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범용 CFD 코드에서 석탄 가스화 및 연소 모델링에 관한 이해

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Understanding Coal Gasification and Combustion Modeling in General Purpose CFD Code

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ABSTRACT

The purpose of this study is to assess approaches to modeling coal gasification and combustion in general purpose CFD codes. Coal gasification and combustion involve complex multiphase flows and chemical reactions with strong influences of turbulence and radiation. CFD codes would treat coal particles as a discrete phase and gas species are considered as a continuous phase. An approach to modeling coal reaction in FLUENT®, selected in this study as a typical commercial CFD code, was evaluated including its devolatilization, gas phase reactions, and char oxidation, turbulence, and radiation submodels. CFD studies in the literature were reviewed to show the uncertainties and limitations of the results. Therefore, the CFD analysis gives useful information, but the results should be carefully interpreted based on understandings on the uncertainties associated with the modelings of coal gasification and combustion.

Key Words : Coal gasification, Coal combustion, Modeling, CFD, General purpose code

1. Introduction

Gasification technology of solid fuel has been getting more interest in the power generation industry because of its great versatility of the fuel[1]. For better understanding of coal gasification and combustion, they have been simulated by many numerical methods. For simulation of coal gasification and combustion process, computational fluid dynamics (CFD) analysis is one of the widely used methods. CFD codes which are used for the simulation have become easily available from commercial vendors, as general purpose codes show superior capability to in-house codes, especially for the user interface.

Mathematical modeling of coal gasification and combustion is ambiguous work because of heterogeneous characteristics of coal combustion, which should be based on many assumptions in the simulation work. Therefore, the CFD analysis of coal gasification and combustion may have many uncertainties, even if, it provides useful information such as distribution of the gas composition and flow field. In this paper, these factors are investigated with evaluating modeling methods of coal gasification and combustion in general purpose CFD code, FLUENT®.

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2. CFD modeling with coal combustion

CFD analysis has been one of the important tools for obtaining basic data to evaluate the performance of the pulverized coal fired boilers. In the same manner, CFD modeling provides insights into the many complex phenomena in a coal reactor, which lead designers and operators to obtain improved performance of the reactor. Comprehensive modeling of pulverized coal gasification and combustion has been developed for several decades. PCGC series developed by advanced combustion engineering research center in Brigham Young university is a representative comprehensive coal combustion model[2]. The comprehensive model means the model considering gas fluid dynamics, turbulence, particle mechanics, gas phase reactions, mixing and gas properties, particle phase reactions, heat transfer, and other physicochemical pheno-

mena. This model can be expanded to advanced models which may contain additional functions or submodels.

2.1. Development of general purpose codes

PCGC is a generalized, three dimensional, and steady state analysis tool that can characterize a variety of reactive fluid flows with entrained particles when these flows can be described locally by general momentum, energy, and chemical element conservation equations[2]. The contents of the general purpose CFD codes for coal modeling are based on the PCGC program. In other words, approaches are the same as the PCGC program in terms of the multiphase and physical systems. Engineering organizations are developing the advanced models based on CFD analysis. For example, national energy technology laboratory (NETL) presented the progress toward developing in-house codes for CFD models of the commercial scale gasifier using commercial CFD software, FLUENT®[3]. In addition, integrated simulation of Aspen Plus® and FLUENT® was introduced[3]. They have been applied to various chemical process and power generation applications. Reaction engineering international (REI), a consulting firm in combustion and environment solutions, has presented a CFD analysis tool for an entrained flow gasifier[4]. Its gasifier models are being constructed using its CFD code, GLACIER®. The code was primarily applied to burner and furnace design, utility boilers, waste incineration, pulverized coal combustion, and it was expanded to simulate the coal gasifiers[4].

2.2. Simulation cases

Over the last few decades, attempts have been made by scholars to simulate coal gasification and combustion. Several papers are devoted to the study of a detailed CFD analysis of coal gasification and combustion using general CFD codes[1-8].

