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Simultaneous Optimisation and Integration of IGCC Plant Using Graphical Method

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

[a]Xi'anJiaotong University, Xian Ning West Road No.28, 710049, China
[b]Hong KongUniversity of Science and Technology, Clear Water Bay, Hong Kong
kehui@ust.hk

As a promising green technology, Integrated Gasification Combined Cycle (IGCC) plant is more efficient and low-pollution electricity generation choice than conventional thermal power plants. Its process is mainly consist of the gasifier, the air separation unit and the combined cycle unit. Going through those key blocks, the fuel, such as coal and biomass, could be converted to syngas and further combusted for power generation. In order to be a viable technology, the bottleneck is located on the high energy production cost, which could be overcame by improving the plant efficiency through process optimisation and Integration. The opportunity and challenge are given by the complicated configuration and extreme operation conditions, which also demands a flexible and robust IGCC plant simulation to complete deep process analysis. In this work, a novel simplified IGCC mathematical model is proposed considering thermodynamics constraints with energy and mass conservation. The gasification is simulated based on the principle of Gibbs free energy minimisation, which holds the good feature of avoiding potential bi-level optimisation problem. The proposed gasification model results in syngas composition similar to the experimental data provided in literature. Meanwhile, the cryogenic air separation unit is selected with the double distillation column configuration, which is simulated considering the novel simplification of thermal coupled distillation columns. What is more, the combined cycle unit is simulated with isentropic assumption plus efficiency to complete the process. To validate the novel simplified IGCC model, one base case is built and compared with literature data. Another highlight of this work is the simultaneous optimisation and integration methodology instead of conventional sequential one, which gives more guarantee for achieving global optimal solution. If the ideal property assumptions are occupied, a graphical approach could be generated for the simultaneous optimization and integration of IGCC plant. The best material and energy integration scheme in proper operation condition could be selected considered with respect to the overall thermal efficiency of the IGCC plant. The good performance is shown by about 10 % power increment compared with the base case in the case study.

1. Introduction

Integrated Gasification Combined Cycle (IGCC) technology is raised as one of the effective “green” electrical power generation technology in last decades. The feedstock such as coal and biomass could be reacted with ox generation. Because of using the pre-combustion gas cleaning approach, the environmental performance of IGCC plants is quite outstanding, which could be proved by the low main contamination emission. Besides that, the significance of developing IGCC technology is according to its high efficiency compared with the conventional coal fired power plants, which could achieve around 40 % based on Lower Heating Value (LHV). (Maurstad, 2005) Even though there are a lot of merits, the high energy production cost still creates the barrier for IGCC technology to enter into the stage of fully commercialisation. As a result, process optimisation and integration technology has a great potential to improve the overall plant efficiency for satisfying above urgent requirement.

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As IGCC main block, GT is an essential part of the combined cycle unit, which is originally developed for Natural Gas Combined Cycle (NGCC) power plant. Many modifications are extremely essential to fit the syngas not previous natural gas and oil as the combustor fuel. Because the syngas contains a lot of hydrogen, the common Dry Low-NOx (DLN) combustors should be replaced by traditional diffusion combustors to prevent quick flame propagation. The low energy density of the syngas causes the increment of flow rate to maintain the same turbine inlet temperature, which not only increases the power output but also makes the turbine easily to achieve compressor surge limitation, gas turbine torque limitation and turbine inlet temperature and material lifetime limitation. Those make the application of GT in IGCC plant holding both of the challenges and opportunities.

In other hand, ASU is the link between the gasification island and the power generation block, which also makes the configuration more complicated and the operation more flexible. For the existing oxygen driven IGCC demonstration sites, commercial cryogenic air separation technology is selected. This choice is made because of the large O_2 production capacity (3,200 t/d) and the high device reliability of cryogenic ASU (Rizk, 2012). What is more, the operation conditions of cryogenic ASU are able to be adjusted in a quite wide range. But the fact is that only a series of stranded ambient pressure schemes is frequently used in the current manufacturing. The improvement may be achieved by applying the non-standard statement in the IGCC plant.

The research about optimisation and integration of IGCC plant has been developed for many years, but the attentions are mainly focus on the single IGCC block. The optimisation and integration researches taking multiple units into consideration are not so much, in which the combination of ASU and GT could be a common example. Kim (2011) has discussed the possible solutions to enhance the GT and ASU performance through changing the integration degree, which works by reducing the GT compressor surge margin. Lee (2009) reports the high integration degree should be preferred, and the high nitrogen injection ratio could be only acceptable in the high air integration degree. What's more, some cases studies are carried out by Frey and Zhu (2006), which puts the guideline of GT and ASU operation as a whole. But there is still a gap in the field of total plant optimisation and integration, especially taking them simultaneously.

In this paper, above gap is fulfilled with case studying. The mathematical simulations of IGCC plant are proposed and developed, which includes the main blocks of gasification unit, air separation unit and gas turbine. To holding enough flexible for further optimisation and integration, the theoretical thermodynamics calculation are occupied to simplify the model as much as possible. One base case is tested with input information collected from the industrial experiences to validate the simulation accuracy. With the proposed graphical simultaneous optimisation and integration method, an improved case is calculated to identify the good performance of proposed methodology.

