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Interpretation of coal gasification modeling in commercial process analysis simulation codes †

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Abstract

The purpose of this study is to recognize modeling methods for coal combustion and gasification in commercial process analysis codes. Many users have appreciated the reliability of commercial process analysis simulation codes; however, it is necessary to understand the physical meaning and limitations of the modeling results. Modeling of coal gasification phenomena has been embodied in commercial process analysis simulators such as Aspen. Commercial code deals with modeling of the gasification system with a number of reactor blocks supported by the specific code, not as a coal gasifier. However, the primary purpose of using process analysis simulation code is to interpret the whole plant cycle rather than an individual unit such as a gasifier. Equilibrium models of a coal gasifier are generally adopted in the commercial codes, where the method of Gibbs free energy minimization of chemical species is applied at the given temperature and pressure. The equilibrium model of the coal gasifier, RGibbs, in commercial codes provides users with helpful information, such as exit syngas temperature, composition, flow rate, performance of coal gasifier model, etc. with various input and operating conditions. This simulation code is being used to generate simple and fast response of results. Limitations and uncertainties are interpreted in the view of the gasification process, chemical reaction, char reactivity, and reactor geometry. In addition, case studies are introduced with examples. Finally, a way to improve the coal gasifier model is indicated, and a kinetically modified model considering reaction rate is proposed.

Keywords: Coal gasification; Modeling; Process analysis; Commercial code; Equilibrium

1. Introduction

As the problem of the green house effect has risen, utilization of clean coal energy has become more important. Oxy-fired pulverized coal combustion and IGCC (integrated gasification combined cycle) systems have attracted more attention. An IGCC system is constituted of four major parts, ASU (air separation unit), gasification, gas clean up, and combined cycle as shown in Fig. 1. A coal gasifier is probably the most important unit which produces synthesis gas at high temperature and pressure. Other solid fuels such as biomass can be also used in the gasifier. The efficiency of an IGCC plant is typically higher than that of the conventional pulverized coal fired power plants, and pollutants such as NO_X and SO_X are also lower. On the other hand, the overall economics of IGCC power generation is yet to be determined. Several projects have been successfully demonstrated, but full scale commercial operation is not common. Also it is difficult to make an experiment with coal gasifiers due to their huge scale and operating condition. Therefore, many tools are being researched and developed to simulate the coal gasifier and IGCC. In addition, the gasifier model should be developed to reduce the technical and financial burden in developing and commercializing coal gasification processes.

As a result, some commercial process analysis simulation codes such as Aspen Plus, Aspen Hysis, and GateCycle have been developed to simulate the whole plant cycle, where coal gasification model is included as a constituent unit. Among them, Aspen Plus of Aspen Technology is being widely used for the conceptual process design for coal industries. Aspen Hysis of Aspen Technology is also the process modeling tool for design and optimization for oil & gas production, petroleum refining, and air separation industries. GateCycle of GE Energy is a tool for both the gas and steam sides of power plant design and analysis.

It is not easy to model the coal combustion and gasification phenomena mathematically because the inherent characteristics of coal are complex. Even with this difficulty, there are

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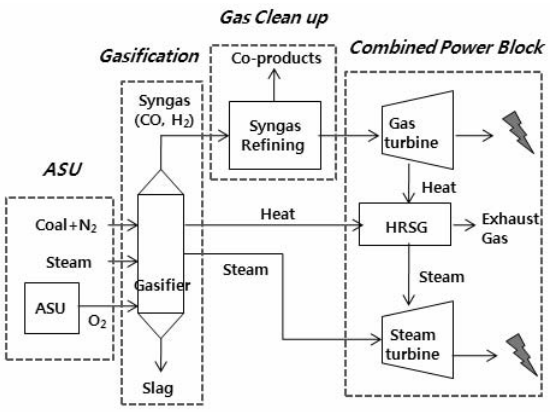

Fig. 1. IGCC diagram.

widely accepted approaches in modeling the coal gasification in the reactor, for example, CFD (computational fluid dynamics), equilibrium, and kinetic models considering reaction rate. Modeling and simulation technology of the coal gasifier has progressed considerably. Recent modeling efforts include the application of equilibrium models to predict the performance of the commercial gasifier, as well as several kinetic models. Although a kinetic model gives essential information on reaction rates, the equilibrium model is valuable because it can predict thermodynamic limits as a guide to process analysis, evaluation and improvement [1].