Hill and Smoot developed a three dimensional coal combustion CFD model, PCGC-3[2]. This code was assumed to equilibrium gas phase chemistry. The turbulent flow field with the chemical reactions was coupled by integrating the equations over a probability density function. Fletcher et al. proposed a CFD analysis model to simulate the flow and reaction in an entrained flow biomass gasifier[5]. The model was based on the commercial code, CFX®. Biomass particulate was modeled by a Lagrangian approach as it enters the gasifier and releases its volatiles. Finally, the particulate undergoes gasification and combustion. The model provided information about the gas composition and temperature at the outlet. Models of finite rate chemistry in the gas phase and char reactions were added to the standard model. Watanabe and Otaka presented modeling of coal gasification reaction using CFX® via a user Fortran interface[6]. This model was used to predict the gasification performance of the entrained flow coal gasifier. This model was composed of pyrolysis, char gasification, and gas phase reaction models. The distribution of the gas temperature and composition was presented. Syred et al. indicated the development of fragmentation model for solid fuel combustion and gasification as subroutines for inclusion in CFD codes, FLUENT®[7]. They recognized that FLUENT® was well developed and had well proven routines for Lagrangian tracking of burning particles through complex flow fields. The difficulties of incorporating models of fragmentation in CFD codes were discussed. Kang et al. constructed a numerical model of the entrained flow coal gasifier to simulate the coal gasification process using FLUENT® [8]. The complicated processes were classified into simplified stages of slurry evaporation, coal devolatilization, and chemical reactions coupled with turbulent flow and heat transfer.

Most of the simulation cases are the comprehensive models. Namely, fluid flow, heat and mass transfer, turbulence, chemical reaction, and reactor geometry are considered for simulation. As a result, thermal and hydrodynamic characteristics are obtained with discretized control volumes in the system.

3. Approaches to modeling coal combustion in the general purpose CFD codes

3.1. Multiphase modeling for hydrodynamics

Since coal combustion and gasification take place simultaneously, multiphase modeling should be considered. A discrete phase is modeled by defining the initial position, velocity, size, and temperature of individual particles. These initial conditions are used to initiate a trajectory. The calculations are based on the force balance on the particle and on the convective and radiative heat transfer, and mass transfer from the particle, using the local continuous phase conditions as the particle moves through the flow. The Lagrange

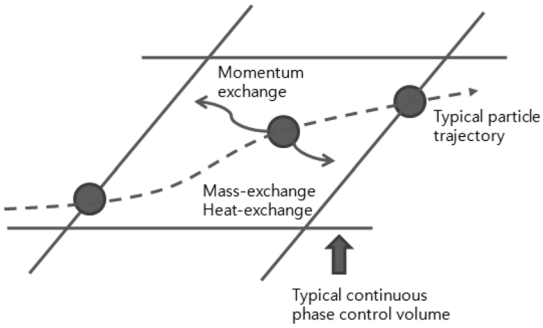

Fig. 1. Transfer relation between discrete and continue phases.

discrete phase model follows the Euler-Lagrange approach. The fluid phase is treated as a continuum to solve the time averaged Navier-Stokes equations, while the dispersed phase is solved by tracking a number of particles through the calculated flow field. The dispersed phase can exchange mass, momentum, and energy with the fluid phase[9]. Fig. 1 shows the transfer relation between discrete and continue phases.

In the Euler-Euler approach, since the volume of a phase cannot be occupied by the other phases, the concept of phasic volume fraction is introduced. These volume fractions are assumed to be continuous functions of space and time. Their sum should be equal to one. Conservation equations for each phase are derived to obtain a set of equations, which have similar structure for all phases. These equations are closed by providing constitutive relations that are obtained from empirical information or by application of kinetic theory[9]. In conclusion, the governing equations between the solid phase and the fluid phase are coupled and the equations are solved with consideration of the fluid mechanics. As a result, the fluid fields and the particle trajectory are obtained at given initial and boundary conditions.

3.2. Coal chemistry

When a coal particle is heated to a temperature higher than 700-1000K the coal devolatilizes. The coal particle is divided into a solid residue, the char, and volatiles. Then, homogeneous reactions of volatiles and heterogeneous reactions of char take place. In general purpose CFD code, modeling coal combustion is generally categorized into non-premixed combustion model. When coal is the only fuel in the system, coal can be modeled by two mixture fractions. One stream is used to represent the char and the other stream is used

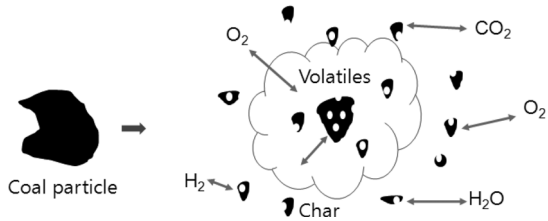

Fig. 2. Coal combustion and gasification process.

to represent volatiles. This process can be simply described as shown in Fig. 2.

