for conservation laws of mass, momentum, and energy are given as:

\[
\nabla \cdot (\rho \mathbf{v}) = S_m \tag{1}
\]

\[
\nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \left( \frac{\tau}{\rho} \right) + \rho \bar{g} + \mathbf{F} \tag{2}
\]

\[
\nabla \cdot (\rho (\mathbf{v} E + p)) = \nabla \cdot \left( \lambda_{\text{eff}} \nabla T - \sum_j h_j \mathbf{J}_j + \left( \tau_{\text{eff}} \cdot \mathbf{v} \right) \right) + S_h \tag{3}
\]

where \( \lambda_{\text{eff}} \) is the effective conductivity which include the molecular thermal conductivity(\( \lambda \)) and the turbulence conductivity \( \lambda_{\text{t}} \). \( \mathbf{J}_j \) is the flux of species \( j \).

The stress tensor \( \tau \) is given by

\[
\tau = \mu \left( \nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) - \frac{2}{3} \nabla \cdot \mathbf{v} I \tag{4}
\]

where \( \mu \) is the molecular dynamic viscosity, \( I \) is the unit tensor, and the second term on the right-hand side is the effect of volume dilatation. The first three terms on the right-hand side of equation (3) represent heat transfer due to conduction, species diffusion, and viscous dissipation. \( S_h \) is a source term including the enthalpy formation from the chemical reaction of the species. The energy \( E \) is defined as

\[
E = h - \frac{p}{\rho} + \frac{v^2}{2} \tag{5}
\]

where \( h \) is the sensible enthalpy and for incompressible flow given as

\[
h = \sum_j Y_j h_j + \frac{p}{\rho} \tag{6}
\]

\( Y_j \) is the mass fraction of species \( j \) and

\[
h = \int_{T_{\text{ref}}}^T c_{p,j} \, dT \tag{7}
\]

where \( T_{\text{ref}} \) is the reference temperature set at 298.15 K.

2.3 Turbulence Model

The standard \( k-\varepsilon \) turbulence model is used in this simulation due to its suitability for a wide range of wall-bound and free-shear flows. The standard \( k-\varepsilon \) turbulence model is robust, economic for computation, and accurate for a wide range of turbulent flows. The turbulence kinetic energy, \( k \), and its rate of dissipations, \( \varepsilon \), are calculated from the equations from the paper by Lauder and Spalding [1972]. Both buoyancy and minor compressibility effects on the turbulence model are considered.

The turbulence models are valid for the turbulent core flows, i.e. the flow in the regions not in the immediate proximity of the wall. The flow very near the walls is affected by the presence of the walls. In the viscous sublayer, where the solution variables change most rapidly, is not solved in this study. Instead, wall functions, which are a collection of semi-empirical formulas and functions, are employed to connect the viscosity-affected region between the wall and the fully-turbulent region [Lauder and Spalding, 1974]. The wall functions consist of (i) laws-of-the-wall for mean velocity and temperature (or other scalars) and (ii) formulas for near-wall turbulent quantities. The standard wall functions for velocity, temperature, and species are employed in this study. See Sailen and Wang [2005 and 2006] for details.
2.4 Radiation Model

The P-1 radiation model is used to calculate the flux of the radiation at the inside walls of the gasifier. The P-1 radiation model is the simplest case of the more general P-N radiation model that is based on the expansion of the radiation intensity I. The P-1 model requires only a little CPU demand and can easily be applied to various complicated geometries. It is suitable for applications where the optical thickness aL is large where “a” is the absorption coefficient, and L is the length scale of the domain.

The heat sources or sinks due to radiation is calculated using the equation

\[-\nabla q_r = aG - 4aG\varepsilon_w \quad (8)\]

where

\[q_r = -\frac{1}{3(a+\sigma_s)}C\sigma_g VG\quad (9)\]

and \(q_r\) is the radiation heat flux, \(\sigma_s\) is the scattering coefficient, \(G\) is the incident radiation, \(C\) is the linear-anisotropic phase function coefficient, and \(\sigma\) is the Stefan-Boltzmann constant.

The flux of the radiation, \(q_{r,w}\), at walls caused by incident radiation \(G_w\) is given as

\[q_{r,w} = -\frac{4\pi\varepsilon_w}{\pi} \frac{\sigma T_w^4}{4(1-\rho_w)} G_w \quad (10)\]

where \(\varepsilon_w\) is the emissivity and is defined as

\[\varepsilon_w = 1 - \rho_w \quad (11)\]

and \(\rho_w\) is the wall reflectivity. See FLUENT user guide for details [2005].

