CHEMICAL ENGINEERING TRANSACTIONS
VOL. 45, 2015
A publication of AIDIC
The Italian Association
of Chemical Engineering
www.aidic.it/cet
Guest Editors: Petar Sabev Varbanov, Jiří Jaromír Klemeš, Sharifah Rafidah Wan Alwi, Jun Yow Yong, Xia Liu

ISBN 978-88-95608-36-5; **ISSN** 2283-9216
DOI: 10.3303/CET1545316

Simultaneous Integration and Optimization of an IGCC Plant

Maojian Wang*[a,b], Ergys Pahija[b], Guilian Liu[a], Chi-Wai Hui[b]

[a]Xi'an Jiao Tong University, Xi'an, Shaanxi Province, China
[b]Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong
kehui@ust.hk

An Integrated Gasification Combined Cycle (IGCC) is a promising green technology applied for thermal power plants. It offers an efficient way to generate electricity from coal, biomass or any other suitable solid or liquid fuels with lower impact to the environment. The biggest challenge of making IGCC to become a viable technology is its high energy production cost. This creates a barrier for this green technology to enter into the stage of a highly competitive electricity market. An IGCC plant is a complex process system which involves processing units operated in very extreme conditions. Proper material and energy integration may provide a hope for cost reduction. In this paper, a mathematical model of an IGCC plant was built that includes a gasification unit, an Air Separation Unit (ASU) and a Combined Cycle unit. A modified Gibbs free energy model is used for predicting the composition of the syngas taking into account material and energy balances. The proposed gasification model results in syngas composition similar to the experimental data provided in literature. What's more, Combined Cycle unit is simulated with isentropic assumption plus efficiency. While ASU is simulated mainly using the rigorous distillation model. Although individual processing unit optimization plays a significant role in enhancing the plant performance, an optimal integration among the three units still has significant potential to improve the efficiency, availability, and operability of a coal-fed IGCC power plant. The proposed mathematical model allows material and energy integration to be performed within and among different processing units while optimizing the IGCC plant as a whole. Different material and energy integration schemes were considered with respect to the overall thermal efficiency of the IGCC plant. The good performance is shown by about 2 % overall efficiency increment in the case study.

1. Introduction

The Integrated Gasification Combined Cycle (IGCC) is a promising green electrical power generation technology. The attractive characteristics are more efficient power generation and less environmental effects compared with conventional coal power plant. Another outstanding feature is the wide range of the feed options, which could be coal, biomass or any other suitable solid or liquid fuels. Any of them is able to be converted to syngas through gasification and finally be utilized to generate electricity.

According to the previous understanding of IGCC technology, the significance of developing it are in three key points, which are its high efficiency, high flexibility and low emission performance. Based on the industrial experiences, IGCC plant efficiency can achieve around 40 % calculated using Lower Heating Value (LHV) (Maurstad, 2005), which is considerably higher than the conventional coal fired power plants. In another hand, the high flexibility is located on both of the feed and product sides, which means its capability to use a wide range of fuels as mentioned above and to produce not only electricity, but a series of chemicals to make poly-generation come true. What's more, the last main advantage can be proved by low main contamination emission, such as SO_2 (Padurean et al., 2012), NO_x (Maurstad, 2005) and mercury (Sofia, 2013). If the IGCC plant is oxygen driven one, the additional cost for Carbon Capture and Storage is lower enough to be added compared with other industry practice to achieve so called "Zero-carbon-emission". The reason why IGCC is such a "green" technology could be theoretically explained by

Please cite this article as: Wang M., Pahija E., Liu G., Hui C.-W., 2015, Simultaneous integration and optimization of an igcc plant, Chemical Engineering Transactions, 45, 1891-1896 DOI:10.3303/CET1545316

the contributions of pre-combustion gas clean-up process, which can easily understand with the help of the process description in next section.

But there are still some bottlenecks of IGCC technology, which creates the barrier for it to enter into the stage of fully commercialization in the highly competitive electricity market. Firstly, the electricity cost of IGCC power plant is still higher than the current market price, particularly the large capital cost. And the efficiency penalty of the CO_2 capture should also be decreased, which is around 6.5 % to 8.6 % (LHV efficiency) (Wheeler, 2003). At the same time, the risk of the low plant availability is still a problem. After the operation for a number of years, most of the plant availability was in the range of 70 % to 80 % (Sahraei et al., 2014).

