# Numerical Investigation of Top Fuel Injection Design in a Coal Gasifier

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## ABSTRACT

Computational Fluid Dynamics (CFD) schemes are employed to simulate the effects of potential fuel injection techniques on gasification performance. The objective is to help design the top-loaded fuel injection arrangement for an entrained flow gasifier using coal water slurry as the input feedstock. Two specific arrangements are investigated: (a) coaxial dual jets impingement with slurry coal in the center and oxygen in the outer jet and (b) four jets impingement with two single slurry coal jets and two single oxygen jets.

When the heterogeneous finite-rate solid-gas reaction scheme is implemented, it is discovered that the particle collision model can't be implemented with the heterogeneous gasification scheme in the present computational model. The instantaneous gasification model is later employed to examine the particle collision phenomenon by implementing the particle collision model, in which the coal (consisting of carbon and volatiles) is injected as gas, and the water is injected as droplets. The result of droplet tracks shows that the droplets are not bounced around, as speculated, at the intersection where the jets meet, and majority of the droplets passes through the jet impingement section and hit the wall as the finite rate case. This implies that the results of the finite rate are acceptable even though the particle collision model is not implemented. The finite-rate result actually presents a worst-case scenario for predicting wall erosion. The particle tracks for both the 2 concentric and 4 separate injection configurations show that the coal particles hit the wall and can accelerate deterioration of the refractory bricks. The case employing two concentric injections provides better fuel-oxidant mixing and higher heating value than the case using four separate injections.

## 1.0 INTRODUCTION

The Industrial Technology Research Institute (ITRI) in Taiwan has installed and operated a small experimental oxygen-blown, entrained-flow coal gasifier in Kaohsiung for four years. Currently, dry pulverized coal is pneumatically transported via nitrogen to the gasifier and injected tangentially from the bottom of the gasifier (see Wang et. al. 2006). A new gasifier is currently on the drawing board, and a different fuel feeding scheme via injecting water slurry coal is under consideration. Instead of injecting the dry pulverized coal from the bottom of the gasifier, the water slurry coal will be injected from the top of the gasifier. Since there are many different means to inject the fuel, conducting experiments to investigate many different options is a time consuming and expensive process. To help narrow the number of experimental variables and guide design direction, the **objective** of this study is to employ a Computational Fluid Dynamics (CFD) scheme to investigate the gasification performance by simulating various fuel injection schemes.

Several potential fuel injection configurations are studied. The schematic of the new gasifier is presented in Fig. 1. Instead of injecting tangentially, the fuel and oxidant are injected 45 degrees downward toward the center from the top of the gasifier. The gas and coal from both injectors will impinge at the center. With these new injectors, the gas and particles flow downward and exit from the bottom. The gasifier's inside diameter is enlarged to 0.6m from the existing 0.3m by replacing the current refractory brick with a thinner but higher thermal resistance brick. The outside diameter of the gasifier remains the same as 0.6m. The height remains the same at 3m. The coal is mixed with water to form a 60%-40% coal/water (by weight) slurry mixture before being fed into the gasifier.

### 1.1 TASKS

This study focuses on the following two specific tasks:

(1) Coaxial dual jets impingement --- The fuel injector consists of two coaxial pipes. The water slurry coal is transported through the inner pipe, and the oxygen is transported through the outer annular passage. Two injectors (Fig. 1) are located diametrically and are oriented in an downward angle (θ) to impinge against each other at the centerline of the gasifier.

(2) Four jets impingement --- Four injectors are arranged as shown in Fig. 2. A pair of injectors is located diametrically and inject coal water slurry. The second pair of injectors is located $90^{o}$ from the first pair and injects oxygen only. Again, all four injectors are oriented azimuthally in an downward angle of $45^{o}$ to impinge against each other at the centerline of the gasifier.

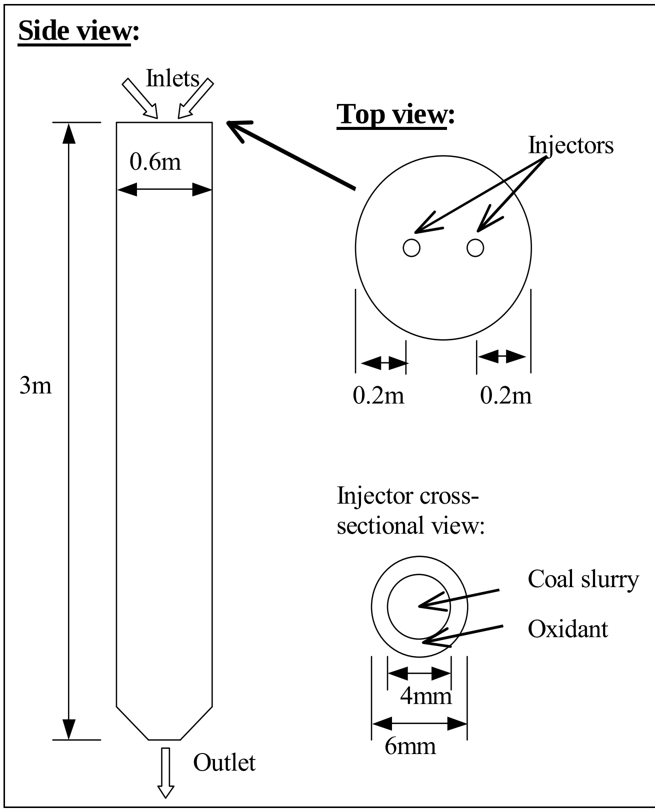


Fig. 1 Modified gasifier with two inclined jets.