Devolatilization. A complete devolatilization model would describe the composition and physical state of the coal or char particle at all stages of devolatilization. However, it is impossible to predict it with numerical simulation because operating conditions have an effect on the quantity of volatiles. The composition and yield of the volatiles released are dependent on the heating rate and the temperature[5]. The yield of volatiles is significantly in excess of the value given by the proximate analysis. Volatile matter is composed of many complex substances. The composition of the volatiles is not arbitrary as it depends on the composition of the original coal.

In FLUENT®, coal is simply classified into anthracite, coal-lv, coal-mv, coal-hv, lignite, and peat as the quantities of the fixed carbon and volatile matter. Table 1 shows the coal type and default properties provided by FLUENT®[9].

The devolatilization model is applied to a combusting particle when the temperature of the particle reaches the vaporization temperature and remains in effect while the mass of the particle exceeds the mass of the non-volatiles in the particle[9]. Composition of the volatiles is represented as $C_XH_YO_Z$, such as mixture of the fuel. The volatile stream composition is defined

Table 1. Coal type provided by FLUENT®[9]

Coal	Property			
	Density (kg/m^3)	CP (J/kg.K)	Component fraction (%)	
			F.C.	V.M.
Anthracite	1550	1680	85.1	6.9
Coal-lv	1400	1680	79.1	12.9
Coal-mv	1400	1680	64.4	27.6
Coal-hv	1400	1680	57.5	34.5
Lignite	1250	1680	44.7	50.4
Peat	1150	2000	30.7	65.3

Table 2. Devolatilization model provided by FLUENT®[9]

Coal	Devolatilization model						
	Constant rate	Single rate		Two competing rate (Kobayashi model)			
	A_0	A	E (kJ/mol)	A_1	E_1 (kJ/mol)	A_2	E_2 (kJ/mol)
Anthracite	50	1.8 E+07	117	2.0 E+05	104.6	1.3 E+07	167.4
Coal-lv	50	3.82 E+05	74				
Coal-mv	50	4.92 E+05	74				
Coal-hv	50	3.12 E+05	74				
Lignite	20	3.12 E+05	74				
Peat	20	3.12 E+05	74				

by selecting appropriate species and setting their mole or mass fraction. There are some models to describe the devolatilization in FLUENT®. They are the constant rate model, the single kinetic rate model, and the two competing rates model (Kobayashi model). Table 2 shows the devolatilization models and rate constants provided by FLUENT®[9].

If the kinetics is considered, a rate constant *k* should be used to model the phenomena. The reaction rate constants are defined by input of an Arrhenius type of equation (1), such as pre-exponential factor, *A*, and activation energy, *E*.

$$\begin{array}{l}\text{Coal - k: Volatile + Residue}\\ \qquad\quad\ \alpha \qquad (1-\alpha)\end{array}$$

$$k = A \cdot \exp(-E/RT) \tag{1}$$

On the other hand, a two competing rate model, the Kobayashi model, is an empirical model based on two competing overall reactions[11]. Equation (2) shows the Kobayashi devolatilization model.

$$\text{Coal} \begin{cases} \text{k}_1\text{: Volatile 1 + Residue 1} \\ \qquad\quad \alpha_1 \qquad (1-\alpha_1) \\ \text{k}_2\text{: Volatile 2 + Residue 2} \\ \qquad\quad \alpha_2 \qquad (1-\alpha_2) \end{cases}$$

$$\begin{aligned} k_1 &= B_1 \cdot \exp(-E_1/RT) \\ k_2 &= B_2 \cdot \exp(-E_2/RT) \end{aligned} \tag{2}$$

The Kobayashi model was made to model the fact that the volatile yields at high temperatures had been found to be considerably higher than the proximate volatiles content. Authors defined that B_1 and B_2 are pseudo pre-exponential factors and E_1 and E_2 are pseudo activation energies. The first reaction is assumed to be dominant at relatively low temperatures leading to the volatile yield α_1. At high temperatures the second reaction is assumed to become faster than the first one, which amounts to requiring that E_2 be much larger than E_1, resulting in larger volatile yields[11]. It should be noted that the model reduces to a single reaction at relatively low temperature where the second reaction is negligibly slow. Therefore, kinetic parameters for the first reaction are uniquely specified under relatively low temperature conditions[11].

