

COMPARISON OF INSTANTANEOUS, EQUILIBRIUM, AND FINITE-RATE GASIFICATION MODELS IN AN ENTRAINED-FLOW COAL GASIFIER

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ABSTRACT

A coal gasification simulation model involves many sub-models and each of the sub-models needs to be investigated and verified. This paper focuses on comparing three different gasification reaction models: instantaneous gasification, global equilibrium, and finite-rate models. The goal is to determine if the simplified instantaneous gasification model can be used to quickly capture acceptable approximations of thermal-flow and reaction behaviors that can be used as a preliminary screening tool of new design ideas for improving gasifiers' performance. The Eulerian-Lagrangian approach is applied to solve the Navier-Stokes equations and eight species transport equations with three heterogeneous global reactions and three homogeneous reactions. The coal particles are tracked with the Lagrangian method. In the instantaneous gasification model, the interphase exchange rates of mass, momentum and energy are assumed to be infinitely fast. Also, the dispersed phase can be simplified as the gas phase, and the complex two-phase flow is then treated as a single-phase flow. Two water shift rates are used. The fast rate is used with the presence of catalyst, while the slow rate is used without catalyst as in a typical entrained-flow gasifier. The results show that reactions in the instantaneous gasification model occur fast and finish quickly; whereas, the reaction in the finite-rate model, which involves gas-solid reactions, occurs slowly. Varying the coal particle size of the finite-rate model shows that the syngas heating value of the smaller particle size is closer to the instantaneous gasification model. The water shift rate plays a very important role on affecting the accurate prediction of the syngas composition. The syngas composition of using fast water shift rate is very close to that calculated from the global equilibrium method. The overall result reveals that the instantaneous gasification approach can provide an overall evaluation of relative changes of gasifier performance in terms of temperature, heating value, and gasification efficiency corresponding to parametric variations, but not adequately capture the local gasification process predicted by the finite rate model in most part of the gasifier.

1.0 INTRODUCTION

Gasification is the process of converting various carbon-based feedstocks to clean synthetic gas (syngas), which is primarily a mixture of hydrogen (H_2) and carbon-monoxide (CO), through an incomplete combustion. Feedstock is partially combusted with oxygen and steam at high temperature and pressure with only less than 30% of the required oxygen for complete combustion being provided. The syngas produced can be used as a fuel, usually as a fuel for boilers or gas turbines to generate electricity, or can be used to make a synthetic natural gas, hydrogen gas or other chemical products. The gasification technology is applicable to any type of carbon-based feedstock, such as coal, heavy refinery residues, petroleum coke, biomass, and municipal wastes.

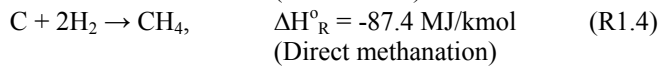
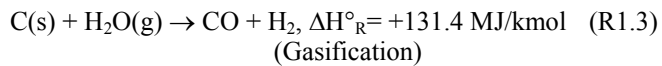
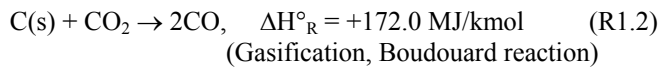
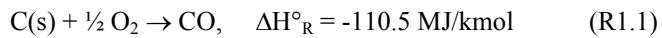
The ultimate goal of the gasification research team at the University of New Orleans is to develop a trustworthy computational tool that can be used to help improve gasifier designs to achieve better performance, efficiency, and reliability. It is also desired to reduce the size of gasifiers, which will lead to reduction of their capital and operational costs. A good understanding of the gasification process inside a gasifier is needed to help achieve these goals. The desired product of a gasifier can mostly be obtained if the gasifier is big enough so the residence time is sufficiently long to achieve chemical equilibrium status. However, the corresponding gasifier will be large and expensive and the product yield will be low due to the lengthy residence time. To reduce the gasifier size while augmenting product yield, the authors believe that performance of a high-efficiency gasifier is closely related to and affected by the thermal-flow behavior inside the gasifier. CFD simulation is an economic and effective tool to help achieve this goal. However, the gasification reaction model is complicated and requires tremendous time to simulate. Therefore, it is desired to see if a simplified approach can be employed to quickly capture acceptable approximations of thermal-flow and reaction behaviors that can be used as a preliminary screening tool of new ideas for improving gasifiers' performance. This study focuses on comparing CFD simulation

results of an entrained-flow coal gasifier using the finite-rate model and the instantaneous gasification model (simplified approach). The finite-rate model solves gas-solid interactions, while the instantaneous gasification model assumes a locally-homogeneous flow and solves the flow as a single-phase flow. The syngas composition of both models are compared with the that calculated by the global equilibrium method.

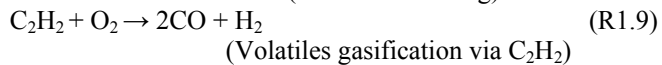
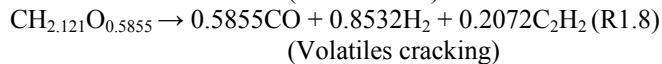
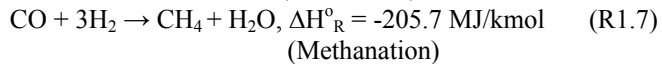
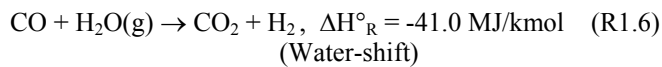
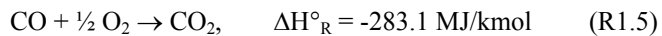
1.1 Global Gasification Chemical Reactions

This study only deals with global chemical reactions of coal gasification (Smoot and Smith, 1985) that can be generalized in reactions (R1.1) through (R1.9) below:

Heterogeneous (solid and gas) phase



Homogenous gas phase



In this study, the methanation reactions are not considered. Reactions (R1.8) and (R1.9) involve volatiles. The volatiles are modeled to go through a thermal cracking (R1.8) and gasification processes (R1.9) via C₂H₂. Coal used in the study is sub-bituminous coal from Indonesia. It has a moisture content of 8.25%. Its moisture-free (MF) proximate and ultimate analyses compositions are listed in Table 1. The compositions of volatiles are derived from the values of coal heating value, proximate analysis, and ultimate analysis.

Table 1 Moisture-free (MF) compositions of Indonesian sub-bituminous coal.