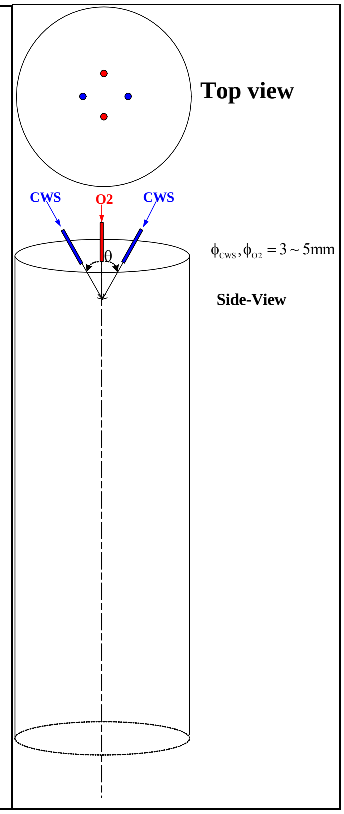


Fig. 2 Four jets impinging.

### 1.3 Global Gasification Chemical Reactions

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

Heterogeneous (solid and gas) phase

$C(s) + \frac{1}{2} O_2 \rightarrow CO$, $\Delta H^\circ_R = -110.5$ MJ/kmol (R1.1)

$C(s) + CO_2 \rightarrow 2CO$, $\Delta H^\circ_R = +172.0$ MJ/kmol (R1.2)
(Gasification, Boudouard reaction)

$C(s) + H_2O(g) \rightarrow CO + H_2$, $\Delta H^\circ_R = +131.4$ MJ/kmol (R1.3)
(Gasification)

Homogenous gas phase

$CO + \frac{1}{2} O_2 \rightarrow CO_2$, $\Delta H^\circ_R = -283.1$ MJ/kmol (R1.5)

$CO + H_2O(g) \rightarrow CO_2 + H_2$, $\Delta H^\circ_R = -41.0$ MJ/kmol (R1.6)
( Water-shift)

$CH_{2.121}O_{0.5855} \rightarrow 0.5855CO + 0.8532H_2 + 0.06907C_6H_6$ (R1.7)
(Volatile cracking)

$C_6H_6 + 3O_2 \rightarrow 6CO + 3H_2$ (R1.8)
(Volatile gasification via benzene)

The volatiles are assumed to go through a thermal cracking (R1.7) and gasification processes (R1.8) via benzene. The Kobayashi two-step model is used for devolatilization. Coal used in the study is from Indonesia. It has a moisture content of 8.25%. Its moisture-free (MF) proximate and ultimate analyses compositions are listed in Table 1.

**Table 1. Moisture-free (MF) composition of Indonesian coal.**

| ***Proximate Analysis (MF), wt%*** | | ***Ultimate Analysis (MF), wt%*** | |
|---|---|---|---|
| Volatile | 51.29 | C | 73.32 |
| Fixed Carbon (FC) | 47.54 | H | 4.56 |
| Ash | 1.17 | O | 20.12 |
| | 100.00 | N | 0.72 |
| | | S | 0.11 |
| | | Ash | 1.17 |
| | | | 100.00 |

In this study, discrete phase model is used to model the coal particles, and finite-rate reaction is used to model their reaction rates. The discrete phase model and the finite-rate reaction will be explained later.

## 2.0 COMPUTATIONAL MODEL

The models used in the study are the same as used by Silaen and Wang (2008). The time-averaged steady-state Navier-Stokes equations as well as the mass and energy conservation equations are solved. The standard k-ε turbulence model is used to provide closure. The flow is solved in Eulerian form as a continuum while the particles are solved in Lagrangian form as a discrete phase. Stochastic model is employed to model the effects of turbulence on the particles. The finite rate combustion model is used for the heterogeneous reactions. Both the finite rate and eddy-dissipation models are used for the homogeneous reactions, and the smaller of the two is used as the reaction rate. Refer to Silaen and Wang (2008) for the detailed devolatilization and gasification models

### 2.2 Computational Domains

Two meshed computational domains are shown in Figs. 3 and 4. In Fig. 3, coal slurry and oxidant are fed through two concentric pipes, with oxidant being injected through the inner pipe, and coal slurry being injected through the outer pipe. In Fig. 4, coal slurry and oxidant are injected through separate injectors and are departed 90 degrees from each other. The grid size of both computational domains is roughly 0.8 millions cells each. FLUENT 6.32 is used as the CFD solver.