Gas phase chemistry. Volatiles react with an oxidizing agent. The gas phase reactions have been dealt with local chemical equilibrium calculated by a method of Gibbs free energy minimization of chemical species or Arrhenius type's chemical kinetics[2,5,6,8,10]. Table 3 shows simplified one-step combustion reactions of volatiles of each coal provided by FLUENT®. The one-step reactions are not recommended to simulate the gas phase chemistry, because surrounding temperature rapidly rises.

The general purpose CFD code provides several models for chemical species transport and reactions to model the gas phase reacting flows. Of the finite-rate chemistry models, the eddy-dissipation model is usually applied to model coal gasification and combustion. The reaction rates that appear as source terms are computed. In that model, the overall rate of reactions is controlled by turbulent mixing. Since turbulence makes mixing of the fuel and oxidizer into the reaction zones slow, chemical kinetic rates are neglected. In real situation, volatiles may burn as soon as they enter the computational domain and that moment is controlled by the chemical reaction rates. Considering that, finite-rate/eddy-dissipation model is often used to model coal gasification and combustion[8]. In this model, the net

Table 3. Combustion reaction of volatiles and property provided by FLUENT®[9]

Coal	Gas phase chemistry				
	Volatiles C_P (J/kg.K)	Volatiles molecular weight (g/mol)	Combustion reaction of volatiles	Rate constant	
				A	E (kJ/mol)
Anthracite	1500	13.21	an_vol+2.207O_2 → 0.1CO_2+4.408H_2O	2.119 E+11	202.7
Coal-lv		23.82	lv_vol+2.979O_2 → CO_2+4.17H_2O		
Coal-mv		17.237	mv_vol+1.706O_2 → CO_2+1.543H_2O		
Coal-hv		18.412	hv_vol+1.598O_2 → CO_2+1.417H_2O		
Lignite		26.631	lig_vol+1.272O_2 → CO_2+1.295H_2O		
Peat		31.085	peat_vol+1.127O_2 → CO_2+1.285H_2O		

rate is taken as the minimum value between reaction rate and turbulent mixing rate. User can determine the number of the chemical reactions. Simple global reactions are mainly used to describe most of the gas phase chemistry and multiple simultaneous chemical reactions can be modeled. User can add or modify the species and input the property data such as density, heat capacity, molecular weight, and enthalpy of additional gas species into the code.

Solid phase chemistry. After the component of the volatiles in the particle is completely evolved, solid phase reactions begin. The char stream composition is generally represented as 100% carbon in general purpose CFD codes. Oxidation and gasification reactions of char have complex mechanism. Turbulent flow and radiative heat transfer complexify them strongly. In addition, there are many variables, such as shape of coal particles, reaction rate, diffusion rate, surface area, a porous condition, ambient temperature, and pressure.

The general purpose CFD code provides char oxidation models as shown in Table 4. For example, FLUENT® provides five surface reaction rate models for combusting particles. They are the carbon burnout kinetics (CBK) model, diffusion limited rate model, the kinetics/diffusion limited rate model, the intrinsic model, and the multiple surface reactions model[9]. In the CBK model, mechanism of char oxidation is predicted to represent the latest stages of burnout. To characterize the extent of char oxidation, the burnout assigned from the mass fraction of combustible remaining is the most useful conversion index. Approximate burning rates can be estimated if the CO/CO_2 product ratio is known[12]. The diffusion limited rate model assumes that the surface reaction proceeds at a rate determined by the diffusion of the gaseous oxidant to the surface of the particle. The kinetics/diffusion limited rate model assumes that the surface reaction rate is determined either by kinetics or by a diffusion rate. The intrinsic combustion model is similar to kinetics/diffusion limited rate model. This model uses the same diffusion rate coefficient but kinetics is explicitly expressed in terms of the intrinsic chemical and

Table 4. Char oxidation model provided by FLUENT®[9]

Coal	Char oxidation model		
CBK combustion model			
	Char intrinsic E (kJ/mol)	CO/CO_2 A	CO/CO_2 E (kJ/mol)
All coal type	146.5	200	37.7
Kinetics/Diffusion-Limited combustion model			
	Mass Diffusion-Limited Rate constant	Kinetics-Limited Rate A	Kinetics-Limited Rate E (kJ/mol)
All coal type	5.0 E-12	0.002	79
Intrinsic combustion model			
	Mass Diffusion-Limited Rate constant	Kinetics-Limited Rate A	Kinetics-Limited Rate E (kJ/mol)
All coal type	5.0 E-12	0.030198	179.4

pore diffusion rates. The multiple surface reactions model describes that the particle surface species can be depleted or produced by the stoichiometry of the particle surface reaction defined by user.