2.5 Combustion Model

The global reaction mechanism is modeled to involve the following chemical species: C, O2, N2, CO, CO2, H2O and H2 (see reactions R1.1 through R1.5). The experimental data shows methanation is insignificant in the studied gasifier, so reactions R1.6 and R1.7 are not included in the simulation. All of the species are assumed to mix in the molecular level. The chemical reactions inside the gasifier are modeled by calculating the transport and mixing of the chemical species by solving the conservation equations which describe convection, diffusion, and reaction of each component species. The general form of the transport equation for each species is given as

\[\frac{\partial}{\partial t} (\rho Y_i) + \nabla \cdot (\rho \nabla Y_i) = -\nabla \cdot \vec{J}_i + R_i. \quad (12)\]

\(R_i\) is the net rate of production of species \(i\) by chemical reaction. \(\vec{J}_i\) is the diffusion flux of species \(i\), which arises due to concentration gradients. Mass diffusion for laminar flows is

\[\vec{J}_i = -\left( \rho D_{i,m} + \frac{\mu_i}{Sc_t} \right) \nabla Y_i \quad (13)\]

where \(D_{i,m}\) is the laminar bidiffusional coefficient and \(Sc_t\) is the turbulent Schmidt number.

In this study, the eddy-dissipation model is used. The assumption in this model is that the chemical reaction is faster than the time scale of the turbulence eddies. Thus, the reaction rate is determined by the turbulence mixing of the species. The reaction is assumed to occur instantaneously when the reactants meet. The sources term \(R_i\) in equation (26) is calculated using the eddy-dissipation model based on the work of Magnusen and Hjertager [1976]. The net rate of production or destruction of species \(i\) as the result of reaction \(r\), \(R_{i,r}\), is given by the smaller of the two expressions below.

\[R_{i,r} = v'_{i,r} M_{i,r} A \rho \varepsilon \min \left( \frac{Y_R}{v'_{r,r} M_{w,r}} \right) \quad (14)\]

and

\[R_{i,r} = v''_{i,r} M_{i,r} B \rho \varepsilon \left( \sum_j v''_{r,j} M_{w,j} \right) \quad (15)\]

where \(v'_{i,r}\) is the stoichiometric coefficient of reactant \(i\) in reaction \(r\) and \(v''_{r,j}\) is stoichiometric coefficient of product \(j\) in reaction \(r\).

In equations (14) and (15), the chemical reaction rate is governed by large-eddy mixing time scale, \(k/\varepsilon\). The smaller of the two expressions (14) and (15) is used because it is the limiting value that determines the reaction rate.

The procedure to solve the reactions is as follows:

1. The net local production or destruction of species \(i\) in each reaction (R1.1 to R1.5) is calculated by solving equations (14) and (15).
2. The smaller of these values is substituted into the corresponding species transport equation (12) to calculate the local species mass fraction, \(Y_i\).
3. \(Y_i\) is then used to calculate the net enthalpy production of each reaction equation.
4. The net enthalpy production becomes the source term in energy equation (3) that affects the temperature distribution. In an endothermic process, the net enthalpy production is negative, which becomes a sink term in the energy equation.

2.6 Discrete Phase (Water Droplets)

When the water spray is used to increase the hydrogen content in the syngas or to reduce the syngas temperature, the discrete phase of water droplets are computed separately by
modeling each individual droplet's heat transfer, water vaporization, and water vapor mass transfer. The interactions among particles are not modeled.

**Droplet Flow and Heat Transfer** — Basically, the droplets in the airflow can encounter inertia and hydrodynamic drags. Because of the forces experienced by a droplet in a flow field, the droplet can be either accelerated or decelerated. The velocity change can be formulated by

\[
m_p \frac{dv_p}{dt} = F_d + F_g + F_o
\]

where \( F_d \) is the drag of the fluid on the droplet and \( F_g \) is the gravity. \( F_o \) represents the other forces, and \( v_p \) is the droplet velocity (vector). Among the forces represented by \( F_o \) are typically included the “virtual mass” force, thermophoretic force, Brownian force, Saffman's lift force, etc.

Theoretically, evaporation occurs at two stages: (a) when temperature is higher than the saturation temperature (based on local water vapor concentration), water evaporates from the droplet's surface, and the evaporation is controlled by the water vapor partial pressure until 100% relative humidity is achieved; (b) when the boiling temperature (determined by the air-water mixture pressure) is reached, water continues to evaporate even though the relative humidity reaches 100%. After the droplet is evaporated due to either high temperature or low moisture partial pressure, the vapor diffuses into the main flow and is transported away. The rate of vaporization is governed by concentration difference between surface and air stream, and the corresponding mass change rate of the droplet can be given by,

\[
\frac{dm_p}{dt} = \pi d^2 k_c (C_e - C_{ie})
\]

where \( k_c \) is the mass transfer coefficient and \( C_e \) is the concentration of the vapor at the droplet surface, which is evaluated by assuming that the flow over the surface is saturated. \( C_{ie} \) is the vapor concentration of the bulk flow, obtained by solving the transport equations. The values of \( k_c \) can be calculated from empirical correlations by [Ranz and Marshall, 1955]:

\[
Sh = \frac{k_c d}{D} = 2.0 + 0.6Re_d^{0.5}Sc^{0.33}
\]

where \( Sh \) is the Sherwood number, \( Sc \) is the Schmidt number (defined as \( v/D \)), \( D \) is the diffusion coefficient of vapor in the bulk flow. \( Re_d \) is the Reynolds number, defined as \( uv/d, \( u \) is the flow velocity.