<i>Proximate Analysis (MF), wt%</i>		<i>Ultimate Analysis (MF), wt%</i>	
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

1.2 Recent Research

Chen et al. (2000) developed a comprehensive three-dimensional simulation model for entrained coal gasifiers which applied an extend coal gas mixture fraction model with the Multi Solids Progress Variables (MSPV) method to simulate the gasification reaction and reactant mixing process. The model employed four mixture fractions separately track the variable coal off-gas from the coal devolatilization, char-O₂, char-CO₂, and char-H₂O reactions. Chen et al. performed a series of numerical simulations for a 200 ton per day (tpd) two-stage air blown entrained flow gasifier developed for an IGCC process under various operation conditions (heterogeneous reaction rate, coal type, particle size, and air/coal partitioning to the two stages).

Bockelie et al. (2002(a)) of Reaction Engineering International (REI) developed a CFD modeling capability of entrained flow gasifiers that focuses on two gasifier configurations: single-stage down fired system and two-stage with multiple feed inlets. The model was constructed using GLACIER, an REI in-house comprehensive coal combustion and gasification tool. The basic combustion flow field was established by employing full equilibrium chemistry. Gas properties were determined through local mixing calculations and are assumed to fluctuate randomly according to a statistical probability density function (PDF), which is characteristic of the turbulence. Gas-phase reactions were assumed to be limited by mixing rates for major species as opposed to chemical kinetic rates. Gaseous reactions were calculated assuming local instantaneous equilibrium. The particle reaction processes include coal devolatilization, char oxidation, particle energy, particle liquid vaporization and gas-particle interchange. The model also includes a flowing slag sub-model.

U.S. Department of Energy/National Energy Technology Laboratory (NETL) developed a 3D CFD model of two commercial-sized coal gasifiers [Guenther and Zitney (2005)]. The commercial FLUENT CFD software is used to model the first gasifier, which is a two-stage entrained-flow coal slurry-fed gasifier. The Eulerian-Lagrangian approach is applied. The second gasifier is a scaled-up design of transport gasifier. The NETL open source MFI (Multiphase Flow Interphase eXchanges) Eulerian-Eulerian model is used for this dense multiphase transport gasifier. NETL also developed an Advanced Process Engineering Co-Simulator (APECS) that combines CFD models and plant-wide simulation. APECS enables NETL to couple its CFD models with steady-state process simulator Aspen Plus.

Silaen and Wang (2005) conducted numerical simulations of the coal gasification process inside a generic two-stage entrained-flow gasifier using the commercial CFD solver FLUENT. They investigated the effects of several parameters on gasification performance including coal mixture (slurry or dry powder), oxidant (oxygen-blown or air-blown), wall cooling, and various coal distributions between the two stages. The simulation results provide the temperature and species distributions inside the gasifier. The results indicate that coal-slurry feed is preferred over coal-powder feed to produce

hydrogen. On the other hand, coal-powder feed is preferred over coal-slurry feed to produce carbon monoxide. The air-blown operation yields poor fuel conversion efficiency and the lowest syngas heating value due to air dilution. The effect of wall cooling has been shown insignificant on the exit gas composition and heating value. The fuel conversion efficiency of the case with coal distribution with 75% (first stage) vs. 25% (second stage) is better than the case with 50% vs. 50% coal distribution. They stated that a two-stage design has an advantage of the flexibility to adjust parameters to achieve desired performance.

In the continuation of that study, Silaen and Wang (2006) carried out a study that focused on the effect of flow injection directions on the gasification performance using the same generic two-stage entrained flow gasifier. Horizontal injection direction was compared to downward and upward direction. The results revealed that the horizontal injection direction gave the best gasifier performance. Changing the direction of the first-stage injectors downward resulted in a carbon fuel conversion reduction, but produce more H₂. Changing the direction of the second-stage injectors, however, does little to affect the overall flow patterns due to the smaller-quantity of coal injection (25%); therefore the gasifier performance is essentially insignificantly affected.

Silaen and Wang (2008) conducted a study that investigates the effects of different parameters on gasification performance including five turbulence models, four devolatilization models and three solid coal sizes. The Eulerian-Lagrangian approach with finite global reaction rates was applied. A two-step decomposition model was applied to volatiles cracking and gasification via benzene. The results reveal that the standard k-ε and the RSM models gave consistent results. High inertia possessed by large coal particles can propel the particles cross the gas streamlines and increase particle-gas mixing which results in enhanced reaction rate. The single rate devolatilization model and the chemical percolation model produced moderate and consistent devolatilization rate.

This study is a continuous work of Silaen and Wang (2005, 2006, 2008) and focuses on comparing two different gasification reaction models – the instantaneous gasification model and the finite-rate model.

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. Species transport equations are solved for all gas species involved. The standard k-ε turbulence model is used to provide closure. Silaen and Wang (2008) reported that the standard k-ε turbulence model yields reasonable results without requiring very much computational time when compared to other turbulence models. Enhanced wall function and variable material property are used. The P1 model is used as the radiation model.

Finite-Rate Model -- The flow (continuous phase) is solved in Eulerian form as a continuum while the particles (dispersed phase) are solved in Lagrangian form as a discrete phase. Stochastic model is employed to model the effects of turbulence on the particles. The continuous phase and discrete phase are communicated through drag forces, lift forces, heat transfer, mass transfer, and species transfer. The finite-rate combustion model is used for the **heterogeneous** reactions, but 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. The finite-rate model calculates the reaction rates based on the kinetics, while the eddy-dissipation model calculates based on the turbulent mixing rate of the flow. Gasification or combustion of coal particles undergoes the following global processes: (i) evaporation of moisture, (ii) devolatilization, (iii) gasification to CO and (iv) combustion of volatiles, CO, and char. The Chemical Percolation Devolatilization (CPD) model [Fletcher and Kerstein (1992), Fletcher et. al (1990), and Grant et. al (1989)] is chosen as the devolatilization model based on the finding by Silaen and Wang (2008) that the Kobayashi two-competing rates devolatilization model [Kobayashi et. al. (1976)] is very slow, while the CPD model gives a reasonable result.

For solid particles, the rate of depletion of the solid due to a surface reaction is expressed as a function of kinetic rate, solid species mass fraction on the surface, and particle surface area. The reaction rates are all **global net rates**, i.e., the backward reaction, calculated by equilibrium constants, are included in the global rate. Therefore, the finite rate employed in this study implicitly applies local equilibrium approach. Reaction rate constants used in this study are summarized in Table 2.