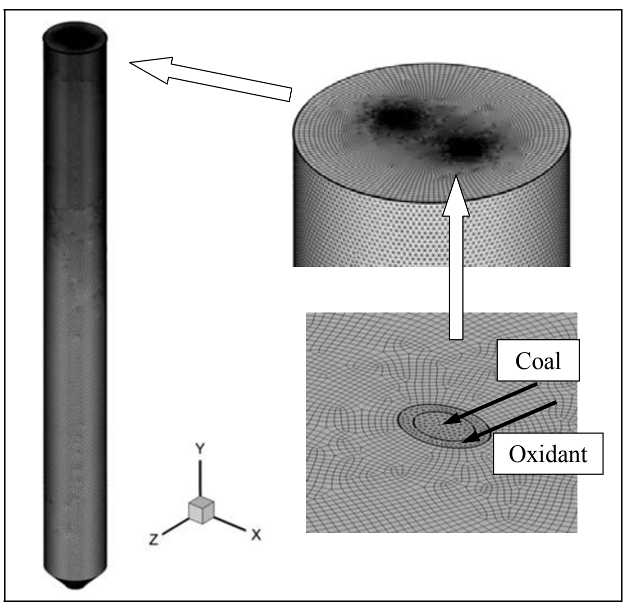


**Fig. 3 Meshed computational domain for two concentric injectors spraying with 45$^o$ downward angle and 90$^o$ interception angle.**

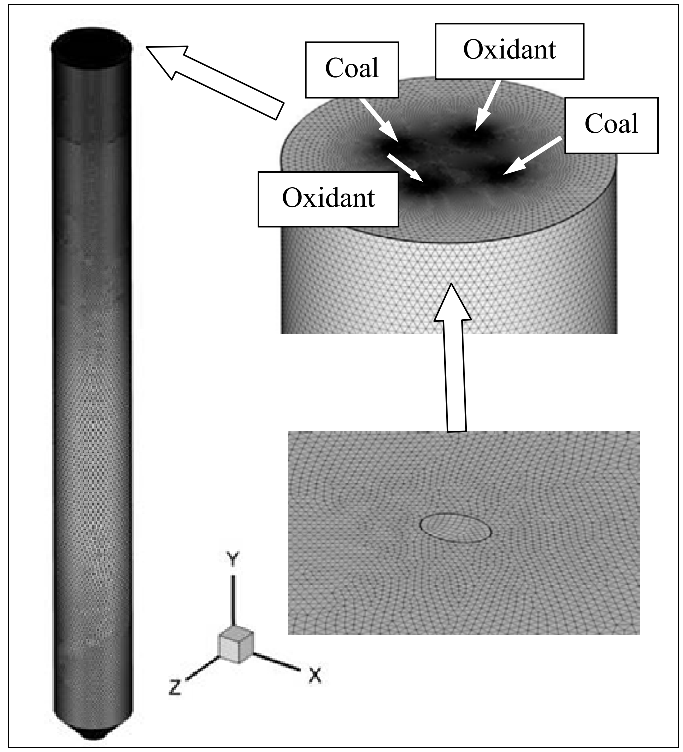


**Fig. 4 Meshed computational domain for four separate injectors spraying with 45$^o$ downward angle and 90$^o$ interception angle.**

### 2.3 Boundary Conditions and Inlet Conditions

The total feed rates of coal slurry and oxidant are listed in Table 4. The coal/water weight ratio of the coal slurry is 60%/40%. The oxidant is 95% $O_2$ and 5% $N_2$. Two tons of coal per day are required to achieve the coal slurry feed rate of 0.0324 kg/s as listed in Table 4. The equivalence ratio between the fixed carbon contained in the coal and the oxygen feed rate is 0.4. The mass flow rate input for each injection is given in Table 5. The temperatures of the coal slurry and the oxidant are provided at 300K and 420K, respectively.

The walls are all adiabatic and with no slip condition (i.e. zero velocity). The particles are assigned to reflect if they hit any wall. The operating pressure inside the gasifier is initially set at 15 bars. The outlet is set as a constant pressure condition at 15 bars. After calculation, the pressure inside the gasifier and at the inlet will be adjusted to accommodate the pressure drop inside the gasifier.

The oxidant is considered as a continuous flow, and coal slurry is considered as a disperse phase consisting of many discrete coal particles, which are composed of the fixed carbon, the original water from the moisture content of coal, and the water added in the slurry. In other words, in the computational model the slurry is modeled as particles with each particle consisting of a fixed carbon particle inside a water droplet. Other components of the coal, such as N, S, and ash, are injected as gas together with the oxidant in the continuous flow. N is treated as $N_2$, while the masses of S and ash are lumped into $N_2$. The coal slurry size is uniformly given as spherical droplets with a uniform arithmetic diameter of 200 µm.

**Table 4 The feed rates of coal slurry and oxidant simulated in this study**

| *Composition* | *Feed rate, kg/s* |
|---|---|
| Coal slurry (60% coal - 40% $H_2O$) | 0.0324 |
| Oxidant (95% $O_2$ - 5% $N_2$) | 0.0113 |

**Table 5 Mass flow rate input for four-injector case (2 coal injections and 2 oxidant injections)**

| *Parameters* | |
|---|---|
| Coal slurry injection mass flow rate, kg/s | 0.0161 |
| Oxidant injection mass flow rate, kg/s | 0.0058 |
| Mass fraction at oxidant injection | |
| $O_2$ | 0.930 |
| $N_2$ | 0.070 |

## 3.0 RESULTS AND ANALYSIS

### 3.1 Results of Two-Concentric Injectors

Finite-Rate Results

The result of particle tracks of two-concentric injectors is shown in Fig. 5. In this figure, particles from each injection are seen to meet and pass each other at the center. No collisions among particles are seen because the particle reaction model can not be used together with the particle collision model in the current computational scheme. The reason for this is explained below.