When the droplet temperature reaches the boiling point, the following equation can be used to evaluate its evaporation rate [Kuo, 1985]:

\[
\frac{dm_p}{dt} = \pi d^2 \left( 2.0 + 0.46Re_d^{0.5} \right) \ln \left( 1 + c_p (T_e - T)/h_{fg} \right)/c_p
\]

where \( \lambda \) is the heat conductivity of the gas/air, and \( h_{fg} \) is the droplet latent heat. \( c_p \) is the specific heat of the bulk flow.

The droplet temperature can also be changed due to heat transfer between droplets and the continuous phase. Without considering radiation heat transfer, the droplet's sensible heat change depends on the convective heat transfer and latent heat (\( h_{fg} \)), as shown in the following equation.

\[
\frac{m_p c_p}{dt} = \pi d^2 h (T_e - T) + \frac{dm_p}{dt} h_{fg}
\]

where the convective heat transfer coefficient (\( h \)) can be obtained with a similar empirical correlation to Eq. 18:

\[
Nu_d = \frac{hd}{\lambda} = 2.0 + 0.6 Re_d^{0.5} Pr^{0.33}
\]

where \( Nu \) is the Nusselt number, and \( Pr \) is the Prandtl number.

In the gasifier, the temperature of main flow will be above the water boiling temperature. Notice the characteristic velocity in \( Re_d \) is the relative velocity between the droplet and gas flow, which is usually small for droplets in micrometers. Therefore, \( Re_d \) is also very small. In addition, the term \( c_p(T_e - T)/h_{fg} \) in Eq. 19 can be much smaller than 1 (0.04 in this study). By ignoring the term with \( Re \) and using \( \ln(1+\delta) = \delta \), the approximate droplet evaporation time can be obtained as:

\[
t = \frac{h_{fg} \rho d^2}{2 \lambda (T_e - T)}
\]

This equation can be used to design the location of the water spray to ensure that water can be fully evaporated before the gasifier exit.

**Stochastic Particle Tracking** - The effects of turbulence on the dispersion of droplets/particles is considered by using stochastic tracking. Basically, the droplet trajectories are calculated by using the instantaneous flow velocity (\( \bar{u} + u' \)) rather than the average velocity (\( \bar{u} \)). The velocity fluctuations are then given as:

\[
u' = \zeta (\bar{u}^2)^{0.5} = \zeta (2k/3)^{0.5}
\]

where \( \zeta \) is a normally distributed random number. This velocity will apply during the characteristic lifetime of the eddy (\( t_e \)), a time scale defined by either of the following equations:

\[
t_e = 0.3k/\epsilon
\]

\[
t_e = -0.15k/\epsilon \log(r)
\]

where \( r \) is a uniform distributed random number ranging from 0 to 1. In case the droplet slip velocity is so large that the time for the droplet to cross the eddy is shorter than the time defined above, the droplet eddy crossing time will be used, which is defined as:
where \( t_p \) is the particle relaxation time with \( t_p = \frac{\rho_p d^2_p}{18 \rho g \nu_g} \), \( L_e \) is the eddy length scale, and \( |u-u_p| \) is the magnitude of the relative velocity. After this time period, the instantaneous velocity will be updated with a new \( \zeta \) value until a full trajectory is obtained. The random effect of the turbulence on the droplets can predicted reasonably only if a sufficient number of trajectories are calculated. In this study, the trajectory number is chosen to be 25 and several test runs indicated that increasing this number does not make the result much different.

### 2.7 Inlet and Boundary Conditions

Indonesian coal is used as feedstock in this study. Its composition is given in Table 1. The inlet and boundary conditions are given in Table 2 and Fig. 2a. A total of 204,509 tetrahedral meshes are used as shown in Fig. 2b.