Table 2 Summary of reaction rate constants used in this study

Reaction	Rate Constant	Parameters
Solid-gas heterogeneous reactions:		
C(s) + ½O ₂ → CO (Combustion)	k = AT ⁿ exp(-E/RT)	n = 0 A = 0.052 kg/m ² .Pa ^{-0.5} E = 6.1x10 ⁷ J/kmol
C(s) + CO ₂ → 2CO (Gasification, Boudouard reaction)	k = AT ⁿ exp(-E/RT)	n = 0 A = 0.0732 kg/m ² .Pa ^{-0.5} E = 1.125x10 ⁸ J/kmol
C(s) + H ₂ O(g) → CO + H ₂ (Gasification)	k = AT ⁿ exp(-E/RT)	n = 0 A = 0.0782 kg/m ² .Pa ^{-0.5} E = 1.15x10 ⁸ J/kmol
Gas phase homogeneous reactions:		
CO + ½ O ₂ → CO ₂	k = AT ⁿ exp(-E/RT)	n = 0 A = 2.2x10 ¹² E = 1.67x10 ⁸ J/kmol
CO + H ₂ O(g) → CO ₂ + H ₂ (Water shift)	k = AT ⁿ exp(-E/RT)	n = 0 A = 2.75x10 ² * E = 8.38x10 ⁷ J/kmol
CH _{2.121} O _{0.5855} → 0.5855CO + 0.8532H ₂ + 0.2072C ₂ H ₂		Eddy-dissipation only
C ₂ H ₂ + O ₂ → 2CO + H ₂		Eddy-dissipation only

* This rate is reduced from the original value of Jones and Lindstedt (1988)

The reaction rate of the water-shift, adopted from Jones and Lindstedt (1988), is found to be too fast in this study because the rate is obtained with the presence of catalyst. Considering no catalyst is added in a typical gasifier, the water shift reaction

rate is purposely slowed down to make the syngas composition consistent with that in the actual production of a commercial entrained-flow gasifier with coal-slurry feed from bottom.

For liquid droplets, water evaporates from the particle's surface when temperature is higher than the saturation temperature (based on local water vapor concentration). The evaporation is controlled by the water vapor partial pressure until 100% relative humidity is achieved. 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 moisture is evaporated due to either high temperature or low moisture partial pressure, the vapor diffuses into the main flow and is transported away. Please refer to Silaen and Wang (2008) for the detailed devolatilization and gasification models.

Instantaneous Gasification Model -- The interphase exchange rates of mass, momentum and energy are assumed to be infinitely fast. 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. The eddy-dissipation model is used to model the chemical reactions. The eddy-dissipation model assumes the chemical reactions are faster than the turbulence eddy transport, so the reaction rate is controlled by the flow motions.

Since the water-shift rate plays an important role on the formation of the final syngas composition, two water shift rates are used. The fast rate is used with the presence of catalyst, while the slow rate is used without catalyst as in a typical entrained-flow gasifier. The fast rate from Jones and Lindstedt (1988) was first used and it was discovered that the results are similar to using the eddy-dissipation rate. Considering using the eddy-dissipation rate is convenient, the fast water shift rate is hence replaced by the eddy-dissipation rate in this study. The slow water shift rate is the same as that used in the previous finite rate simulation as shown in Table 2.

The instantaneous gasification model can significantly reduce the computational time but can only provide a qualitative trend of gasification process. Although the instantaneous gasification model is crude, it catches the effect of thermal-fluid field (including turbulence structure) on chemical reactions, which are not readily available from the equilibrium method.

Chemical Equilibrium Method – In the chemical equilibrium method, CFD scheme is not employed. The C-H₂O gasification process (R1.3) is assumed to consume the steam first before the water-shift takes place to use up the remaining steam. This assumption is based on the fact that water shift is slow without catalyst in a typical gasifier.

The computation is carried out using the finite-volume-based commercial CFD software FLUENT (Version 6.3.26) from Ansys, Inc. The simulation is steady-state and uses the pressure-based solver, which employs an implicit pressure-correction scheme and decouples the momentum and energy equations. SIMPLE algorithm is used to couple the pressure and velocity. Second order upwind scheme is selected for spatial discretization of the convective terms. For the finite rate model where the Eulerian-Lagrangian approach is used, the iterations are conducted alternatively between the continuous and the dispersed phases. After twenty continuous phase iterations, one dispersed phase iteration is performed. The drag, particle surface reaction, and mass transfer between the dispersed and the continuous phases are calculated. The continuous phase is updated in the next iteration based on the dispersed phase calculation results, and the process is repeated. Converged results are obtained when the residuals satisfy mass residual of 10^{-3} , energy residual of 10^{-5} , and momentum and turbulence kinetic energy residuals of 10^{-4} . These residuals are the summation of the imbalance in each cell, scaled by a representative for the flow rate. The computation was carried out in parallel processing on two dual-core Pentium clusters with 12 nodes each.

2.1 Physical Characteristics of the Model and Assumptions

This paper studies a one-stage entrained flow coal gasifier. Fundamental investigation is first conducted on a simplified 2-D geometry (Fig. 1) to perform a parametric study of the effect of coal particle sizes on gasification performance and two different approaches of modeling coal slurry.