2. Simulation of gasification process

As the commercial code such as Aspen is an overall process analysis simulation code, it was developed for interpretation of the whole plant. That is the primary purpose of the process analysis simulation code although small sections of complex and integrated systems can be created and tested as separate modules before they are integrated [2]. A concern of this study is the interpretation of the coal gasification part of a coal IGCC plant in commercial process analysis simulation codes, which are used focusing on the modeling of coal combustion and gasification.

2.1 Previous research using commercial codes

The modeling of coal gasification using commercial process analysis simulation codes has been extensively researched domestically and worldwide. In domestic researches, J. Kim et al. developed an analysis model using Aspen Plus for an IGCC system consisting a dry coal feeding and oxygen blown entrained gasification process [3]. Sensitivity analysis was carried out by using the developed model. J. Kim et al. proposed exergy analysis of IGCC system including Shell® gasification using Aspen Plus [4]. A new approach to exergy analysis was proposed for calculating the consumption of energy as the minimum driving force and of exergy consumption that is avoidable. S. Jung et al. studied a simulation model of 300MWe IGCC plant using Aspen Plus [5]. The efficiency

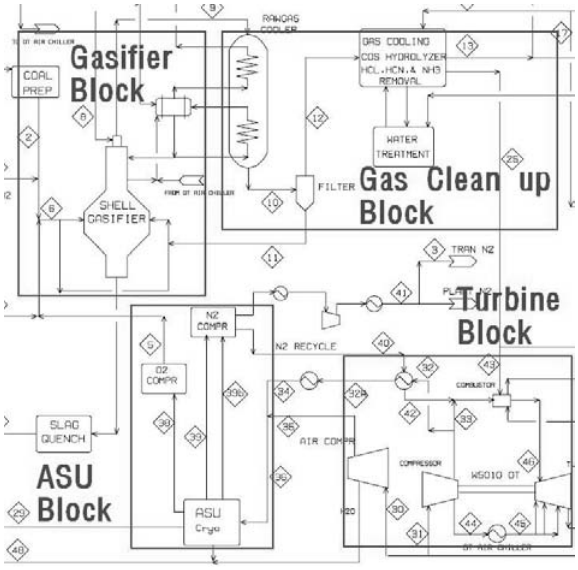

Fig. 2. IGCC process in Aspen modified from [9].

of the gasifier and the whole IGCC plant was estimated on variable coal types. H. Shim et al. studied the comparison on the operating condition of gasification plant on different feedstocks such as pulverized dry coal, coal water slurry, bunker-C, and naphtha by using Aspen Plus [6].

Among international researchers, Ong'iro et al. developed a simulation model with Aspen Plus, which was used to study the effects of design and performance parameters on the efficiency and emissions from IGCC cycles [2]. Fiaschi et al. proposed the possibility of reducing CO_2 emissions from an IGCC plant using Aspen Plus [7]. They focused on an emission removal system among IGCC units. Yan et al. studied a fluidized bed coal gasifier process using Aspen Plus and compared modeling results with experimental results for validation [8].

As shown in previous researches, coal gasification modeling using commercial code generally inclines to interpretation of the whole process analysis of the plant cycle.

2.2 Modeling using a commercial code

Aspen, one of the widely used chemical process simulators, is mainly used to predict the performance of the plant, based on the mass and heat balance, and the phase and chemical equilibrium, at the steady state condition. As an example, Aspen has been used for analysis of the IGCC process as shown in Fig. 2 [9].

The Aspen model consists of flow sheets of the important sections of the IGCC system. The flow sheets are connected by material, heat, and/or work streams. Each flow sheet consists of unit operation blocks and may also include design specifications or blocks using own codes. The gasifier model is included in one of the unit operation blocks. The main reactor models of Aspen are briefly described and illustrated in Table 1 from reference [10]. It is modeled through connection of some reactor blocks.