**Table 1 Composition of Indonesia Coal.** The 38.81% (wt) of volatiles are absorbed as C and H.

<table>
<thead>
<tr>
<th>Solids or Liquids</th>
<th>Weight %</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>61.52</td>
</tr>
<tr>
<td>H</td>
<td>4.35</td>
</tr>
<tr>
<td>O</td>
<td>12.82</td>
</tr>
<tr>
<td>N</td>
<td>1.12</td>
</tr>
<tr>
<td>S</td>
<td>0.5</td>
</tr>
<tr>
<td>Ash</td>
<td>6.32</td>
</tr>
<tr>
<td>Moisture</td>
<td>13.37</td>
</tr>
<tr>
<td><strong>Total, wt %</strong></td>
<td><strong>100</strong></td>
</tr>
<tr>
<td><strong>HHV kcal/kg</strong></td>
<td><strong>5690</strong></td>
</tr>
</tbody>
</table>

**Table 2 Input and boundary conditions for the baseline full-load case**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal feed rate (kg/h)</td>
<td>83.5</td>
</tr>
<tr>
<td>Steam feed rate (kg/h)</td>
<td>3.14</td>
</tr>
<tr>
<td>Oxidant feed rate (kg/h)</td>
<td>76.23</td>
</tr>
<tr>
<td>Transport nitrogen feed (kg/h)</td>
<td>24.05</td>
</tr>
<tr>
<td>Water spray (kg/h)</td>
<td>24.01</td>
</tr>
</tbody>
</table>

### 3.0 COMPUTATIONAL PROCESS

The preprocessing tool used in the study is GAMBIT, which provides one interface to build and mesh the geometry.

The CFD solver used in this study is the commercial CFD code FLUENT Version 6.1.22 [2005]. Fig. 3 illustrates the basic program structure that can be used to support CFD simulation in FLUENT. FLUENT is a finite-volume-based CFD solver written in C language and has the ability to solve fluid flow, heat transfer and chemical reactions in complex geometries and supports both structured and unstructured meshes. Buoyancy induced flow is calculated. The density in the buoyancy term in the momentum equation is calculated using the ideal gas law.

![Figure 2](image-url)  
(a) Boundary conditions  
(b) Meshed computational domain

The segregated solution method is used. Segregated solution solves the governing equations of continuity, momentum, energy, and species transport sequentially (segregated from one another). The non-linear governing equations are linearized implicitly with respect to the dependent variables. The second order discretization scheme is applied for the momentum, the turbulence kinetic energy, the turbulence kinetic dissipation, the energy, and all the species. The SIMPLE algorithm Patankar et. al [1980] is used in this study as the algorithm for pressure-velocity coupling. The built-in standard \( k-\varepsilon \) turbulence model is used. Lagrangian trajectory calculations are employed to model the dispersed phase of droplets. The impact of droplets on the continuous phase is considered as source terms to the governing equations. After obtaining an approximate flow field of the continuous phase (gasflow in this study), droplets are injected and their trajectories are calculated. At the same time, drag, heat and mass transfer between the droplets and the gasflow is calculated. Ten iterations are performed in the continuous phase for every one iteration performed in the discrete phase.
Converged results are obtained after the specified residuals are met. A converged result renders mass residual of $10^{-3}$, energy residual of $10^{-6}$, and momentum and turbulence kinetic energy residuals of $10^{-5}$. These residuals are the summation of the imbalance for each cell, scaled by a representative of the flow rate. Typically, 2000 to 3000 iterations are needed to obtain a converged result, which takes about three hours on a parallel processor with four 2.8 GHz Pentium 4 personal computers.

**Figure 3 Segregated solution method.**

**4.0 RESULTS AND DISCUSSIONS**

The total water spray rate (24.01 kg/h) is based on the value for the full-load operation with 83.5 kg/h of coal and 186.84 kg/hr total of feedstock at the operating pressure of 14.8 bars. Seven cases are simulated in this study:

Case 1: Full load with water spray at 14.8 bars — baseline.
Case 2: 50% load with prorated 50% water spray at 14.8 bars.
Case 3: Full load without water spray at 14.8 bars.
Case 4: Simulating experimental case at 49.7% load via one injector with prorated water spray at 2.04 bars.
Case 5: Simulating experimental case at 20.3% load via one injector with prorated water spray at 4.32 bars.
Case 6: Simulation of Case 4 with three fuel injectors feeding the same total mass flow as in Case 4. Each fuel injector in Case 6 is 1/3rd of the load in Case 4.
Case 7: Simulation of Case 4 with all three fuel injectors feeding the same mass flow as in Case 4. The total mass flow rate in Case 7 is three times the total load in Case 4.

Parameters for seven simulated cases are listed in Table 3. The simulation results on the gas temperature, carbon fuel conversion efficiency, and the mass-weighted average mole fractions of species at the gasifier outlet are listed in Table 4.