Therefore, there is an urgent requirement to upgrade the IGCC technology by improving the plant efficiency and reducing the cost. According to the complicated configuration, process optimization and integration technology can play a significant role of filling this gap. Each individual block of IGCC plant is based on some conventional technology which is well investigated during past decades. But in order to suit for the IGCC application, the difficulty not only lies in the configuration aspect, but also in suitable adjustment of block design or operation. Optimization of combining the capture of H_2S and CO_2 can have a significant cost saving, which can be quantified of the benefit around 25 % (Wheeler, 2003). Both of the heat and mass integration between different units can make the additional efficiency improvement come true. For example, the level of gasifier and gas turbine combustor integration can be optimized to achieve higher thermal efficiency based on the study by Emun (2010). Even though there is a number of achievement already, some gaps are still existing related with simultaneous optimization and integration method, which will be expanded in deep in the methodology section. With the help of this method, further efficiency progress can be identified. In this paper, the framework of simultaneous integration and optimization methodology is generally explained. The essential modelling gaps to guarantee the simultaneity is demonstrated and fulfilled. According to the results of case study, the good performance of simultaneous integration and optimization methodology can be easily proved.

2. Process description

Until now, there is not a standard principle of the IGCC plant process, but the main blocks are quite similar. In this paper, IGCC process without CCS is selected in order to make the process a little bit simple and clear to help us be focus on the methodology.

The process flow diagram is given in Figure 1. The coal or other fuel like biomass, is crushed and supplied into the gasifier sometime with water, where it is partially oxidized. If pure oxygen is used as oxidant instead of air, there will be an air separation unit (ASU). The operating pressure and temperature of gasifier are different based on the fuel supplied and gasifier type, which are in the range of 0.1 to 8 MPa and 700 to 1,800 K. Gasification product the crude syngas is mainly composed of H_2, CO, CO_2 and H_2O. Besides the chemical energy, the crude syngas contains sensible heat which can be recovered to produce steam for steam turbine. After cooling, gas cleaning is completed at near ambient temperature with proven technologies. The clean syngas drives a gas turbine after combustion with additional oxygen and injected nitrogen. The heat of flue gases from gas turbine is used to generate superheated steam in the heat recovery steam generator (HRSG). A steam turbine is drove by that steam to product additional power. The gas turbine process and the steam turbine process plus HRSG consist of the Combined Cycle, which is similar to the technology used in modern natural gas fired power plants.

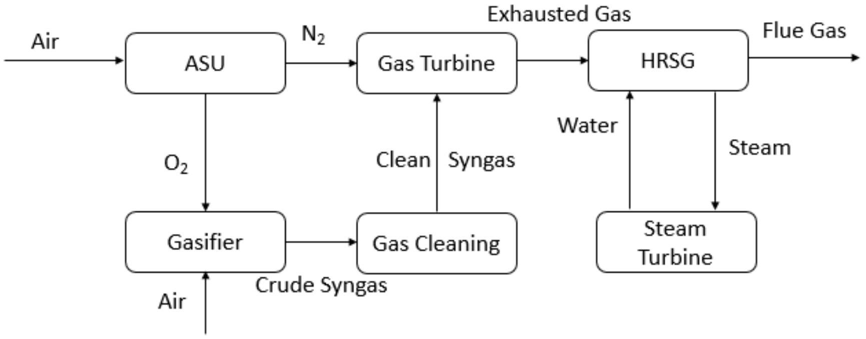

Figure 1: Schematic diagram of the IGCC process without CCS

3. Methodology

Process integration and process optimization are two close but individual topics in the previous research experiences. There are two main aspects of process integration, which are heat integration and mass integration. Both of them are well developed and could have a good contribution to improve the performance of the system. With the process of chemical plant becoming more and more complicated, the individual improvement from heat or mass integration cannot satisfied the expectation. So the possibility of the combination of heat and mass integration are explored, which occasionally has the same problem for IGCC technology. The promotion from heat integration for IGCC plant can generally identified in unit scale and plant scale. Good examples can be easily found in the recent publications. Not only the blocks, but also the whole decarbonised coal IGCC sites integrated with CCS can improve the electricity cost by maximizing site-wide heat recovery according to Ng (2010) work. In this work, the combination of heat and mass integrations are mainly located between the ASU and Gas Turbine (GT) considering the waste heat recovery, nitrogen injection and air integration.