To model particle collisions, the CFD model has to track all particles one by one at the same time. For each particle, the model has to predict the possibility of collision between that particle and other particles. So, if there are N particles, each particle will have N-1 possible collision partners. Because the collision between particle A and particle B is the same as the collision between particle B and particle A, the number of possible collision pairs is $\frac{1}{2}N^2$. To calculate $\frac{1}{2}N^2$ possible collisions for each time step is beyond the computational capability of a cluster of 64 nodes in the authors' research group. Therefore, to save computational time and power, the collision model tracks particles in groups/parcels instead of individually; so each parcel is a statistical representation of a number of individual particles. As an example, if the model tracks a group of parcels, where each parcel represents 100 particles, the number of collision calculation is decreased by a factor of $10^4$ (or $100^2$). While the parcel tracking technique is good at saving collision calculation, it does not allow us to track the species fractions inside the particles, which is required in the particle reaction model. Thus, the particle collision model cannot be used together with the particle reaction model in the current computational scheme.

Even with the current limitation of adequately simulating the coal particle collisions, the results are still very useful because they can be treated as a worst-case scenario of wall erosion with more coal particles hitting the wall than in the real case. The results show that the time needed for the particles to burn out is just less than 0.2 seconds. Many of the particles burn near the wall, which is after they hit the wall and reflect. Figure 6 shows the temperature and species distribution on two perpendicular vertical center planes inside the top 1/3rd of the gasifier. The gas species distributions in the lower 2/3rd of the gasifier are almost uniform, so they are not shown. The temperature distribution shows two hot spots near the wall. These are the locations where the coal particles hit the wall, reflect, and burn out. At the same locations, the CO species fraction is the highest while the $CO_2$ fraction is the lowest. But $O_2$ is already fully depleted by the time the particles reach the walls. It is suspected that reaction $C + CO_2 \rightarrow 2CO$ are dominant at those locations. The particles hitting the wall combined with the high gas temperature could damage wall refractory bricks. As explained earlier, the presented results are a worst-case scenario.

No CO is observed in the upper part of the gasifier near the inlets, but the $CO_2$ concentration is higher in that area. It seems complete combustion occurs there because CO reacts immediately with $O_2$ to produce $CO_2$ and release energy to support endothermic gasification reactions R1.2 and R1.3.

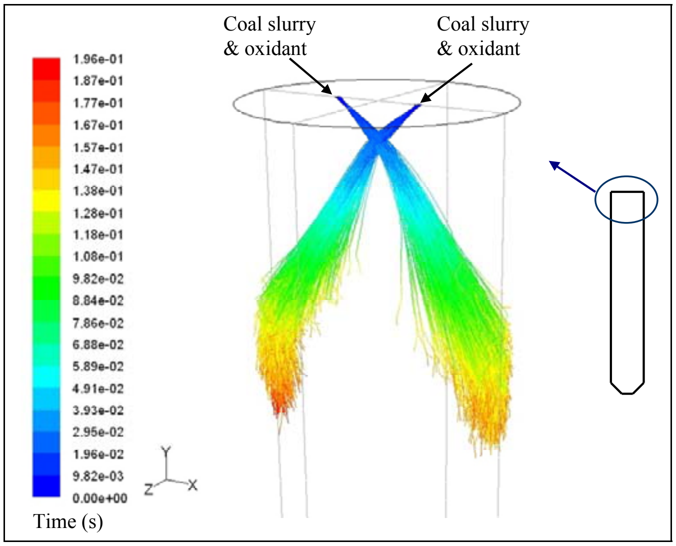


**Fig. 5 Coal particle tracks for two concentric coal slurry and oxidant injections with heterogeneous finite rate solid-gas reactions. (Note that Particle collision model can't be implemented together with the heterogeneous particle reaction model.)**

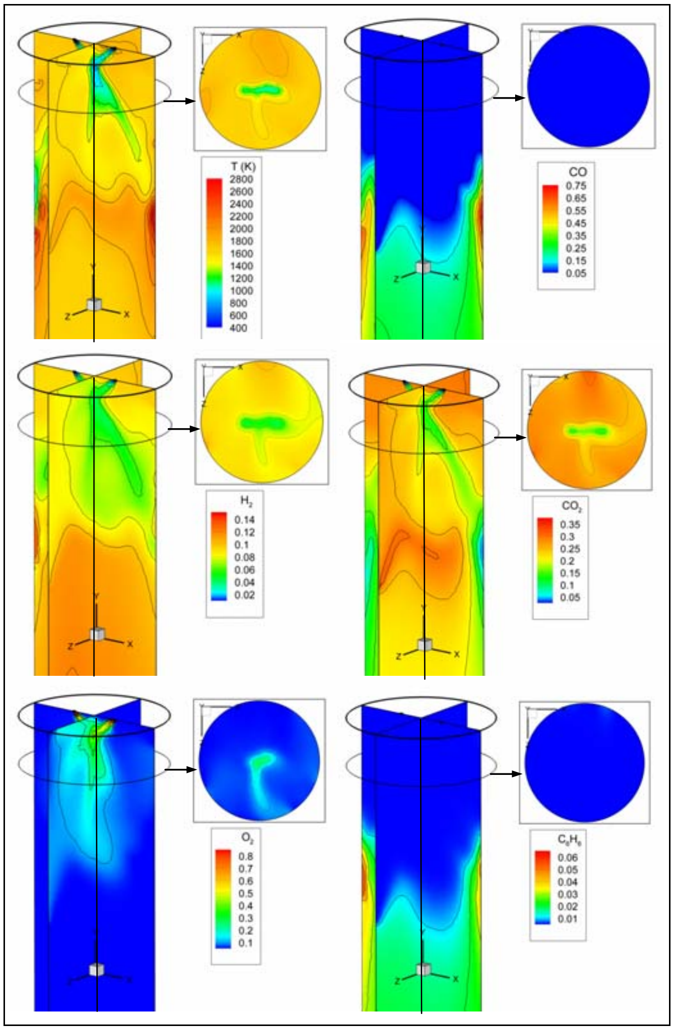


**Fig. 6 Temperature and species mole fraction distributions on two perpendicular vertical center plane inside gasifier for concentric coal-oxidant injection case with heterogeneous finite rate solid-gas reaction model.**