**Table 3 Parameters for simulated cases**

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Case 1</th>
<th>Case 2</th>
<th>Case 3</th>
<th>Case 4</th>
<th>Case 5</th>
<th>Case 6</th>
<th>Case 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel</td>
<td>100%</td>
<td>100%</td>
<td>100%</td>
<td>49.7%</td>
<td>49.7%</td>
<td>49.7%</td>
<td>149.1%</td>
</tr>
<tr>
<td>Spray</td>
<td>100%</td>
<td>50%</td>
<td>0%</td>
<td>49.7%</td>
<td>49.7%</td>
<td>49.7%</td>
<td>49.7%</td>
</tr>
<tr>
<td>Pressure, bar</td>
<td>14.8</td>
<td>14.8</td>
<td>14.8</td>
<td>2.04</td>
<td>4.32</td>
<td>2.04</td>
<td>2.04</td>
</tr>
<tr>
<td>Total mass flow rate, kg/s</td>
<td>0.0519</td>
<td>0.0258</td>
<td>0.0519</td>
<td>0.0241</td>
<td>0.0105</td>
<td>0.0241</td>
<td>0.0722</td>
</tr>
<tr>
<td>Coal mass flow rate, kg/s</td>
<td>0.0232</td>
<td>0.0116</td>
<td>0.0232</td>
<td>0.0115</td>
<td>0.0047</td>
<td>0.0115</td>
<td>0.0346</td>
</tr>
<tr>
<td>Water spray, kg/s</td>
<td>0.0067</td>
<td>0.0033</td>
<td>0.0000</td>
<td>0.0033</td>
<td>0.0014</td>
<td>0.0033</td>
<td>0.0099</td>
</tr>
<tr>
<td>Mass fraction at inlet</td>
<td>C</td>
<td>0.2751</td>
<td>0.2751</td>
<td>0.2751</td>
<td>0.2947</td>
<td>0.2621</td>
<td>0.2947</td>
</tr>
<tr>
<td></td>
<td>H₂O</td>
<td>0.107</td>
<td>0.107</td>
<td>0.107</td>
<td>0.1147</td>
<td>0.102</td>
<td>0.1147</td>
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<tr>
<td></td>
<td>H₂</td>
<td>0.0195</td>
<td>0.0195</td>
<td>0.0195</td>
<td>0.0208</td>
<td>0.0185</td>
<td>0.0208</td>
</tr>
<tr>
<td></td>
<td>O₂</td>
<td>0.4443</td>
<td>0.4443</td>
<td>0.4443</td>
<td>0.4072</td>
<td>0.467</td>
<td>0.4072</td>
</tr>
<tr>
<td></td>
<td>N₂</td>
<td>0.1541</td>
<td>0.1541</td>
<td>0.1541</td>
<td>0.1625</td>
<td>0.154</td>
<td>0.1625</td>
</tr>
</tbody>
</table>
Components at exit:
efficiency, %  
Fuel conversion  
Gasification efficiency, %  
Carbon fuel conversion efficiency  
Exit temperature, K  
Heating value (MJ/kg)  

Parameters  
sectional area along the height of the gasifier as shown in  
of each gas component is calculated across the cross-
height of 0.3 m are due to the injections of coal, steam, and  

Fig. 5. The dips of temperature and CO curves in Fig. 5 at  

reacts with the remaining O$_2$ to produce CO$_2$ through  
This process is not an efficient process to produce fuel or heating  
value because it converts the fuel CO to H$_2$ and CO$_2$.  The  
production of CO$_2$ reduces the fuel heating value. It is more  
efficient to produce H$_2$ from the gasification reaction C +  
H$_2$O$ightarrow$ CO + H$_2$ (R1.3), in which no CO$_2$ is produced.  
The production of CO$_2$ reduces the fuel heating value. It is more  
efficient to produce H$_2$ from the gasification reaction C +  
H$_2$O$ightarrow$ CO + H$_2$ (R1.3), in which no CO$_2$ is produced.  
However, if more H$_2$ is needed as the end product, the water  
shift process is an optional process to produce H$_2$ among  
several other alternative methods.

As listed in Table 4, 100% of the carbon has reacted  
before the gas exits the gasifier. This fast reaction could be  
due to the eddy-dissipation model used in this study. In the  
eddy-dissipation model, the chemical reactions are assumed  
to be faster than the turbulence time scale; so for the size of  
this gasifier, the residence time is sufficient for all the  
reactions to be completed when the flow exits the gasifier.  
To evaluate the gasifier performance, four different  
indicators are defined in this study:

- The carbon conversion efficiency  
- The carbon fuel conversion efficiency  
- The fuel conversion efficiency  
- Gasification efficiency

The carbon conversion efficiency is defined as  
Carbon conversion  

\[
\text{carbon conversion} = 1 - \frac{\text{carbon at the exit}}{\text{raw carbon} + \text{recycled carbon}} 
\]  

\[(27)\]
Although the carbon conversion efficiency is 100% in Case 1 (i.e. no carbon is left, C = 0%), not all carbon is converted to useful fuel. The portion of carbon that is converted to CO\(_2\) is not beneficial, so the indicator "carbon conversion efficiency" does not inform how much carbon is converted to the useful fuels, CO or CH\(_4\), in this study. Therefore, another term "carbon fuel conversion efficiency" is adopted and defined as the percentage of carbon converted into the useful fuels, CO or CH\(_4\), and written as,

\[
\text{Carbon fuel conversion efficiency} = \frac{[\text{CO} + \text{CH}_4\text{]}}{[\text{raw carbon}]} \tag{28}\]

So, the useful carbon conversion of Case 1 is not 100% even though 100% of carbon reacts, but rather 20% is converted to CO. Eighty percent of the carbon reacts to produce CO\(_2\), which is not a useful fuel, in the final product.