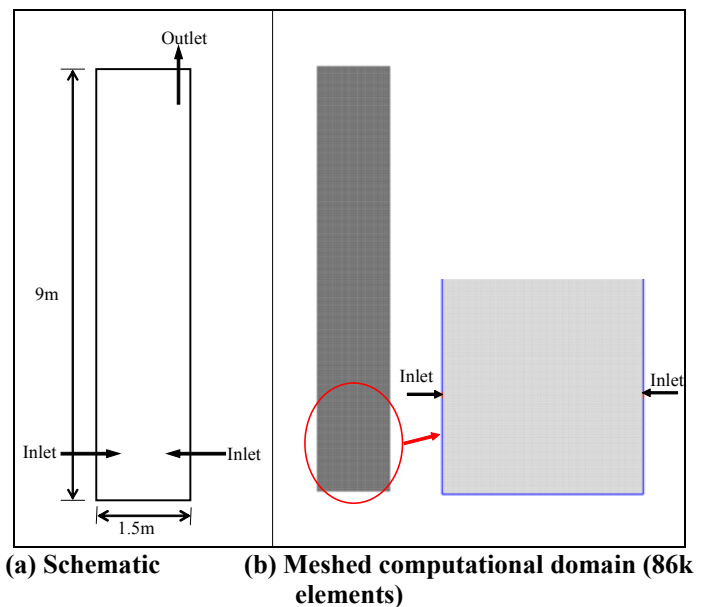
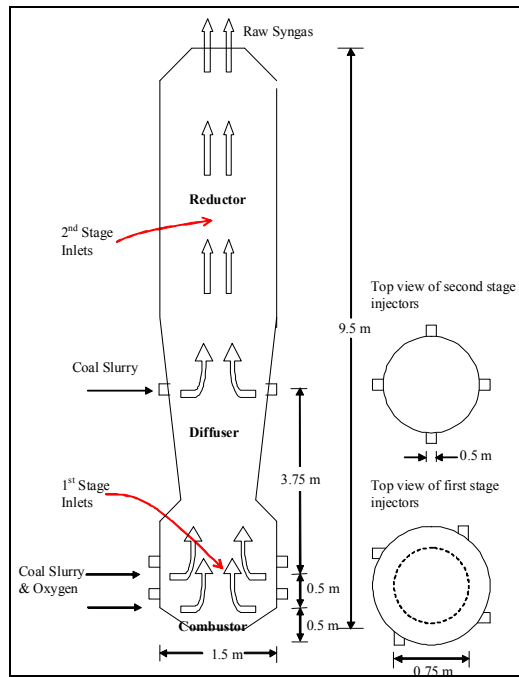
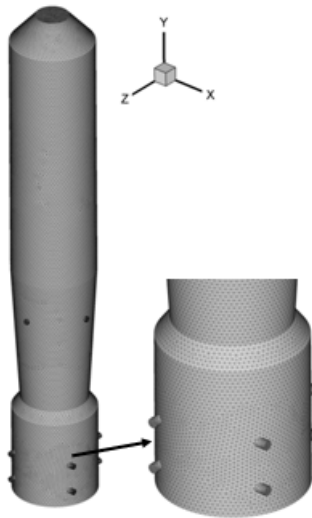


Fig. 1 Schematics of a simplified 2-D one-stage entrained flow gasifier configuration studied and its meshed computational domain.



(a) Schematic of 3-D gasifier



(b) Meshed computational domain (969k elements)

Fig. 2 Schematics of 3-D one-stage entrained flow gasifier configuration (adopted from Bockelie et al. 2002a) and its meshed computational domain. The second stage is not used in this study.

From the 2-D results, a fixed coal particle size and one coal slurry model are selected to conduct 3-D simulation. The geometry of the 3-D one-stage gasifier is adopted from Bockelie et al. (2002a) and is shown in Fig. 2. Two opposing injectors are located near the bottom of the gasifier. In the simulations, the buoyancy force is considered, varying fluid properties are calculated for each species and the gas mixture, and the walls are impermeable. The following general assumptions are made: the flow is steady and no-slip condition (zero velocity) is imposed on wall surfaces.

3.0 BOUNDARY AND INLET CONDITIONS

Indonesian sub-bituminous coal is used as feedstock in this study. Its composition is given in Table 1 and the feed rates used are given in Table 3. The 2-D feed rate is prorated lower from the 3D feed rate to the extent that the injection velocity is comparable to the 3-D case. The coal/water weight ratio of the coal slurry is 60%-40%. The oxidant used is 95% O₂ and 5% N₂. Oxidant/coal slurry feed rate used in Table 3 gives O₂/coal equivalence ratio of 0.3.

Table 3 Feed rates used in the study

	Feed rate (kg/s)	
	2D gasifier	3D gasifier
Coal slurry	18.15	21.39
Oxidant	6.04	7.12

In the finite-rate model, the oxidant is considered as a continuous flow and coal slurry is considered as a discrete flow. The discrete phase only includes the fixed carbon and water from the moisture content of coal and water added to make the slurry. Two approaches are adopted to model the coal slurry injection. The first approach injects the slurry coal with each particle containing both coal and liquid water. The second approach injects coal (as a solid particle) and liquid water (as droplets) separately. Other components of the coal, such as N, H, S, O, and ash, are injected as gas, together with the oxidant in the continuous flow. N is treated as N₂, H as H₂, and O as O₂. S and ash are lumped into N₂. The coal slurry size is uniformly given as 50 μm respectively in the baseline case. In the instantaneous gasification model, all species are injected as gas.

The walls are assigned as adiabatic with internal emissivity of 0.8. The boundary condition of the discrete phase at walls is assigned as “reflect”, which means the discrete phase elastically rebound off once reaching the wall. At the outlet, the discrete phase simply escapes/exits the computational domain. The gasifier is operating at 24 atm.

4.0 RESULTS AND DISCUSSIONS

4.1 Comparison of Finite-Rate, Chemical Equilibrium , and Instantaneous Gasification Cases

Table 4 presents the exit syngas temperature and compositions for the finite-rate and instantaneous gasification cases. Carbon conversion is defined as the amount of unburned char contained in the exit gas divided by the total char injected through the inlets. Carbon conversion for the finite-rate case is 91% while the carbon conversion for the instantaneous gasification is 100%. As mentioned earlier, carbon particles are made to gasify instantaneously in the instantaneous gasification model. Thus, the solid-gas reaction process can be modeled as homogeneous combustion reactions. The homogenous reactions of char in the instantaneous gasification model are much faster

than the heterogeneous reactions of char in the finite-rate model. In the instantaneous gasification, char is injected as gas which means that it can immediately react as soon as it leaves the inlets. Coal particles in the finite-rate model have to undergo evaporation and devolatilization before the char can be burned. The existence of unburned chars in the exit gas is consistent with the operating of current gasifiers reported in available literatures.

Table 4 Exit syngas temperature and compositions for 2D cases with 50 μm particles .

2D	Finite rate	Instantaneous gasification, slow water shift	Instantaneous gasification, fast water shift	Equilibrium
Temperature (K)	1181	1179	1204	N/A
Carbon conversion	91.0%	100.0%	100.0%	100.0%
Cold gasification efficiency	78%	84%	84%	85%
Mole fraction:				
CO	28.4%	28.9%	4.3%	6.1%
H ₂	29.7%	36.4%	59.6%	59.4%
CO ₂	8.5%	10.5%	34.7%	33.4%
CH _{2.121} O _{0.5855}	0.0%	0.0%	0.0%	0.0%
H ₂ O	31.2%	23.1%	0.0%	0.0%
C ₂ H ₂	1.0%	0.0%	0.3%	0.0%
N ₂	1.0%	1.1%	1.1%	1.1%
O ₂	0.0%	0.0%	0.0%	0
HHV at 25C (MJ/kg)	9.7	10.4	10.4	10.5

Syngas temperature for both finite-rate and instantaneous gasification cases with a slow water shift rate, listed in Table 4, are almost identical. The exit syngas compositions are also close except more hydrogen is produced in the instantaneous gasification model at the expense of steam. However, Figs. 4 and 5 show very different local temperature and mass-weighted species distributions between these two cases. The reactions happen and finish very quickly as expected, but the CFD results provide a quantitative measure of the reaction time. On the other hand, the finite-rate model shows a hot region (around 2200 K) below the injection points and a gradual increase above the injection points. The heating value of the finite rate is a bit low as expected.