Instantaneous Gasification Results

As a compromise to resolving the limitation of modeling the particle-particle interactions when the particle reaction model is used, the "instantaneous gasification" method is employed as an alternative approach to examine the particle collision phenomenon. Under the "instantaneous gasification" approach, carbon particles are made to gasify instantaneously, thus the solid-gas reaction process can be modeled as homogeneous combustion reactions. This approach is based on the locally-homogeneous flow (LHF) model proposed by Faeth [1987], implying infinitely-fast interphase transport rates. The instantaneous gasification model can effectively reveal the overall combustion process and results without dealing with the details of the otherwise complicated heterogeneous particle surface reactions, heat transfer, species transport, and particle tracking in turbulent reacting flow.

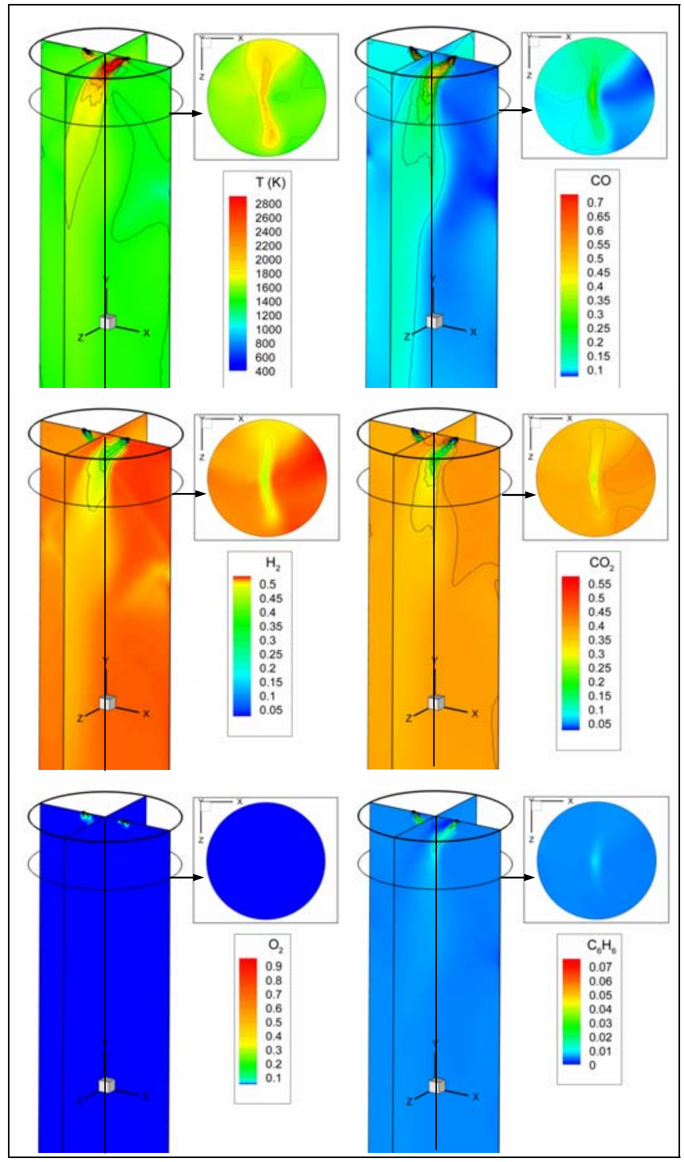


**Fig. 7 Temperature and species mole fraction distributions on two perpendicular vertical center-planes inside gasifier for concentric coal-oxidant injection case using the instantaneous gasification model implemented with particle collision model.**

Featured with a simpler mechanism, the gas combustion model is robust and less costly in computation. But it should be noted that this model lacks accuracy and detail in describing the physical process and usually over- predicts the reaction rate. With the instantaneous gasification approach, the fuel (fixed carbon and volatiles) is injected as gas, but the water component of the coal slurry and the moisture content of the coal are injected as water droplets (a discrete phase). The model is then able to track the particle-particle interactions among the droplets. Unsteady particle tracking is used to enable the tracking of the particle-particle interactions. The particle collision model includes elastic collision, particle breakup, and coalescence sub-models. It is speculated that the particles may be bounced off in different directions when the jets meet.

The temperature and species distributions on two vertical mid-planes in the top 1/3 of the gasifier is presented in Fig. 7. Hot spots occur near the injection point, where the CO species fraction is also high. These are the locations where carbon actively reacts and is very different from the finite rate solid-gas reaction model simulated earlier where solid carbon burns near the wall. In the instantaneous gasification model, carbon is instantly converted into gas at the injection locations. As a result, carbon reacts much sooner than in the finite rate gasification model where the particle has to go through evaporation and devolatilization before it undergoes chemical reactions.