The third performance indicator, fuel conversion efficiency, is defined as the ratio of the total moles of the useful fuel gases produced (H\(_2\), CO, and CH\(_4\)) to the total moles of value of the raw carbon, water, and oxygen injected in the process. This definition can fairly compare the effectiveness of conversion of hydrogen and oxygen into useful fuels between oxygen-blown and air-blown schemes as well as dry and wet feed methods. The fuel conversion efficiency is written as,

\[
\text{Fuel conversion efficiency} = \frac{[\text{H}_2 + \text{CO} + \text{CH}_4]}{[\text{raw carbon} + \text{H}_2\text{O} + \text{O}_2]} \tag{29}\]

The ultimate gasification performance indicator, gasification efficiency, is defined as the ratio of the total heating value of the useful syngas produced (H\(_2\), CO, and CH\(_4\)) to the total heating value of the coal injected in the process. The gasification efficiency is written as,
Gasification efficiency = \frac{[H_2 + CO + CH_4]_{heating\ value}}{[coal]_{heating\ value}} \quad (30)

The fuel conversion efficiency and gasification efficiency in Case 1, as given in Table 4, are 54% and 70%, respectively, which are relatively low. The heating value of the syngas is 6.9 MJ/kg, which is also low compared to a typical oxygen-blown gasifier. The reason for this low fuel conversion efficiency is postulated to be caused by the low steam injection accompanied by over-supplied oxygen (34% in Case 1 versus a typical 25%-30% of the stoichiometric value for a gasifier). When steam is not sufficiently available, the gasification process \(C(s) + H_2O(g) \rightarrow CO + H_2\) (R1.3) does not occur. With oversupplied oxygen, the condition is favorable for burning carbon monoxide via \(CO + \frac{1}{2} O_2 \rightarrow CO_2\) (R1.4). This can be evidenced by the very high temperature (2800K) in the gasifier as combustion is stronger than needed. A later stage of water spray near the gasifier exit exacerbates the endothermic water-shift reaction \(CO + H_2O(g) \rightarrow CO_2 + H_2\) (R1.5), which produces H2 in a less effective process (than the endothermic gasification process, R1.3) by producing CO2. This can be evidenced by the drop of CO and rise of CO2 at a height of 2.8 m in the gasifier in Fig. 5. One approach to improve the fuel conversion efficiency is to take advantage of the gasification reaction R1.3 by injecting more steam near the fuel injector when carbon is still available rather than at the exit when carbon has been converted to CO.

4.2 Effect of Different Fuel Feed Rates with Prorated Water Spray

Case 2 is simulated to investigate the effects of using a different fuel feed rate. The fuel load percentage for Cases 2 is 50% of the full load. The water spray rate is also changed in proportion to the change of fuel feed rate. The result listed in Table 4 shows that Cases 1 and 2 have nearly the same exit gas temperature and compositions. Reducing fuel feed 50% does not affect the exit gas composition.

4.3 Effects of Removing Water Spray

Since Case 1 shows that water spray near the gasifier exit ineffectively converts CO to H2 with co-production of CO2, it is interesting to see if the syngas heating value can be improved by eliminating water spray. This is investigated as Case 3. The result given in Table 4 shows that the exit gas temperature (2032 K) is higher than that of Case 1 (1774 K). As expected, the exit gas contains a much higher mole fraction of CO (28%) than in Case 1 (9%), lower H2 (35.4% vs. 44.3%) and lower CO2 (24.1% vs. 35.9%). As a result, the fuel conversion efficiency is higher (65% vs. 54%) as well as the heating value (8.0 MJ/kg vs. 6.9 MJ/kg).

The mass-weighted averages of gas composition and temperature distributions are shown in Fig. 6. The mole fractions of CO, H2, and CO2 maintain almost constant values in the gasifier higher than 0.5m after the fuel injection. In contrast, the gas temperature drops about 400 K from 0.5 m to the exit. This temperature drop is a manifestation of the two endothermic gasification reactions \(C(s) + CO_2 \rightarrow 2CO\) and \(C(s) + H_2O(g) \rightarrow CO + H_2\), even though the increases of CO and H2 and the reduction of CO2 are slight (see Fig. 6).

4.4 Comparison With the Experimental Data

Two experimental cases, Cases 4 and 5, are simulated, and their results are compared to the measured data. The experiments were conducted for part-load conditions with only one fuel injector in operation at low operating pressures. The exact water spray feed rates are not recorded, so amounts of water prorated from the full load are used in the simulation.