Table 1. Main reactor model provided by Aspen [10].

Reactor	Purpose
RYield	Reactor with specified yield
RStoic	Stoichiometric reactor with specified reaction extent of conversion
REquil	Chemical & phase equilibrium by stoichiometric minimization
RGibbs	Chemical & phase equilibrium by Gibbs energy minimization
RCSTR	Continuous stirred tank reactor
Flash2	Determine thermal and phase conditions

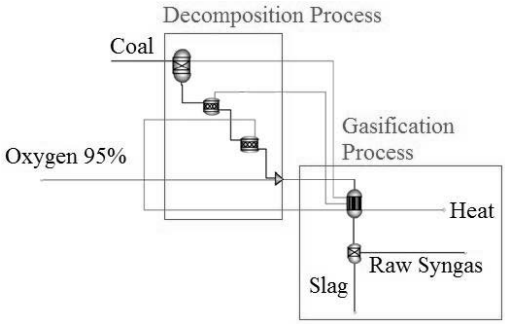

Fig. 3. Simulation model of a model gasifier in Aspen redrawn from [6].

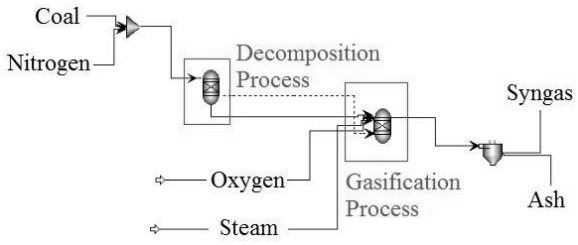

Fig. 4. Gasification model of IGCC in Aspen from [11].

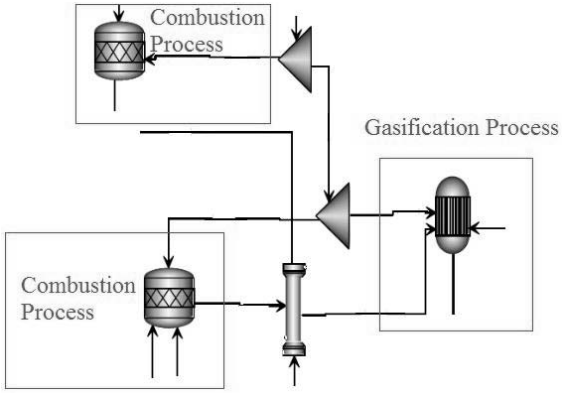

Fig. 5. Biomass gasification model in Aspen from [12].

For example, a dryer of the plant units is described by an RStoic reactor and a gasifier is described by an RGibbs reactor in a coal gasification and combustion system. It is explained with some examples of gasification simulation.

2.3 Examples using commercial codes

Gasification of solid fuels such as coal or biomass can be embodied with reactor blocks provided by the commercial process analysis code. The gasification part modeling was reviewed with some examples.

Shim et al. focused on the determination of operating conditions for a 300MWe scale IGCC plant with various feedstocks through Aspen Plus [6]. The model was composed of fuel preparation, gasification, ash removal, acid gas removal, gas turbine, and steam turbine. After the gasification process was simulated, the simulation results were verified by comparing with reference data. In the gasifier simulation, the fuel preparation process consisted of coal pulverizing, drying, and transporting system. The gasifier model was divided into four sectors such as decomposition, gasification, soot and slag generation as shown in Fig. 3 [6].

RYield reactor block was used to specify the yield distribution based on ultimate analysis of desired coal. The authors chose eleven major chemical reactions generated in the gasifier and those were calculated by approaching minimization of Gibbs free energy in the RGibbs reactor block. In the gasifier model using the RGibbs reactor, the gas composition was calculated at equilibrium state between reactants and products of the chemical reactions. After passing decomposition and gasification process, unburned carbon and slag are generated. This step was described by RStoic reactor block.