Figure 8 shows plots of the velocity vectors and water droplet tracks at two vertical mid-planes for the instantaneous gasification model case. The XY plane plots show that the water droplets deviate from the direction of the velocity vectors once they pass the impingement point. The result of droplet tracks shows that the droplets spread more but are not severely bounced around, as speculated, at the intersection where the jets meet, and majority of the droplets passes through the jet impingement section and hit the wall as the finite rate case. This implies that the results of the finite rate are acceptable even though the particle collision model is not implemented.

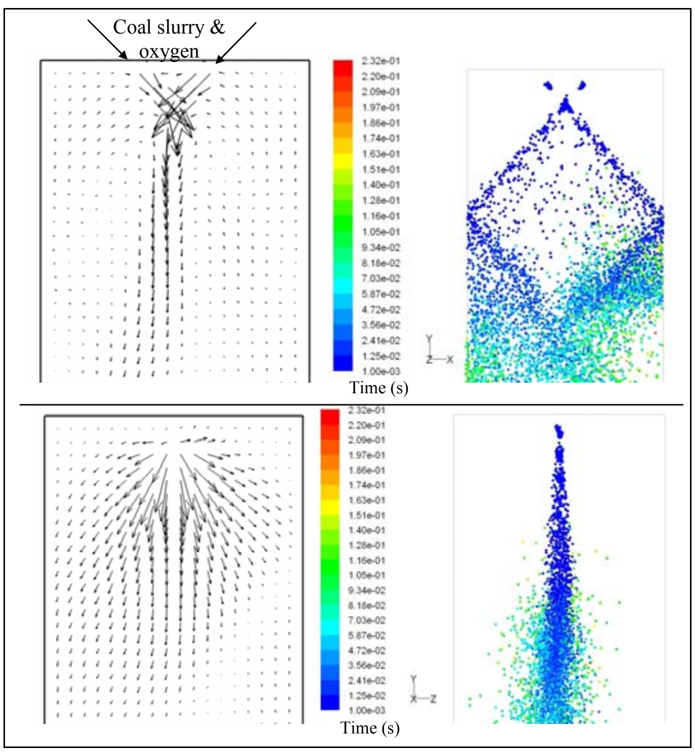


**Fig. 8 Velocity vectors and water droplet tracks on two perpendicular vertical center-plans for the concentric coal-oxidant injections using the instantaneous gasification model implemented with particle collision model.**

### 3.2 Results of Four Separate Coal and Oxidant Injectors

Finite-Rate Results

A plot of particle tracks for the four separate coal and oxidant injection cases is presented in Fig. 9. These cases show that the particles need longer time (~ 1 second) to burn out compared to approximately 0.2 seconds in the case of two concentric coal-oxidant injections. Injecting coal slurry separately from the oxidant does not provide good gas-particle mixing that is needed for effective heterogeneous reactions to occur. In a real situation, the reaction could be faster than the predicted results because most particles would collide, change direction, and achieve a better mixing with the oxidant, which also impinges at the center.

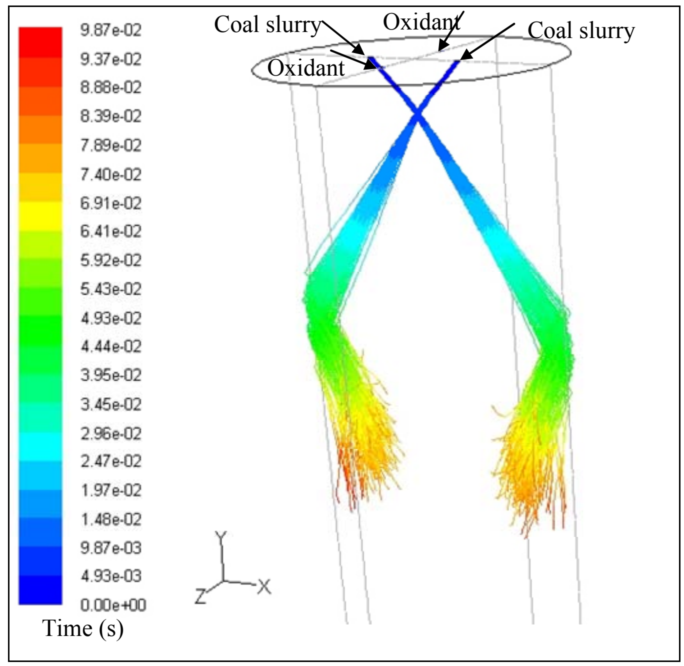


**Fig. 9 Coal particle tracks for four separate coal slurry and oxidant injections using finite rate reaction. (Note: Particle collision model can not be implemented.)**

The temperature and gas species distributions in Fig. 10 show a few similar characteristics as those of the two concentric injections case in Fig. 6. The hottest spots occur at the locations where the particles burn out, and the CO is highest and $CO_2$ is lowest at those locations. Also, there is no CO in the upper part near the inlet, but $CO_2$ is highest in the same area.

The exit gas temperature of the separate injection case is roughly 200K lower than that of the concentric injection case. Its $H_2$ concentration in the exit gas is higher by 4 percentage points, but its CO concentration is lower by 2.5 percentage points than the concentric injection case. The syngas heating value of 298K, listed in Table 6, for the separate injection is 5.5 MJ/kg and is 2 percentage points lower than the concentric injection.