As shown in Tables 2, 3, and 4, the default properties provided by FLUENT® are almost same for each coal type. However, they are different as various coals, namely, they are not fixed values. User should consider appropriate rate constants of simulated coal. The reactants and products among chemical reactions affect each other. Therefore, many rate constants for different chemical reactions are required for the modeling. User will have to take this circumstances into consideration.

3.3. Turbulence and radiation

This study focuses on modeling coal gasification and combustion itself in general CFD codes. Modeling turbulence and radiation is also important because they are closely related with coal gasification and combustion. For example, turbulent flow and radiative heat transfer complexify the phenomena in the entrained bed coal gasifier. General purpose CFD codes provide physical models to simulate turbulence and radiation [9]. It is necessary to verify the validity of the models. In this study, the effect of each model on the results is shown as simple coal combustion is simulated using FLUENT®. Fig. 3 shows the three dimensional reactor to simulate coal combustion.

Standard k-ε, standard k-ω, and Reynolds stress (RS) models were selected as turbulence models. P1, discrete ordinates (DO), and discrete transfer (DTRM) models were selected as radiation models. Table 5 shows initial and boundary conditions.

Turbulent flows are characterized by fluctuating velocity fields. This fluctuation can be of small scale and high frequency. Modified set of equations with averaging is used for removing the small scales. The modified equations contain additional unknown variables, and turbulence model is needed to determine these variables[9]. Fig. 4 and 5 show the axial velocity and turbulence viscosity distribution across the center of the reactor at a height 4 m from the base. Difference of the results is shown based on same conditions except for turbulence models. It is beyond

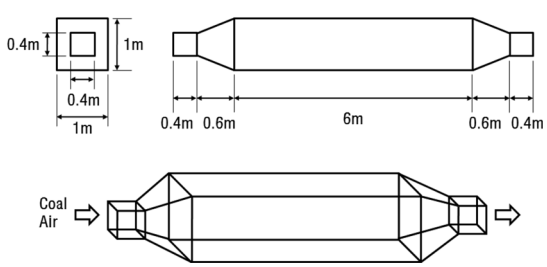

Fig. 3. The shape of an example reactor.

Table 5. Initial and boundary conditions

Property		Value
Fuel (Coal-mv)	mass flow rate	2 kg/s
	mean diameter	134 μm
	initial temperature	300 K
Oxidizer (Air)	mass flow rate	4 kg/s
	initial temperature	1500 K
Operating pressure		101325 Pa
Wall temperature		300 K
Wall thickness		0.1 m

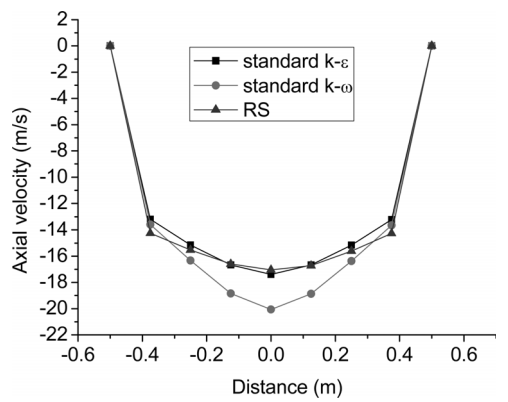

Fig. 4. Comparison of the axial velocity distribution across the center of the reactor at a height of 4 m from the base.

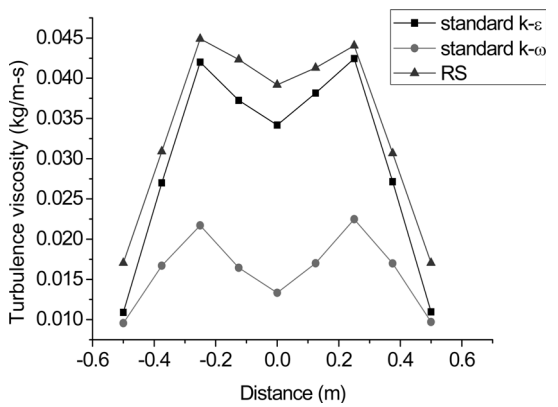

Fig. 5. Comparison of the turbulence viscosity distribution across the center of the reactor at a height of 4 m from the base.