The simulated results are listed in Table 4 and are compared with the measured data in Table 5. The gas mole fractions given in Table 5 are the values that have been normalized excluding N2. This study does not include reactions that involve CH4 so no CH4 mole fractions are available from the CFD results in Table 4. The comparison shows CFD of Case 4 underpredicts CO and CO2 by approximately 2.5 and 8 percentage points, respectively. On the other hand, it overpredicts H2 by roughly 9 percentage points. This might be caused by injecting water in the simulation than actually being sprayed, so more CO is converted to H2 via the water shift reaction. It also overpredicts the carbon conversion efficiency. The simulation predicts that all the carbon reacts, i.e. 100% carbon conversion efficiency, while the measured data shows that only 66% of carbon reacts. The gasification efficiency is significantly overpredicted. This could be contributed by the eddy-dissipation model which tends to overpredict the rates of the reactions that consume char (R1.1 through R1.3).
Table 5  Comparison of simulated result to measured data for Cases 4 and 5.  $N_2$ is not included in the mole fraction calculation.

<table>
<thead>
<tr>
<th></th>
<th>Case 4 Measured</th>
<th>Case 5 Measured</th>
<th>Case 4 CFD</th>
<th>Case 5 CFD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exit gas mole fraction:</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$CO$</td>
<td>22.00%</td>
<td>19.48%</td>
<td>36.86%</td>
<td>4.50%</td>
</tr>
<tr>
<td>$H_2$</td>
<td>38.52%</td>
<td>49.61%</td>
<td>26.49%</td>
<td>49.55%</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>39.27%</td>
<td>30.91%</td>
<td>35.81%</td>
<td>45.95%</td>
</tr>
<tr>
<td>$CH_4$</td>
<td>0.21%</td>
<td>-</td>
<td>0.85%</td>
<td>-</td>
</tr>
<tr>
<td>Gas temp above inlet, K</td>
<td>1594 1700-2000</td>
<td>1495 1500-2500</td>
<td>1500-2500</td>
<td></td>
</tr>
<tr>
<td>Carbon conv. efficiency</td>
<td>66%</td>
<td>100%</td>
<td>94%</td>
<td>100%</td>
</tr>
<tr>
<td>Gasification efficiency</td>
<td>39%</td>
<td>81%</td>
<td>52%</td>
<td>64%</td>
</tr>
</tbody>
</table>

A reading from a thermocouple inserted immediately above the feedstock injection port recorded a local temperature at 1594 K. The simulated temperature at the same location is about 2000 K, which is approximately 400 K above the measured value. The temperature difference between the simulated and measured value seems large; however, the temperature field (Fig. 7) near the thermocouple measuring location shows large temperature gradient and gives a gas temperature range from 1700 K to 2000 K within a few centimeters. Considering the uncertainty in accurately determining the measuring locations during the experiment and the uncertainty in predicting the flame fronts near the fuel injectors, it could be fair to state that the simulated temperature is roughly 100-400 K higher than the measured data. Similarly, strong temperature gradients, actually stronger than in Case 4, exist near the thermocouple measurement location in Case 5 (Fig. 7). The temperature drops almost 1,000 K within a short distance above the fuel injectors. The higher predicted temperature is also attributed to the adiabatic wall assumption made for the simulation.

The comparison between the simulated and measured data for Case 5 shows the simulation significantly underpredicts the CO mole fraction but overpredicts $H_2$ and $CO_2$ mole fractions and the carbon conversion efficiency. This might be caused by injecting too much water before the gasifier exit in the simulation and consequently converts too much CO into $H_2$ and $CO_2$ than in the experiment. Predicted exit gas composition in Case 4 is closer to the experimental data than in Case 5; it seems also more water is injected in the simulation than in the experiment. Therefore, it is important to accurately record the amounts of water spray in future experiments. The prediction of coal gasification efficiency is off by 12 percentage points in Case 5 but significantly overpredicted in Case 4.

The discrepancies between the simulated and the experimental results could be attributed by the following possible reasons:

- The eddy-dissipation model of the reaction rates could provide faster rates and earlier equilibrium status than the real reaction, so the gasification efficiency and carbon conversion efficiency are both overpredicted. Finite rate reaction model is recommended for future analysis.
- Since the data were obtained under off-design, part-load conditions, the data could be taken under transient or nonequilibrium conditions, which might render less-efficient gasification than under the steady-state and equilibrium condition in simulations.
- Higher temperature gradients exist near the feedstock injection region. A minor mismatch in the measurement locations with those in the computational results would cause large temperature difference.
- The amount of water spray is not known. This would throw the simulations in either the under or over prediction direction.