Besides that, the relationship between process integration and process optimization is another key point, which is essential to be mentioned. In the beginning, the process integration is completed after the process optimization, which means that the process is sequentially optimized and integrated. The concept of simultaneous optimization and integration has been introduced firstly through Grossmann (1986). The Pinch Analysis is occupied in the analysis as a mature technology, which is also taken into consideration in our work. The advantage of the simultaneous optimization and integration method is to get a better solution compared with the previous sequential one, which means there is higher possibility to catch the global optimal solution rather than local optimal solution. The excellent performance of this simultaneous method has been briefly concluded in previous research papers for simple industrial example. When it comes to the specific application in IGCC plant, the general framework is consecutive with what mentioned above. Different heat and mass integration options are included in the constraints by transforming to mathematical equations in advanced. The objective function should be set as the minimization of the whole IGCC plant efficiency, which can be described as below:

$$\eta_{plant} = \frac{P_{GT} + P_{ST} - W_{ax}}{HHV} \quad (1)$$

Where P_{GT} is the power output from Gas Turbine, P_{ST} is the power output from Steam Turbine, W_{ax} is the work consumption from the auxiliary equipment such as ASU compressor and HHV is the total Higher Heating Value of the coal feed in stock.

Besides that, the heat and mass balance also have been occupied. The simulation is built as a Macro in Excel 2013 cooperating with Standard GRG Non-linear Solver and Water 97 add-in, which is property database using the industrial standard IAPWS-IF97.

4. Modelling of Gasification process

Gasification is completed in the gasifier, including a series of reactions which can convert the solid fuel to combustible gases, such as carbon monoxide and hydrogen, by supplying gasifying agent like oxygen (Minchener, 2005). Different types of models have been developed to predict the gasifier performance. Using the computational fluid dynamics (CFD) technology with considering the details of reaction and flow, one of the most fidelity models can be achieve requiring the input information about equipment geometry and reaction kinetics data. But the shortcoming is that it is hard to be used in the context of an integrated plant process simulation model. Some other choices of gasifier simulation are trying to capture the reaction (char formation, combustion, gasification, slag formation etc.) and the underlying heat and mass transfer phenomena (Biagini et al., 2009). Aspen Plus modelling can be taken as an example with less fidelity than the CFD models.

In order to complete feasibility analysis, simulation and optimization of IGCC systems, The equilibrium-based models (Hau et al., 2008) are the simplest in terms of computational effort and ease of implementation as the best choice, which is also the choice in this work. The effects of feed option, equipment geometry and reaction details have no influence of this kind of model. So the advantage of occupying this approach is making the problem tractable. And more attentions could be emphasized on the integration and optimization of the process in the broader scope.

4.1 ideal Gibbs free energy model

The crude syngas is assumed as a mixture of CH_4, H_2, CO, CO_2, H_2S, COS, NH_3, NO_2, SO_2, N_2O, SO_3. The composition is calculated simultaneously with the equilibrium temperature in adiabatic statement. At the equilibrium state, the total Gibbs free energy of the system is minimized. The total Gibbs free energy of a system, G_{system}, is defined:

$$G_{system} = \sum_{i=1}^{N} n_i (G_{f,i}^0 + RT \ln \frac{\hat{f}_i}{f_i^0}) \tag{2}$$

Where $G^0_{f,\,i}$ is the standard Gibbs free energy of formation (kJ/mol), n_i (mol) is amount of component i of the system. T (K) is system temperature and R is gas constant. With ideal gas assumption, $\hat{f}_i$ is related with system mole composition y_i and pressure P (Pa):

$$\hat{f}_i = y_i P \tag{3}$$

When at low pressures, f_i^0 is taken as the standard state pressure. $G_{f,i}^0$, is the calculated based on the concept using Eq(4) which is presented as:

$$G_{f,i}^0(T) = \Delta H_{f,i}^0(T) - T\Delta S_i^0(T) \tag{4}$$

The enthalpy and entropy changes from standard state to system state at T (K), $\Delta H_{f,i}^0(T)$ and $\Delta S_i^0(T)$, are calculate based on the Eq(5), Eq(6) and Eq(7). Heat balance and mass balance are also achieved for the gasifier as a whole.

$$t = T/1{,}000 \tag{5}$$

$$\Delta H_{f,i}^0(T) - H_{298.15}^o = At + B\,{t^2}/{2} + C\,{t^3}/{3} + D\,{t^4}/{4} - {E}/{t} - H \tag{6}$$

$$\Delta S_i^0(T) = Aln(t) + Bt + C\,{t^2}/{2} + D\,{t^3}/{3} - E/(2t^2) + G \tag{7}$$

Where H^o is standard enthalpy (kJ/mol) and A, B, C, D, E, H are constant values supplied by National Institute of Standards and Technology (NIST) chemistry database.