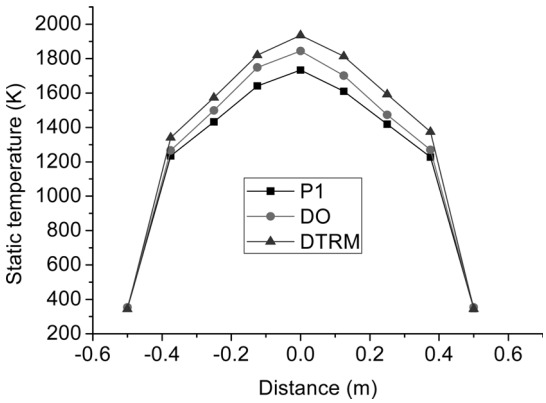

Fig. 6. Comparison of the temperature distribution across the center of the reactor at a height of 4 m from the base.

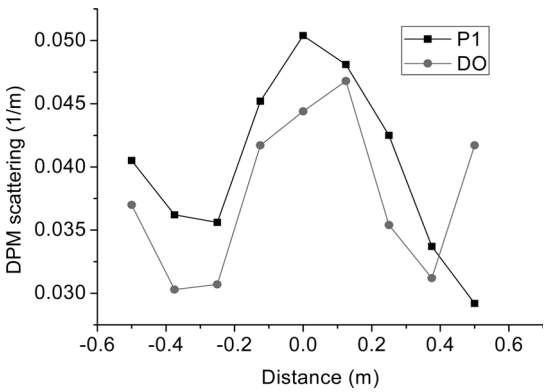

Fig. 7. Comparison of the particle scattering distribution across the center of the reactor at a height of 4 m from the base.

our scope to analyze mathematically the reason. It is necessary to recognize that each turbulence model may give different results in different combustion environment.

Radiation in solid phase is more important than radiation in gas phase. Since it is difficult to predict the behavior of particles as combustion environment, radiative heat transfer is difficult to analysis. Radiation is sensitive to the many variables, such as absorption and scattering coefficients. Fig. 6 and 7 show the temperature and particle scattering distribution across the center of the reactor at a height 4m from the base. Difference of the results is shown based on same conditions except for radiation models. Therefore, appropriate physical model should be used considering combustion environment.

4. Availability and uncertainty

4.1. Availability

Flow field. By solving the governing differential equations, flow fields are calculated over the system. As a result, the distribution of gas composition, temperature, pressure, and velocity is contoured. They can be used for the operation and for the considerations on the engineering designs, such as flame shape, oxygen concentration, and heat flux to wall.

Reactor geometry. User can design the reactor geometry by producing the mesh in the control volume. It is important because the flow field is changeable as the reactor geometry. For example, flow recirculation can be formed at a corner and flow velocity is sensitive to burner dimension or complex geometry of the reactor.

Mixing effect. The effect of mixing of the reactants is important with respect to multiphase reaction, such as coal gasification and combustion. Gasification mechanism is generally induced due to mixing by turbulence and chemical reaction. There is no mixing effect in equilibrium model, whereas the general purpose CFD code has considered the mixing effect as controlling mixing rate.

4.2. Uncertainty

Coal chemistry. Although there are many coal types, they are simply classified into six coals. User can define the component of coal by using user defined function (UDF), but it does not indicate the change of the physical characteristics. User can determine the fraction of volatile matter as $C_XH_YO_Z$ form. In real situation, less volatile matter is released at elevated pressure. Tar production is associated with reaction mechanisms that are especially sensitive to pressure variations[12]. General CFD codes do not consider those points.

Chemical reaction. A lot of chemical reactions take place in the reactor. They are quantitatively complex because of heterogeneous characteristics of coal reaction. User can determine the number of the chemical reaction but most of the reactions are simple global reactions. It is a rough approach to apply the simple global reaction to chemical kinetic model. Although the rate constants change on ambient conditions, they are fixed values in commercial CFD code. This is one of the uncertainties.