![Temperature distributions for Cases 4 and 5.](image)

**Figure 7** Temperature distributions for Cases 4 and 5.

### 4.5 Effects of Number of Injections

Cases 6 and 7 are simulated to investigate the effects of the number of injectors on the gasifier performance. In Case 6, the same total fuel feed rates as in Case 4 is used, but it is injected through all three injectors, as opposed to only one injector as in Case 4. Changing from Case 6 to Case 4 is similar to a situation when two of the three injectors are under
maintenance, and the only operating injector has to take the entire load. In Case 7, the same fuel feed rate injected through the one injector in Case 4 is injected through each of the three injectors. Changing from Case 7 to Case 4 is similar to a situation when two of the three injectors fail and the remaining injector continues to inject at the same rate. The total fuel feed rate in Case 4 is therefore 1/3rd of Case 7.

The result in Table 4 shows that Case 4 has a better performance than Case 6. The exit gas for both cases have nearly the same H₂ content (roughly 44%), but the CO content of Case 4 (17.4%) is six percentage points higher than that of Case 6. As a result, the heating value of the syngas for Case 4 (8.5 MJ/kg) is higher than Case 6 (7.4 MJ/kg). This is contrary to our intuition that employing three injectors would give a better performance because three injectors usually produces more uniform and stronger reactions than employing only one injector. Since the major difference between operating one and three injectors is associated with flow pattern, investigation is then directed towards studying the flow field of these two cases.

The flow pathlines for Cases 4, 6 and 7 are shown in Fig. 8a, 8b, and 8c, respectively. The flow leaving the single injector in Case 4 is nine times stronger in momentum than the flow leaving each of the three injectors in Case 6. Thus, the cyclonic flow in Case 4 is stronger than in Case 6 and creates faster mixing and reactions. Flow animation movie (not shown in this paper) shows that there is a strong twisting flow moves towards bottom in Case 4 due to the strong cyclone-induced low-pressure core. This patch of gas later spirals upward from the bottom moving opposite to the downward moving core. This downward moving flow is also observed in Case 6, but it is weaker. It is postulated that this downward mixing would enhance gasification and fuel conversion efficiencies.

The gasification performance and syngas composition of Case 7 are on par with Case 4 even though the total mass flow rate in Case 7 is three times more than Case 4. It is postulated that the strength of each injector is the primary factor that strongly affected the cyclone strength because the momentum and speed from each injector is identical between Cases 4 and 7. When compared with syngas composition in Case 4, the CO mole fraction is higher but the H₂ and CO₂ mole fractions are lower in Case 7. This may indicate that the water-shift reaction after the water injection in Case 7 is not as strong as in Case 4. The higher gas velocity induced by the higher total mass flow rate of Case 7 may lead to insufficient time to allow sprayed water to effectively react with CO through the water-shift reaction. As a result, less CO reacts with H₂O and less H₂ and CO₂ are produced. A small amount of water is noticed to remain at the exit. Figure 8 shows that flow pathlines of Case 7 is similar to Case 6 except the water-shift process downstream of the water injection is pushed towards the water injector site by the faster and stronger through-gas flow.
CONCLUSIONS

The results of the baseline case (100% fuel feed rate, 100% water spray) shows that spraying water near the exit of the gasifier is not an effective approach to produce H₂ because the water shift process $CO + H_2O(g) \rightarrow CO_2 + H_2$, is likely to take place by converting CO (a good fuel) to CO₂ and H₂. The production of CO₂ during water shift process reduces the fuel heating value. Rather, it is more efficient to produce H₂ from the gasification reaction $C + H_2O \rightarrow CO + H_2$, in which no CO₂ is produced. If more H₂ is needed as the end product, it is recommended that steam be injected near the feedstock injection ports when plenty carbon is available and temperature is high. The steam can be generated from waste heat without consuming the gas flow energy. Spraying water will take energy away from the gas flow and reduce efficiency. Furthermore, with reduced temperature, the water shift reaction is more likely to take place than the more effective gasification reaction.

Comparison between the simulated and the part-load experimental data shows discrepancies. The CFD simulation usually overpredicts the carbon conversion efficiency and gasification performance. This could be attributed to the eddy-dissipation reaction rate model, which seems to produce faster than the actual reaction rates in this study. The simulation also overpredicts H₂ but underpredicts CO, possibly caused by injecting more water than the unknown actual amounts. The discrepancy in temperature comparison could be contributed by the uncertainty of thermocouple measurement location and the extremely large temperature gradients surrounding the measurement locations.

Employing fuel injection through a single injector unexpectedly performs better than applying three injectors. The results indicate the injection velocity speed and momentum strength of each injector, rather than the total momentum, could be more influential in affecting the gasification efficiency. The computational model developed in this study, although complex as it seems, is still rudimentary in predicting the complicated gasification process. Further improvements are required including incorporating finite rate reactions and imposing temperature and pressure factors upon the reaction rates.

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REFERENCES