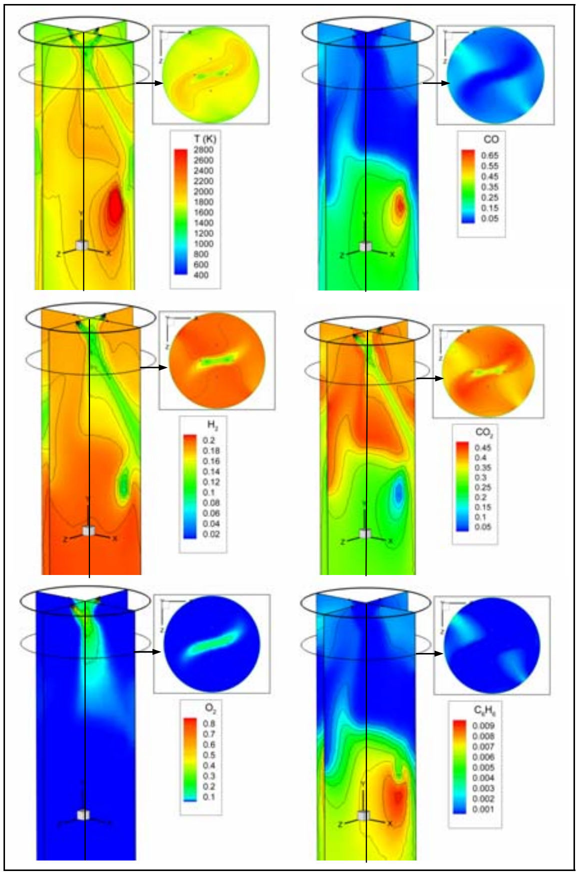


**Fig. 10 Temperature and species mole fraction distributions on two perpendicular vertical center-planes inside gasifier for separate coal-oxygen injection case with finite- rate reactions.**

**Table 6 Flow mass weighted average exit gas temperature and compositions for both 2 concentric and 4 separate injections cases.**

| | Concentric injection | Separate injection |
|---|---|---|
| | Finite-rate | Finite-rate |
| T (K) | 1329 | 1182 |
| Mole fraction: | | |
| CO | 23.1% | 19.6% |
| $H_2$ | 17.3% | 21.4% |
| $CO_2$ | 24.1% | 30.0% |
| VM | 0.0% | 0.0% |
| $H_2O$ | 31.7% | 27.0% |
| $C_6H_6$ | 2.3% | 0.6% |
| $N_2$ | 1.5% | 1.4% |
| C | 0.0% | 0.0% |
| HHV at 25°C (MJ/kg) | 7.5 | 5.5 |

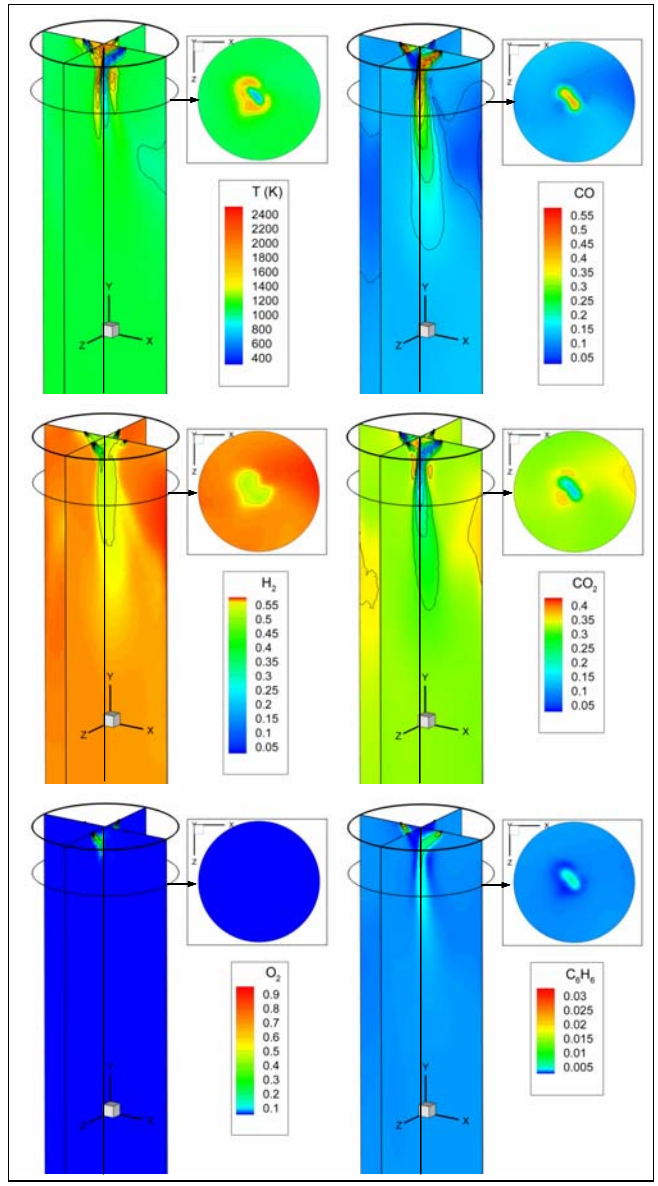


**Fig. 11 Temperature and species mole fraction distributions on two perpendicular vertical center-planes inside gasifier for separate coal-oxygen injection case modeled using the instantaneous gasification model implemented with particle collision model.**

Instantaneous Gasification Results

Similar to the concentric coal-oxidant case, a simulation case using the instantaneous gasification model is conducted for the four separate injection configuration. The temperature distribution given in Fig. 11 shows that the hot region occurs in the area near the injectors, which is different from the case using the finite-rate model where the hot region occurs near the wall away from the injectors. As mentioned earlier, this is due to the instantaneously conversion of carbon into gas at the inlets. The carbon can instantaneously react with other gases without having to wait for the evaporation and devolatilization process to occur as modeled in the finite-rate model.