4.2 Modified Gibbs free energy model

Ideal Gibbs free energy modelling of the gasification process is applied as a part of the IGCC plant simulation and prepared to be the platform about studying the simultaneous optimization and integration methodology. But there is a negligible issue that insert this model inside the whole plant simulation may lead to a bi-level optimization problem, which significantly increase the difficulty of the solving procedure with the danger of local optimum block. To overcome this problem, some modifications become necessary to switch the minimization constraints to others equality constraints. One solution is proposed through using Karush-Kuhn-Tucker (KKT) optimality conditions for the minimization of the Gibbs free energy (Kamath, 2012). In this section, another method using the Gibbs free energy is proposed with the assumption of zero methane component.

Among the series of the gasification reactions, the reversible gas phase water-gas shift reaction reaches equilibrium very fast at the temperatures in a gasifier. It can balance the concentrations of carbon monoxide, steam, carbon dioxide and hydrogen with the reaction equation as below:

$$CO + H_2O \longrightarrow CO_2 + H_2 \tag{8}$$

For each temperature, in theory, equilibrium constants (K_w) can represent the reaction performance. The first time to introduce this concept into gasifier product gas composition calculation is taken by Groeneveld (1979). Firstly, Gibbs free energy of formation in T (K), $G_{f,i}^0(T)$, can be calculated by Eq(4). And the Gibbs free energy of that reaction, $\Delta G_{r,i}^0(T)$, can be calculated as below:

$$\Delta G_{r,i}^0(T) = \sum\nolimits_{product} G_{f,i}^0(T) - \sum\nolimits_{reactant} G_{f,i}^0(T) \tag{9}$$

And the equilibrium constants (K_w) can be calculated by Eq(9) using $\Delta G_{r,i}^0(T)$,

$$\Delta G_{r,i}^{0}(T) = -RTlnK_w \tag{10}$$

Where R is the Gas Constant, and the T is the temperature in K. According to the concept of the equilibrium constant, K_w can be related with syngas compositions. And with the element and heat balances, the problem can be solved without minimization.

5. Modelling of other IGCC units

Besides the gasification unit, ASU and Combined Cycle unit also should be considered as essential components of IGCC plant. The simulation of those parts are introduced as below using conventional design.

The combined cycle is referred to the combination of gas turbine, steam turbine and HRSG. Simplified mathematical model of the gas turbine is consist of three key units: a compressor, a combustor and a turbine. In another hand, the process of steam turbine is proposed including a turbine and a pump. Those two sections are connected by HRSG to recover fuel gas sensible heat. The principle of modelling the combined cycle unit is idealizing the process then adding the efficiency. Isentropic process is assumed as the ideal process for the compressor, turbine and pump in the combined cycle unit. For steam turbine and HRSG, the isentropic process is calculated based on the concept using Water-97 database. Those differences are due to the ideal gas, then the entropy equation is not related with the pressure.

Cryogenic ASU is selected to use in this work, which is consist of a feed compression section, two multi-phase heat exchangers (MHEX), a distillation section (low-pressure (LP) column and high-pressure (HP) column) and a product compression section. Compressed air is separated into pure oxygen and main nitrogen stream after going through the LP column and HP column. Heat exchange is happened not only in MHEX but also between the LP column condenser and HP column reboiler. In the simulation, the ideal properties of air is assumed only including oxygen and nitrogen. The models of the compressors are built similar as the ones in combined cycled. MHEX is simplified as the general heat exchanger with the temperature constraints and satisfying the energy balance.

6. Results and discussions

6.1 Modified Gibbs free energy model validation

The validation is based on the study (Forestry Department, 1986), which claims that the modelling of gasification process based on the experimental data can have a good agreement with experimental results found. Comparing the equilibrium constant we calculated through Gibbs free energy with the experiential ones they referred. The differences are very small, which is described in the Table 1. Then the model can be validated.