Above is the comparison between the finite rate and the instantaneous gasification using the same slow water shift rate as shown in Table 2. . If the slow water shift rate is replaced with the fast rate using the eddy-dissipation approach, the exit syngas composition changes drastically with a large reduction of CO and steam and a significant increase of H₂ and CO₂ – an unmistakable result due to the water shift reaction (R1.6). Unsurprisingly, the exit syngas composition is almost the same as the equilibrium results. The little bit higher exit temperature is resulted from the heat released from the exothermic water shift process.

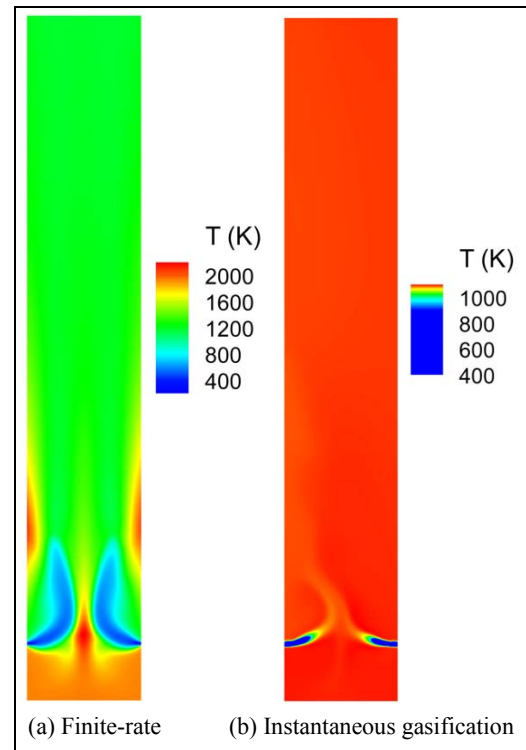


Fig. 4 Temperature distribution for 2D finite-rate case and instantaneous gasification case with a slow water shift rate.

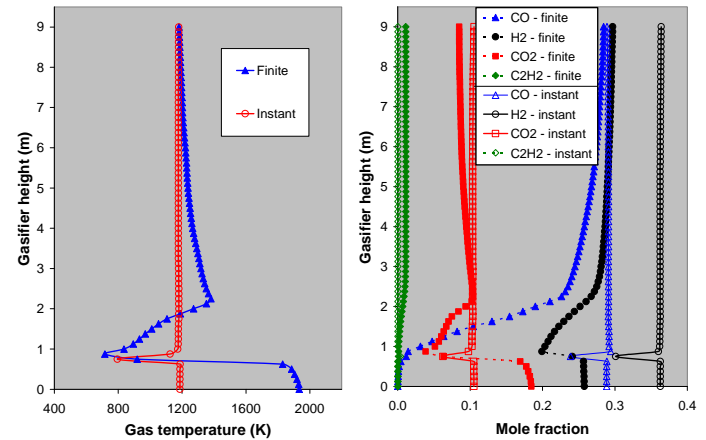


Fig. 5 Mass weighted average of gas temperature and species mole fraction for 2D finite-rate and instantaneous gasification cases with a slow water shift rate.

4.2 Effects of Different Coal Particle Sizes

As mentioned earlier, the reaction rates in the instantaneous gasification are much faster than those in the finite-rate model. Several cases with different coal particle diameters are studied to examine if perhaps the results would be similar if particle size is reduced because smaller particle sizes have larger surface areas, which can help expedite the reaction. Three other different coal slurry particle diameters used are 1 μm , 10 μm , and 100 μm . The results, along with the results for the 50 μm -diameter coal slurry particle case above, are compared in Table 5 with the instantaneous gasification case using the slow water shift rate.

The results show a trend of increased carbon conversion and CO mole fraction but reduced H₂ and CO₂ fractions. The smaller particles require less time to complete gasification as expected. Carbon conversion is 100% for the 1 μ m coal slurry diameter case. Syngas heating value becomes closer to that of the instantaneous gasification as particle diameter decreases.

Table 5 Effect of coal slurry particle diameters on 2D exit syngas temperature and compositions

Particle diameter (μ m)	1	10	50	100	Instantaneous
Temperature (K)	1199	1189	1181	1387	1179
Carbon conversion	100.0%	99.7%	91.0%	70.0%	100.0%
Cold gasification	82%	82%	78%	67%	84%
Mole fraction:					
CO	30.5%	30.1%	28.4%	20.6%	28.9%
H ₂	29.7%	30.1%	29.7%	31.5%	36.4%
CO ₂	7.9%	8.2%	8.5%	13.2%	10.5%
CH _{2.121} O _{0.5855}	0.0%	0.0%	0.0%	0.0%	0.0%
H ₂ O	29.4%	29.2%	31.2%	33.2%	23.1%
C ₂ H ₂	1.4%	1.3%	1.0%	0.4%	0.0%
N ₂	1.1%	1.1%	1.0%	1.1%	1.1%
O ₂	0.0%	0.0%	0.0%	0.0%	0.0%
HHV at 25°C (MJ/kg)	10.2	10.2	9.7	8.3	10.4

4.3 Effect of Two Different Slurry Coal Injection Models

In the finite-rate cases presented above, the coal slurry injection has been modeled following the first approach, i.e. each coal slurry particle consists of char, moisture contained in the coal, and water to make the slurry. The results are now compared with those obtained by employing the second approach, i.e. the water to make slurry is injected separately as water droplets from the coal particles. In this second approach, two adjacent injections are used at each inlet. One is the injection for the coal particle, which consists of char and moisture contained in the coal. The other is the injection for the water droplets that makes the slurry.