Downstream of the impingement location, the water droplets deviate from the gas flow path and is shown in Fig.12. Again, the result of droplet tracks shows that the droplets spread broader but are not severely bounced around, as speculated, at the intersection where the jets meet, and majority of the droplets passes through the jet impingement section and hit the wall as the finite rate case. This implies that the results of the finite rate are largely acceptable even though the particle collision model is not implemented.

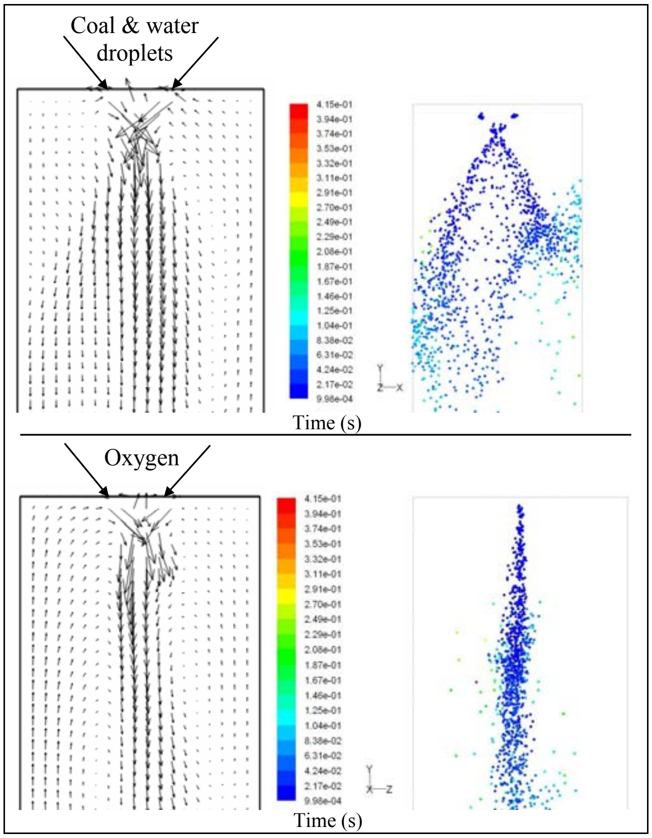


**Fig. 12 Velocity vectors and water droplet tracks for the four separate coal-oxygen injections case modeled using the instantaneous gasification model.**

## 5.0 CONCLUSIONS

A computational study of two proposed coal-slurry fuel injection has been conducted in an entrained flow oxygen-blown gasifier. The limitation of the current computational model does not allow coal particle collision to be included in the heterogeneous finite-rate solid-gas reaction model. To examine the particle collision phenomenon, the instantaneous gasification model is implemented, in which the coal (consisting of carbon and volatiles) is injected as gas and the water is injected as droplets. The result of droplet tracks shows that the droplets are not bounced around, as speculated, at the intersection where the jets meet, and majority of the droplets passes through the jet impingement section and hit the wall as the finite rate case. This implies that the results of the finite rate are acceptable even though the particle collision model is not implemented. The finite-rate result actually presents a worst-case scenario for predicting wall erosion. The particle tracks for both the 2 concentric and 4 separate injection configurations show that the coal particles hit the wall and can accelerate deterioration of the refractory bricks. The two concentric injection cases provide better fuel-oxidant mixing and higher heating value than the case using four separate injections

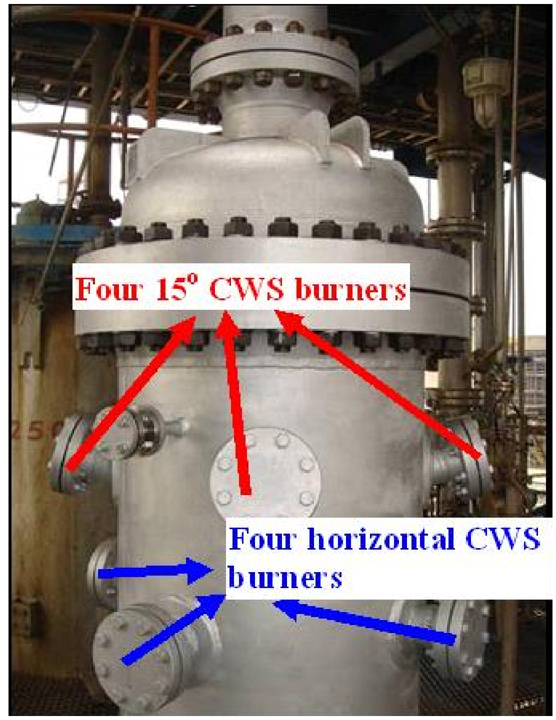


**Fig. 13 The top-loaded injectors in the ITRI experimental gasifier facility.**

## 6.0 ACKNOWLEDGEMENTS


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