Table 1: The equilibrium constants (K_w) validation

Temperature (K)	Experimental K_w	Calculated K_w
873	0.38	0.3875
973	0.62	0.6198
1,073	0.92	0.9229
1,173	1.27	1.2720
1,273	1.6	1.6

6.2 Case study

One improved case has been built to test the performance of the simultaneous integration and optimization method. Another base case has been created to be compared. Some main simulation assumptions and results are listed in the Table 2. The base case has been validated with other examples from literatures and industrial data. After simultaneous integration and optimization of the base case, there are some improvements in different aspects. With recovering the waste heat mainly from ASU compressor, the electricity generation is increased, which leads the increment of overall plant efficiency about 2 %. Also, some contributions are from the air integration and nitrogen injection between ASU and GT. The good performance of simultaneous integration and optimization method has been preliminarily demonstrated, but the further development is also essential to handle more complicated problem including more schemes.

Table 2: Simulation details of base case

Parameters	Values
Reference fuel type	Illinois No.6 coal
Coal feed flow rate	15 kg/s
Gasifier pressure	4.2 MPa
Air flow rate	10,000 kmol/h
Gasification temperature	1,475 K
Power output of Gas Turbine	152.8 MW
Power output of Steam Turbine	86.7 MW
Overall efficiency	39.8 %

7. Conclusion

In this paper, the framework of the methodology, simultaneous integration and optimization, has been explained, especially associated with the IGCC technology. The difficulty to achieve the simultaneity in modelling aspect is in the gasification process about simplification of the bi-level optimization problem. One modified approach is proposed and validated with good performance. Using the mathematical model we built, a case study is completed. Different heat and mass integration schemes are considered. The good performance of the simultaneous optimization and integration method is shown through about 2 % overall efficiency increment in the improved case compared with the base case.

References

Biagini E., Bardi A., Pannocchia G., Tognotti L., 2009, Development of an entrained flow gasifier model for process optimization study, Industrial & Engineering Chemistry Research, 48, 9028-9033, DOI: 10.1021/ie801804g.

Duran M.A., Grossmann I.E., 1986, Simultaneous optimization and heat integration of chemical processes, AIChE Journal, 32, 123-138, DOI: 10.1002/aic.690320114.

Emun F., Gadalla M., Majozi T., Boer D., 2010, Integrated gasification combined cycle (IGCC) process simulation and optimization, Computers & Chemical Engineering, 34, 331–338, DOI: 10.1016/j.compchemeng.2009.04.007.

Forestry Department, 1986, Wood gas as engine fuel, Food and Agriculture Organization, United Nation

Groeneveld M. J., Van Swaaij W. P. M., 1979, Gasification of solid waste—potential and application of co-current moving bed gasifiers, Applied Energy, 5, 165-178, DOI: 10.1016/0306-2619(79)90034-5.

Hau J., Ray R., Thorpe R., Azapagic A., 2008, A thermodynamic model of the outputs of gasification of solid waste, International Journal of Chemical Reactor Engineering, 6, 347-354, DOI: 10.2202/1542-6580.1523.

Kamath R. S., 2012, Strategies for Optimization and Heat Integration in Integrated Gasification Combined Cycle Systems, Carnegie Mellon University, PA, USA.

Maurstad O., 2005, An overview of coal based Integrated Gasification Combined Cycle (IGCC) technology, Laboratory for Energy and the Environment, Massachusetts Institute of Technology, Cambridge, MA, U.S.A.

Minchener A.J., 2005, Coal gasification for advanced power generation, Fuel, 84, 2222-2235, DOI: 10.1016/j.fuel.2005.08.035.

Ng K.S., Lopez Y., Campbell G.M., Sadhukhan J., 2010, Heat integration and analysis of decarbonised IGCC sites, Chemical Engineering Research and Design, 88, 170-188, DOI: 10.1016/ j.cherd.2009.08.002.

Padurean A., Cormos C.C., Agachi P.S., 2012, Pre-combustion carbon dioxide capture by gas–liquid absorption for Integrated Gasification Combined Cycle power plants, International Journal of Greenhouse Gas Control, 7, 1-11, DOI: 10.1016/j.ijggc.2011.12.007.

Sahraei M.H., McCalden D., Hughes R., Ricardez-Sandoval L. A., 2014, A survey on current advanced IGCC power plant technologies, sensors and control systems, Fuel, 137, 245-259, DOI: 10.1016/j.fuel.2014.07.086.

Sofia D., Giuliano A., Barletta D, 2013, Techno-economic assessment of co-gasification of coal-petcoke and biomass in IGCC power plants, Chemical Engineering Transactions, 32, 1231-1237, DOI: 10.3303/CET1332206.

Wheeler F., 2003, Potential for improvement in gasification combined cycle power generation with CO_2 capture, IEA Report No. PH4/19, Paris, France.