It is initially thought that when the water slurry is included in the coal particles, the coal particles need longer time to complete the evaporation process due to more water content inside the particle than if the slurry water is injected separately as water droplets. Thus, the devolatilization and char reactions will be delayed, which could result in a lower carbon conversion. However, the results listed in Table 6 shows that carbon conversion is almost the same but the cold gasification efficiency is eight percentage points higher when water slurry is injected as a part of the coal particles than when it is injected separately as water droplets. Particle concentration distributions shown in Fig. 6 reveal that the particles react a little bit slower for the case where slurry water is injected separately from coal particles (approach 2). The combined coal-water injection model seems to perform more closely to the real condition and results. The difference in result, solely from the different injection models, indicates the uncertainty of current CFD model. A close calibration with experimental data is needed, but it is very difficult to obtain such data from current gasifier operators since most of the data are highly-guarded as proprietary information.

Table 6 Exit syngas temperature and compositions for finite-rate 2D cases with two different coal slurry injection models

Water slurry injection	Combined coal-water particles	Separated coal & water particles
Temperature (K)	1181	987
Carbon conversion	91.0%	90.0%
Cold gasification efficiency	78%	70%
Mole fraction:		
CO	28.4%	22.5%
H ₂	29.7%	29.5%
CO ₂	8.5%	11.9%
CH _{2.121} O _{0.5855}	0.0%	0.0%
H ₂ O	31.2%	33.8%
C ₂ H ₂	1.0%	1.2%
N ₂	1.0%	1.1%
O ₂	0.0%	0.0%
HHV at 25°C (MJ/kg)	9.7	8.7

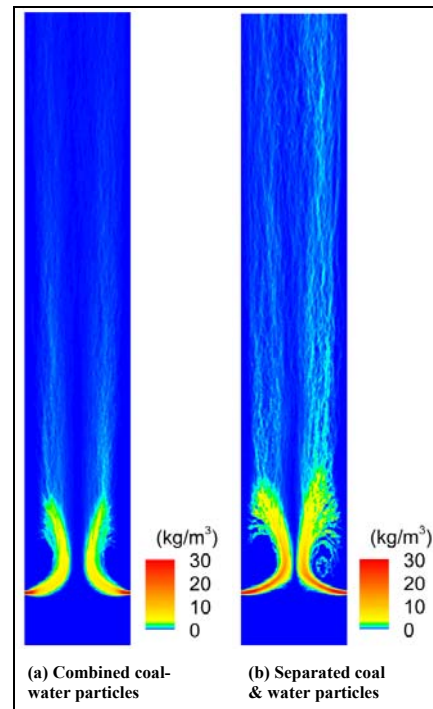


Fig. 6 Particle concentrations for finite-rate cases with (a) combined coal-water particles and (b) slurry water injected as separated water droplets from coal particles.

4.4 Discussion of Results in the 3D Gasifier

A similar comparison between the finite-rate model and the instantaneous gasification model in the 3D gasifier follows by using 50 μ m coal particles and water slurry in coal particles. Table 7 shows the results. Syngas temperature for the instantaneous gasification case (with the slow water shift) is much lower compared to the temperature for the finite-rate case (874K compared to 1221K), which is different from the 2D gasifier case where the syngas temperature for the instantaneous gasification case and the finite-rate case are almost identical

(1179K and 1181K, respectively). One of the plausible explanations is that the 3D gasifier provides better mixing than the 2D gasifier and results in more complete and faster **endothermic** char-CO₂ (R1.2) and char-steam gasification (R1.3) for the instantaneous gasification model and thus the syngas temperature decreases to provide energy for these two gasification reactions. These better gasification reactions are evidenced by increased CO and H₂ mole fractions with reduced CO content.

Table 7 Comparison of exit syngas temperatures and compositions of the 3D gasifier between finite-rate model and instantaneous gasification model.

3D	Finite-rate	Instantaneous gasification, slow water shift	Instantaneous gasification, fast water shift	Equilibrium
Temperature (K)	1221	874	1064	N/A
Carbon conversion	98.1%	100.0%	100.0%	100.0%
Cold gasification efficiency	79%	88%	87%	85%
Mole fraction:				
CO	28.6%	31.0%	7.7%	6.1%
H ₂	31.8%	36.3%	58.2%	59.4%
CO ₂	9.9%	7.5%	30.6%	33.4%
CH _{2.121} O _{0.5855}	0.0%	0.0%	0.0%	0.0%
H ₂ O	28.0%	22.0%	0.0%	0.0%
C ₂ H ₂	0.7%	0.0%	0.3%	0.0%
N ₂	1.0%	3.2%	3.2%	1.1%
O ₂	0.0%	0.0%	0.0%	0
HHV at 25C (MJ/kg)	9.8	10.9	10.9	10.5

The plots of the average gas temperature and species mole fractions along the gasifier's height in Fig. 7 show that, similar to the 2D gasifier, the instantaneous gasification model predicts faster reactions than the finite-rate model does.

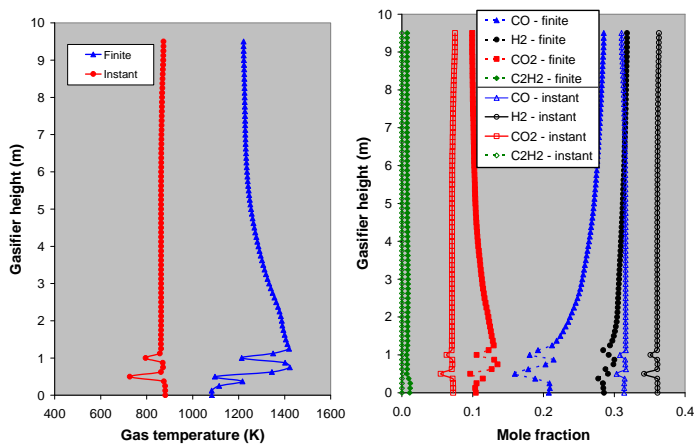


Fig. 7 Mass weighted average of gas temperature species mole fraction distributions for 3D gasifier from cases of finite-rate and instantaneous gasification with slow water shift rate.

Close-up views of the region near the injections for both the finite-rate case and the instantaneous gasification case (with slow water shift rate) are presented in Fig. 8. In the finite-rate case, the hottest region is near the wall just downstream of (or above) the injectors. The CO₂ mole fraction in those locations is the highest. This may indicate that CO produced by the char combustion R1.1 ($C + \frac{1}{2}O_2 \rightarrow CO$) in that area is burned via R1.2 to produce CO₂. The temperature and species distributions plot on vertical mid-plane for the finite-rate case shown in Fig. 8. Figures 8 and 9 show that temperature and species distributions are still changing and reactions are still occurring away from the injection regions. On the other hand, the instantaneous gasification case shows that strong reaction and temperature changes occur not too far away from the injection points. The reactions occur very fast and also finish quickly. Finite-rate case shows a minor trace of unreacted C₂ H₂ and more water vapor content in the syngas.