Park et al. carried out the simulation of gasification of IGCC system with Aspen Plus [11]. The gasifier model was also described with equilibrium concept. The Shell® type gasifier was selected as the subject gasifier of IGCC. Asa result of the modeling, gasifier exit gas composition was obtained. Fig. 4 is a part of the gasification model. It was composed of devolatilization part and gasification part of the gasifier and slag separation part from the product gas. The authors determined the input conditions of coal, transport gas nitrogen, and oxygen (purity 95%) as oxidizer. The gasification was simulated in two reactor blocks, RYield and RGibbs. Finally, products gas and ash were separated at the latter part of the gasifier.

As mentioned above, biomass gasification can be simulated as well as coal as fuel. As an example, Elbaccouch and Ali presented an Aspen process model for the hydrogen production [12]. The processes were divided into four sections: dryer, gasifier, clean up system, and pressure swing adsorption. Fig. 5 shows a diagram of the biomass gasifier model. The gasification unit contains a combustor and a gasifier to volatilize the biomass. Combustion and gasification processes were modeled using RStoic and RGibbs reactor blocks, respectively.

3. Features of commercial code model

As shown in the above examples, the gasification model of plant system is embodied with designated blocks such as RYield, RStoic, and RGibbs in Aspen. Then, it should be discussed whether coal gasification processes such as devolatilization, gas phase reactions, and solid phase reactions, are truly embodied with these blocks or not. Features of gasification modeling in process analysis simulator are discussed.

3.1 Usefulness

Theoretical limits of coal gasification. Coal gasification is a heterogeneous reaction progress. Turbulent flow and radiative heat transfer complexify the phenomena in the gasifier. Coal itself cannot be treated as fuel. It should be decomposed by RYield block and subsequently calculated by RGibbs block to reach an equilibrium state. The chemical equilibrium approach for gasification gives the physical meaning as theoretical limits of coal gasification. Gibbs free energy minimization method is used to predict the composition of the products at equilibrium state. Although reaching the chemical equilibrium requires enough gas/sold residence time in actual reactors, sufficiently high temperatures with good gaseous mixing will bring the chemical composition to that at the equilibrium. It shows an approximate value close to experimental data [1, 5, 6, 8].

Flexible response. The purpose of using the commercial process analysis code is to get the performance of the whole plant cycle on variables. By using a gasification model of commercial codes, it is also possible to predict the properties at the coal gasifier exit such as gas composition, temperature, flow rate, and the performance. The results are predicted in response to variable input and operating conditions. It is ideal when it is incorporated into a process simulation for a gasification system, which requires quick prediction of a whole system with physical meaning.

3.2 Limitations and uncertainties

Although coal gasification can be embodied by using commercial code, many assumptions are needed for modeling. Consequently, there are limitations and uncertainties for description to demonstration.

Gasification process. In real gasifiers, coal gasification phenomena take place simultaneously [13]. The commercial process analysis code treats it by a simple sequence diagram using the model blocks. There exist a number of sub-processes such as feedstocks mixing, pyrolysis, combustion, gasification, heat transfer, turbulence, coal swelling, diffusion, chemical reactions, coal structure, reaction rate, slagging, and other factors having their own effect. In the commercial process simulation codes, however, the gasifier is represented as a simplified lumped parameter, restricted equilibrium reactor model. The Gibbs free energy of coal cannot be calculated because it is a non-conventional component in the commercial code [14]. Therefore, before feeding the coal to the RGibbs block, the coal should be decomposed into its constituent elements in the RYield block. The heat of reaction associated with the decomposition of coal must be considered in the coal combustion, so this heat of reaction is carried from the RYield block to the RGibbs block. It is impossible to describe exactly this concurrent gasification by using a sequence diagram of the code.