Turbulence. Fluid flow predicted by CFD analysis has largely depended on turbulence model for analysis of turbulent flow. However, it is reported that general turbulence models predict the phenomena uncertainly, such as swirling flow, separated flow, flow at stagnation point, and recirculation flow. The choice of turbulence model is dependent on the considerations such as the physics in the flow, the established practice for a specific class of problem, and the level of accuracy required[9]. To model the multiphase turbulent flow, the governing equations are calculated with numerical values averaged. Although there are some models, the Reynolds averaged approach has been generally adopted for the turbulence modeling. The k-ε model has been adopted in many previous studies for coal gasification modeling[1,2,4-6,8,13], because it is semi-empirical model and the derivation of the model equations depends on empiricism and phenomenological consideration. Current CFD codes can analyze complex flow in the arbitrary geometry of the system, but it shows limitations of modeling flow field in the corner of the system. Since recirculation flow with separation is generally required for longer residence time in the coal gasifier, it needs to improve the performance in this area.

Radiation. In CFD analysis for coal combustion, modeling the heat transfer is one of the most difficult points because the reactor operates at high temperature and pulverized coal particles emit light strongly. It affects interactive radiation and makes analysis difficult. Radiation is dominant heat transfer mechanism in the coal reactor and it is difficult to understand the obvious mechanism, particularly for the entrained bed coal gasification having short residence time. Corrosive slags that form and flow on the inner walls of a slagging gasifier can quickly degrade the refractory lining in the gasifier vessel[14]. Therefore, quantitative analysis of the heat transfer to the wall is important. General purpose CFD code provides the radiative heat transfer equation for an absorbing, emitting, and scattering medium at position in the direction. The code also provides some radiative heat transfer models. The choice of the models will be depend on considerations such as optical thickness, scattering, emissivity, and particulate effects. User should determine the absorption and scattering coefficients for the modeling. The CFD code gives the effect of coal particles on the absorption coefficient as a constant. However, the constant depends on combustion conditions and a common way of justifying the property is based on comparison of the results of modeling with available experimental data. As one of the examples, ref. 15. presented the uncertainty of application of radiation model to the coal combustion modeling[15].

4.3. Case review

The uncertainty may be quantitatively understood as reviewing the modeling cases for coal gasification and combustion using general purpose CFD code. First case is a numerical simulation for coal gasification using FLUENT® code[8]. In this paper, the following submodels were considered as shown in Table 6 for comprehensive modeling.

Authors selected cold gas efficiency (CGE) and carbon conversion efficiency (CCE) as an index indicating the gasifier performance. Generally, CCE increases as O_2/coal mass ratio increases and vice versa. Fig. 8 shows different trend in the vicinity of O_2/coal mass ratio 0.3. It is difficult to clarify the reason because there are many interactive submodels. However,

Table 6. Main submodels considered[8]

Subject	Submodel
Coal particle	Discrete phase model
Gas phase	Finite rate/eddy dissipation
Turbulence	RNG k-ε
Radiant	Discrete ordinate
Particle dispersion	Stochastic tracking
Devolatilization	Two competing rates (Kobayashi model)
Char reaction	Multiple surface reaction

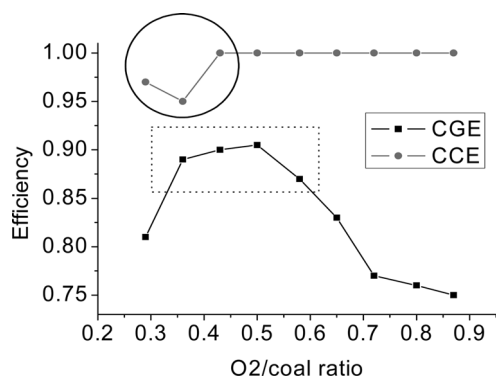

Fig. 8. Effect of O_2/coal ratio on efficiency of the gasifier[8].

Table 7. Chemical reactions[8]

Phase	Chemical reaction
Gas phase	Volatile matter + $1.706O_2 \rightarrow 1.543CO_2 + H_2O$
	$H_2 + 0.5O_2 \rightarrow H_2O$
	$CO + 0.5O_2 \rightarrow CO_2$
	$CO + H_2O \leftrightarrow CO_2 + H_2$
Char gasification	$C(s) + 0.5O_2 \rightarrow CO$
	$C(s) + CO_2 \rightarrow 2CO$
	$C(s) + H_2O \rightarrow CO + H_2$

it is considered that rate constants are inappropriate to this system because the rate constants were collected from different references. Since the rate constants depend on experiment conditions, it is unclear to apply to different conditions. Therefore, a feasibility study is needed.