Similar to the 2D cases, the carbon conversion for the instantaneous gasification model case is also 100%, while there are about 2% unburned chars in the finite-rate model case. Carbon conversion for the 3D finite-rate model case (98.1%) is 7.1 percentage points higher than that of the 2D finite-rate model case (91.0%). The tangential fuel injection in 3D gasifier causes the flow to swirl and lengthens particle residence time which benefits carbon conversion and fuel production. Without tangential swirl, the residence time of the through flow is around 1 second; whereas the tangential injection increases the average particle residence time to 3.8 seconds. This tangential injection can't be simulated in the 2D gasifier.

When the reduced water shift rate is lifted by employing the eddy-dissipation rate, the exit syngas temperature rises from 874K to 1064K. Similar to the 2D case, the exit syngas composition changes drastically with a large reduction of CO and steam and a significant increase of H₂ and CO₂ – a clear signature of the effective water shift reaction (R1.6). As expected, the exit syngas composition is almost the same as the equilibrium results. The heating value of the instantaneous gasification model produces higher heating value than the finite rate, irrespective of the water-shift rate.

In summary, the instantaneous gasification approach with slow water shift can provide approximately adequate syngas composition and heating value of the finite rate result, but it can't adequately capture the local gasification process predicted by the finite rate model in most parts of the gasifier.

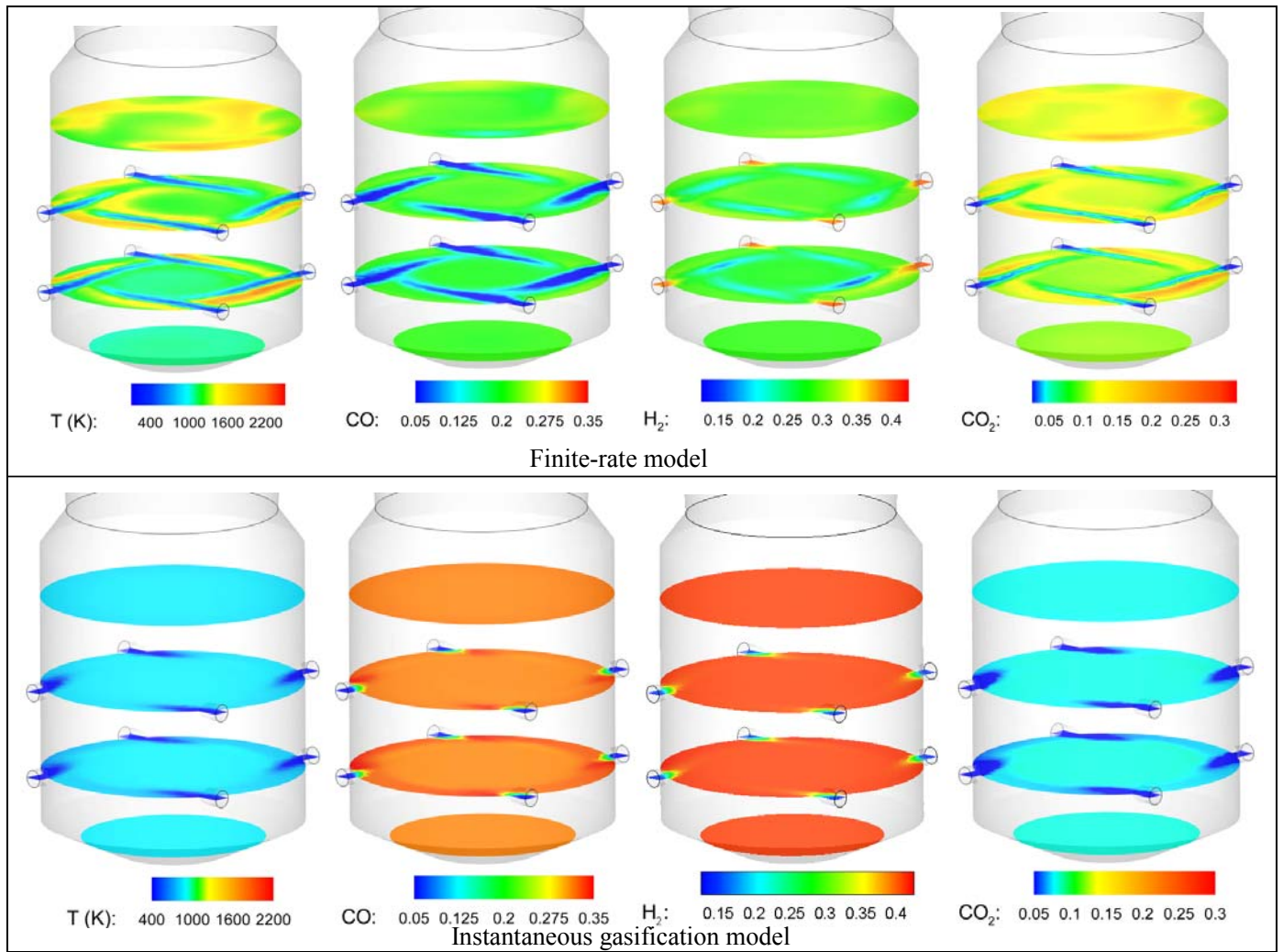
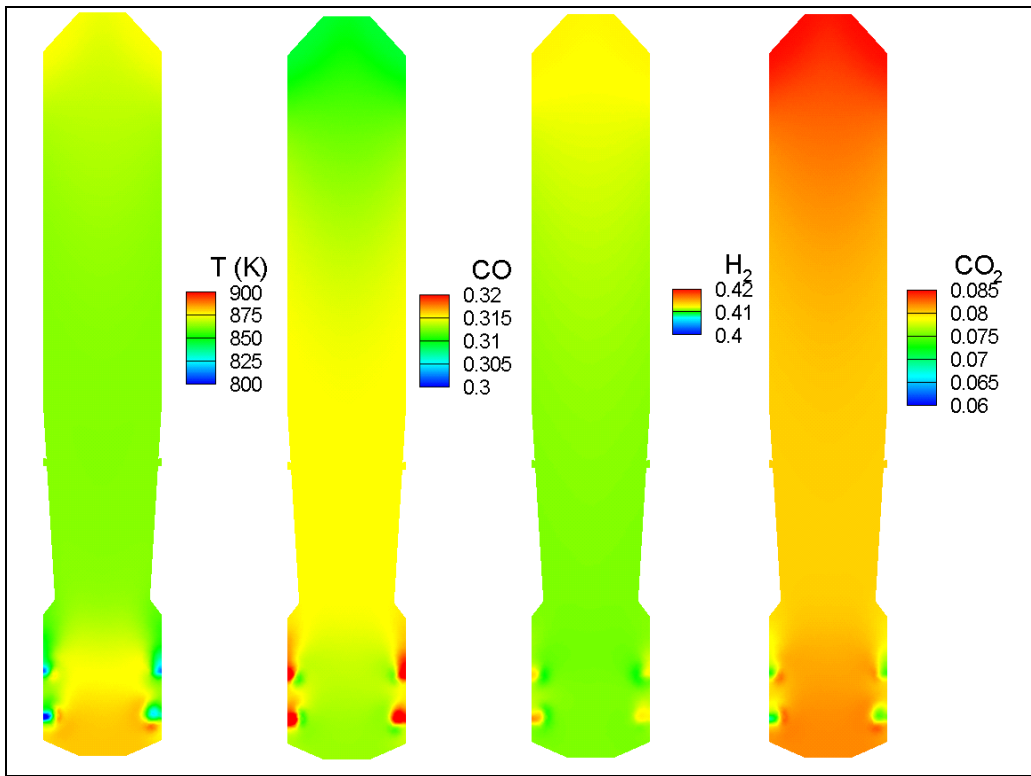
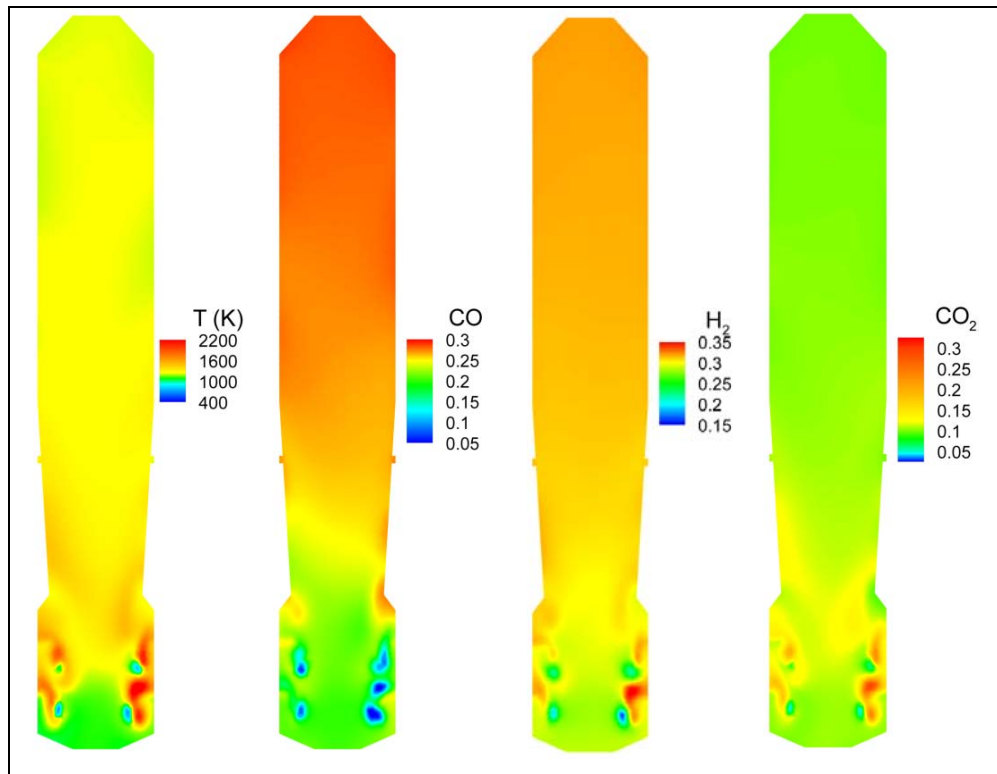