Reaction rate. The chemical equilibrium approach could be considered as one-step reaction approach to determine the gas composition and properties at the gasifier exit. It means that an equilibrium model does not consider reactivity or kinetics of coal reaction. Each of the coals has its own reactivity, and various types of coal are introduced into the gasifier. Therefore, the reactivity should be considered for an individual coal. In heterogeneous reactions, for instance, there are representative reactions, C(s)-O_2, C(s)-H_2O, C(s)-CO_2, and C(s)-H_2. Walker *et al*. estimated the relative rates of the reactions at 1073K and 10kPa pressure as being $3x10^{-3}$ for H_2, 1 for CO_2, 3 for H_2O, and 10^5 for O_2 [13]. It requires a reaction rate model considering the kinetic and diffusion rates and local concentrations of reactants. Although the equilibrium model gives useful information, the interaction between the chemical reactions is not considered [15-18]. The reaction rate is a function of temperature. In relatively low temperature, for example, the reactivity of endothermic reactions becomes low. In the case of an entrained flow gasifier, the residence time is 3-4 seconds [19], which may not be enough to attain chemical equilibrium due to slow char burnout and incomplete gaseous mixing. In an equilibrium model, this point is not considered and it may cause uncertainty.

Volatile yield. The quantity of volatiles determined from proximate analysis is usually less than that which results from pyrolysis. It depends on peak temperature and heating rate [13]. However, it is not predicted in the code. The composition of the volatiles is not arbitrary as it depends on the composition of the original coal. Therefore, the product of the volatiles combustion reaction is changeable for different coal types and combustion environment. It would be one of the reasons for uncertainty.

Reactor geometry. Only output conditions are known through equilibrium calculation. In that concept, all spaces of the gasifier have same properties such as a CSTR (continuous stirred tank reactor). However, the properties are variable on the reactor geometry. For example, flow recirculation may affect the mixing and reaction of the reactants as geometry of the gasifier. It may give uncertainty.

3.3 Case studies

By investigating cases with respect to coal gasification modeling quantitatively, usefulness and uncertainty can be

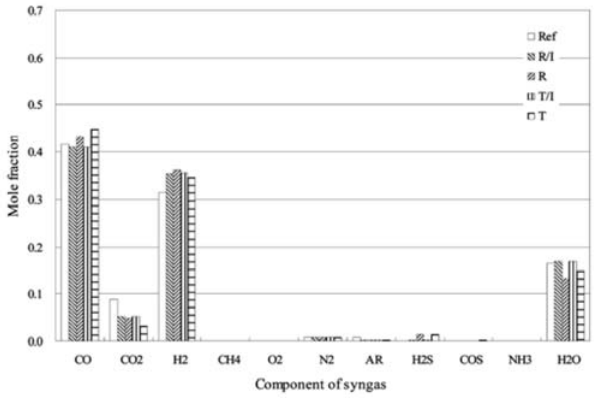

Fig. 6. Evaluation result for coal water slurry from [6].

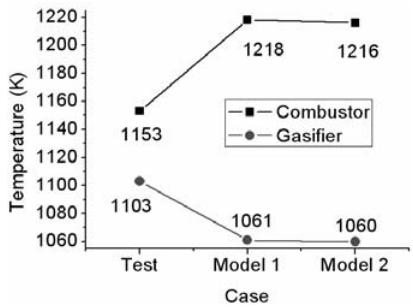

Fig. 7. Evaluation result for temperature.

easily understood. First case is a comparison study on the operating condition of a gasification plant with various feedstocks using Aspen Plus [6]. In this study, the simulation results are verified by comparing with reference data. As to the comparison of syngas yield, in the case of coal water slurry as fuel, CO_2 and H_2 components show comparable results with reference tendency as shown in Fig. 6 [6].

Simplified reactions. The authors chose eleven chemical reactions generated in the gasifier [6]. It is a good assumption that they are dominant reactions. However, gasification cannot be explained with only these reactions. In this study, CO_2 and H_2 components show a contrary difference with reference tendency (less CO_2 and more H_2 based on reference composition).

Isothermal condition. In this study, the temperature and pressure condition is chosen to describe actual operating plants, 2.7MPa, 1693K for pulverized dry coal type gasifier and 4.2MPa, 1643K for coal water slurry type gasifier, respectively. However operating condition varies on spatial location in the gasifier, which means it is non-isothermal condition. Temperature is the most sensitive factor, which has an influence on the variation of properties. Therefore, temperature variation should be considered from the lower to the upper side of the gasifier.