Another point is the level of CGE. Fig. 8 shows that CGE value is close to 0.92 in the vicinity of O_2/coal mass ratio 0.5. CGE is generally about 0.8 as maximum level for this dry-feeding type entrained bed coal gasifier. This is a problem from setting of chemical reactions. Table 7 shows chemical reactions considered for the coal gasification modeling.

The definition of CGE was,

$$\mathrm{CGE} = \frac{\text{HHV in product gas}}{\text{HHV in feedstock}} \tag{3}$$

Four gas phase reactions and three solid phase reactions were considered. Products of the char gasification reactions are all CO and H_2. They are main components having a heating value. It seems that most of the CO_2 and H_2O are simply converted to CO and H_2. It may cause excessive CGE value.

Table 8. Main submodels[5]

Subject	Submodel
Gas phase	Finite rate chemistry
Char reaction	Finite rate chemistry
Turbulence	1) Reynolds stress model 2) k-ε
Effect of turbulence on the particles	Eddy interaction model
Turbulent mixing rate	Eddy breakup model
Particle dispersion	Rossin Rammler distribution
Convective heat transfer	Ranz-Marshal correlation

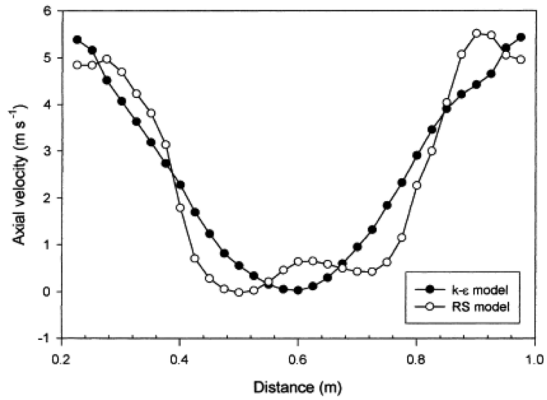

Fig. 9. Comparison of the axial velocity distribution across the center of the gasifier[5].

Second case is CFD analysis for an entrained flow biomass gasification using CFX® code[5]. In this paper, the following submodels were considered for comprehensive modeling as shown in Table 8.

This study shows that the differences between full Reynolds stress model and k-ε model in the reacting case. Fig. 9 shows the axial velocity distributions across the center of the vessel.

There are differences in the axial velocity distribution near the center of the gasifier. It shows the importance of selecting turbulence model on a case by case basis.

Third case is CFD analysis of an entrained flow coal gasification using built-in code[1]. This is not a model using general purpose CFD code but it is meaningful work to find the uncertainty in built-in code, because if this code is incorporated into other general purpose codes. The uncertainty is found in temperature distribution as shown in Fig. 10.

Temperature is over predicted by around 150 K to 350 K. Authors explained that the absorptivity and scattering value may be the main cause for this over

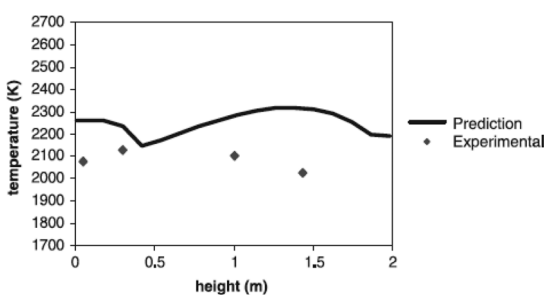

Fig. 10. Axial evolution of gas temperature along with the gasifier[1].

prediction. As mentioned above, finding appropriate absorption and scattering coefficients are very difficult in solid fuel combustion. It would be based on experimental result.

5. Conclusion

This study focuses on understanding approaches to modeling coal gasification and combustion in general purpose CFD codes, FLUENT®. Approaches to modeling devolatilization, gas phase, and solid phase chemistry were described. As a case study, coal combustion was simulated with different turbulence and radiation models. Each of the models showed different results at same conditions and it was necessary to use the appropriate model as different combustion environment. Availability and uncertainties of using the CFD codes was discussed and uncertainty can be understood by reviewing the cases using the commercial codes based on quantitative comparison in terms of flow field. Users would recognize these points and it is necessary to upgrade the uncertainty for advanced CFD analysis of coal gasification and combustion.

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