Fig. 8 Comparison of gas temperature and species mole fraction distributions near the injection regions for the finite-rate and the instantaneous gasification (with a slow water shift rate) cases. The same color map is used for both cases for an easy comparison.



(a) Instantaneous gasification model



(b) Finite-rate model

Fig. 9 Gas temperature and species mole fraction distributions on vertical mid-plane for 3D gasifier with (a) Instantaneous gasification model with slow water shift rate (b) finite-rate model. Different color maps are used between these two cases to allow more clear presentations of local parametric distributions.

5.0 CONCLUSIONS

Four different models are simulated and analyzed in this paper: (a) finite rate model with heterogeneous solid reactions and homogeneous gas reactions, (b) instantaneous gasification model with a slow water shift rate, (c) instantaneous gasification model with a fast water shift using eddy-dissipation rate, and (d) chemical global equilibrium model. The results show:

- (1) Reactions in the instantaneous gasification model occur fast and finish quickly; whereas, the reaction in the finite-rate model, which involves gas-solid reactions, occurs slowly.
- (2) The water shift rate plays a very important role on affecting the accurate prediction of the syngas composition. The syngas composition of using fast water shift rate is very close to that calculated from the global equilibrium method.
- (3) When slow water shift rate is used, the instantaneous gasification model and finite rate achieve similar exit syngas composition and temperature, but local species and temperature distributions in the gasifier are very different.
- (4) The fast water shift rate can be used with the presence of catalyst, while the slow rate should be used without catalyst as in a typical entrained-flow gasifier. Furthermore, forward water shift reaction occurs in low temperature environment, so it is more appropriate to use slow water shift rate for simulating coal gasification in entrained-flow gasifiers.
- (5) Varying the coal particle size of the finite-rate model shows that the syngas composition and heating value of the smaller particle size is closer to the instantaneous gasification model.
- (6) The coal slurry injection has been modeled by two approaches (a) combining coal with water into combined droplets and (b) separating coal particles from water droplets. The combined coal-water injection model seems to perform more closely to the real condition and results. The difference in result, solely from the different injection models, indicates the uncertainty of current CFD model.
- (7) The overall result reveals that the instantaneous gasification approach can provide an overall evaluation of relative changes of gasifier performance in terms of temperature, heating value, and gasification efficiency corresponding to parametric variations, but not adequately capture the local gasification process predicted by the finite rate model in most part of the gasifier.

6.0 ACKNOWLEDGEMENTS

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