Second case is the modeling of a fluidized bed coal gasifier process through Aspen Plus [8]. The author used sub-model blocks made by using Fortran code in addition to the default blocks. In this study, there are also comparisons between the main experimental results and predictions from the Aspen model. The predicted model shows incorrect operating temperature results a little, as shown in Fig. 7.

Heat transfer. The predicted temperature in the combustor is about 60K higher than the experimental results. This is probably because the heat loss model does not consider the energy carried away by a cooling system on the combustor side and lost to the environment due to some damaged insulation layer around the reactor (In the Aspen model, a uniform insulation layer around the reactor was assumed). The predicted gasifier temperatures are about 40K lower than the measured values. It is probably because the liquid water content of the steam was not quite correct.

4. Potential approach for improvement

Although a coal gasification model of the commercial process analysis simulator is useful for interpretation of the whole plant cycle, the coal gasifier model itself has to be improved. The conventional equilibrium model leads to better understanding of the underlying thermodynamic principles governing coal gasification and is useful in predicting what is thermodynamically attainable [1]. It cannot embody real coal gasification phenomena; however, a kinetically modified model is introduced for better modeling results. Devolatilization of coal is an important step of gasification and it should be modeled, not simply as decomposition, in the commercial code because it has influence on the following gasification steps such as homogeneous and heterogeneous reactions. In this modeling, the reaction rate should be considered because the yield of volatiles is sensitive to temperature and heating rate. Each of the chemical reactions has different reaction rates from the devolatilization to the char gasification, so an adequate kinetic model is required. For example, a two-stage equilibrium model is being developed to advance the conventional one-stage equilibrium model [20]. In the conventional one-stage equilibrium model, all reactions are solved simultaneously such as solid-vapor reactions and vapor-vapor reactions. On the other hand, the two-stage model considers that the 1st stage of coal gasification is solid-vapor reactions and the 2nd stage is vapor-vapor reactions due to difference of reactivity. Carbon conversion is calculated at the 1st stage and final gas composition is calculated at the 2nd stage with products of the 1st stage. These processes are also solved through an equilibrium calculation. As a result, the two-stage model predicts more accurate carbon conversion as well as gasification performance of the coal gasifier than that of the one-stage model. Reaction rate varies on variable conditions such as temperature or concentration, so the variation of the properties in the gasifier should be checked on variable operating condition. If this model is linked with commercial code such as Aspen, a better gasifier model may be established.

5. Conclusions

As the coal gasifier is the core process of IGCC systems, effective modeling and uncertainty analysis of the gasification process constitutes an important element of overall IGCC process design and operation. This study focuses on understanding the coal gasification modeling in commercial process analysis simulation codes such as Aspen. Particularly, the limitations and uncertainties as well as usefulness of the gasifier model in the commercial process analysis codes are studied.

Commercial code such as Aspen focuses on overall cycle analysis but not specifically on the gasifier modeling, so it is necessary to interpret modeling in the commercial process analysis simulator. The coal gasification system is modeled with connection of reactor blocks such as RGibbs, RStoic, and RYield. For example, RGibbs block calculates the equilibrium state of reactants and products of chemical species based on the minimization of Gibbs free energy. Usefulness and uncertainty were interpreted based on the modeling process of coal gasification. Usefulness is mainly introduced in the point of the equilibrium model. The chemical equilibrium approach for gasification gives the physical meaning as theoretical limits of coal gasification in whole cycle analysis. However, uncertainty was discussed in the case of a simplified sequence process of complex phenomena, reaction rate, volatile yield, and reactor geometry. As a result, some examples which show the uncertainty were introduced. This paper has significance as an initial consideration for coal gasification modeling in commercial process analysis code. With detailed description and case studies, this paper provides useful information on the modeling approach in commercial process analysis code, which would be helpful for those using such commercial codes.

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References

[1] X. Li, J. R. Grace, A. P. Watkinson, C. J. Lim and A. Ergudenler, Equilibrium modeling of gasification: a free energy minimization approach and its application to a circulating fluidized bed coal gasifier, *Fuel*, 80 (2001) 195-207.

[2] A. O. Ong'iro, V. I. Ugursal, A. M. Al Taweel and D. K. Blamire, Simulation of combined cycle power plants using the Aspen Plus Shell, *Heat recovery systems & CHP*, 15 (2) (1995) 105-113.

[3] J. Kim, M. Park, K. Song and S. Cho, Performance analysis of Shell coal gasification combined cycle systems, *Energy Eng. J*, 6 (1) (1997) 104-113.

[4] J. Kim, M. Park and C. Kim, Performance improvement of integrated coal gasification combined cycle by a new approach in energy analysis, *Korean J. Chem. Eng.*, 18 (1) (2001) 94-100.

[5] S. Jung and H. Kim, Thermal estimation of 300MW IGCC processing system, *Proc. of 2nd International Freiberg Conference on IGCC & XtL Technologies*, Saxony, Germany. (2007).

[6] H. Shim, S. Jung, H. Wang and H. Kim, The comparison study on the operating condition of gasification power plant with various feedstocks, *Korean J. Chem. Eng.*, 26 (2) (2009) 324-331.

[7] Daniele Fiaschi and Lidia Lombardi, Integrated gasifier combined cycle plant with integrated CO_2-H_2S removal: Performance analysis, life cycle assessment and exergetic life cycle assessment, *Int. J. Applied Thermodynamics*, 5 (1) (2002) 13-24.

[8] Hong-Ming Yan and Victor Rudolph, Modeling a compartmented fluidized bed coal gasifier process using Aspen Plus, *Chem. Eng. Comm.*, 183 (2000) 1-38.

[9] *Shell gasifier IGCC base cases*, US DOE/NETL Report PED-IGCC-98-002 (1998).

[10] *Process modeling using Aspen Plus-Aspen Tech Customer Education Training Manual*, Course Number ES200.06.12.

[11] J. Park, T. Kim, Y. Go and S. Choi, Modeling of the gasifier section for IGCC plant, *Proc. of the Korean Society for New Renewable Energy*, Busan, Korea. (2007) 445-448.

[12] Mohamed M. Elbaccouch and Ali T-Raissi, *Aspen Plus process model for the production of gaseous hydrogen via steam gasification of bagasse*, Florida Solar Energy Center, University of Central Florida, Cocoa, FL, USA. (2003).

[13] L. Douglas Smoot and David T. Pratt, *Pulverized coal combustion and gasification: Theory and applications for continuous flow processes*, A Division of Plenum Publishing Corporation, New York. (1979) 218-219.

[14] *Aspen Plus: Getting started modeling processes with solids*, Aspen Technology, Inc. (2000).

[15] B. Kim, J. Yoo and Y. Kim, A study on heat and mass balance in a coal gasifier, *Proc. of the Korean Society for New Renewable Energy*, Busan, Korea, (2007) 424-428.

[16] A. P. Watkinson, J. P. Lucas and C. J. Lim, A prediction of performance of commercial coal gasifiers, *Fuel*, 70 (1991) 519-527.

[17] Qizhi Ni and Alan Williams, A simulation study on the performance of an entrained flow coal gasifier, *Fuel*, 74 (1995) 102-110.

[18] Hiroki Yoshida, Fumio Kiyono, Hideo Tajima, Akihiro Yamasaki, Keiichi Ogasawara and Tadashi Masuyama, Two stage equilibrium model for a coal gasifier to predict the accurate carbon conversion in hydrogen production, *Fuel*, 87 (2008) 2186-2193.

[19] A. C. Beath, *Mathematical Modeling of Entrained Flow Coal Gasification*, Ph.D. thesis, University of Newcastle, Australia, (1996).

[20] Thanh D. B. Nguyen, Y. Lim, B. Song, S. Kim, Y. Joo and

D. Ahn, A numerical study on a two-stage equilibrium model for the gasification process in an entrained-flow coal gasifier, *Proc. of the US-Korea Conference*, Raleigh, USA, (2009).

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