2. Process description

So far, IGCC plant doesn't has a standard process configuration, but the gasification unit, air separation unit and gas turbine can be considered as the essential components. In the Figure 1, the IGCC plant process is described and simulated later, which owns those three key blocks as mentioned above. In the gasification unit, the oxygen generated from the ASU are reacted with the steam and fuel, like coal. Oxygen plays the role of the oxidizing agent in the gasification. The produced syngas has the settled compositions relying on the operation condition, which could have the pressure and temperature as about 40 bar and 1,300 K. In another hand, the compressed air from ASU main compressor or GT compressor is separated into two parts, namely oxygen product and nitrogen product. Some part of nitrogen could be rejected into the gas turbine combustor for dilution. As shown in Figure 1, the ambient air is compressed in the compressor, which is one of three elements to comprise GT. The compressed air is used in potential three ways. They are oxidant in the GT combustor, the cooling agent for GT combustor and GT turbine blades and finally the feed of the ASU. The main portion of it is engaged into the GT combustion in around 11 bar and 1,300 K. (Boyce, 2009) According to the requirement from design constraints, the feed streams for the isobaric combustor is not only the oxidising agent (compressed air) and the fuel (pre-treated syngas) but also the nitrogen from ASU and the water vapour to moistening the syngas. The dilution from the inert components is contributed for both the flame temperature controlling in the GT combustor and the power generation enhancement. After that, the exhausted combustion gas in high temperature and pressure is delivered to the following turbine for power generation. A shaft is used to connect the turbine and compressor. So the net electricity power generation of GT is the turbine output minus the work consumption of compressor. The exhausted gas from the turbine still has the sensible heat with the temperature about 700 K, which will be recovered by the other IGCC blocks not including in the discussion of this work. (Boyce, 2009)

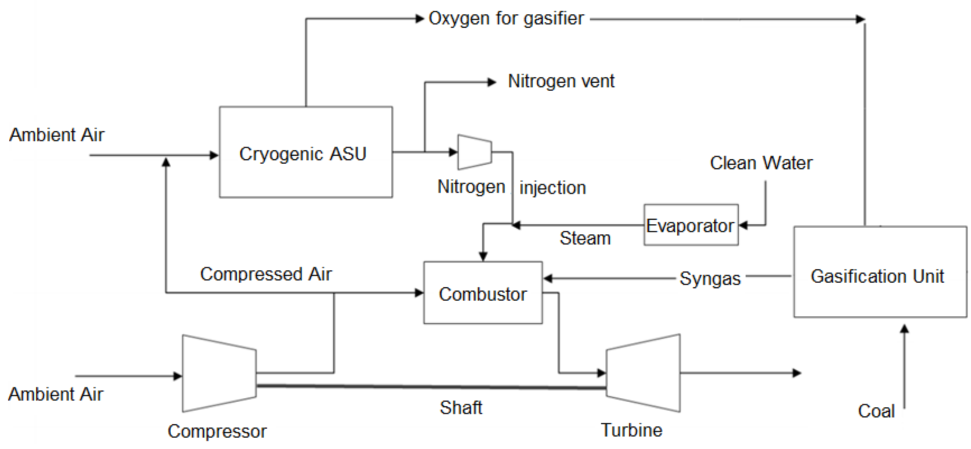

Figure 1: Schematic diagram of the IGCC process.

3. 3.Simulation method

3.1 Gasification unit modelling

After the reaction in the gasification unit, the produced crude syngas is assumed to have the components of CH_4, H_2, CO, CO_2, H_2O and N_2. The composition is calculated simultaneously with the equilibrium temperature in adiabatic statement, in which the ideal properties are selected. 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:

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

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):

$$\hat{f}_i = y_i P \quad (2)$$

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 (3) which is presented as:

$$G_{f,i}^0(T) = \Delta H_{f,i}^0(T) - T\Delta S_i^0(T) \quad (3)$$

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 (4), (5) and (6). Heat balance and mass balance are also achieved for the gasifier as a whole.

$$t = T/1,000 \quad (4)$$

$$\Delta H_{f,i}^0(T) - H_{298.15}^0 = At + B\,{t^2}/{2} + C\,{t^3}/{3} + D\,{t^4}/{4} - {E}/{t} - H \quad (5)$$

$$\Delta S_i^0(T) = A ln(t) \;+\; Bt \;+\; C\,{t^2}/{2} \;+\; D\,{t^3}/{3} \;-\; E/(2t^2) \;+\; G \quad (6)$$

WhereH^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.

3.2 Air separation unit modelling

In order to satisfy the purity and productivity of the oxygen product for gasification, the conventional cryogenic ASU is selected in this paper. The ideal gas is assumed for the air with only two components, 79 % nitrogen and 21 % oxygen. Double distillation column configuration is chosen. Main three steps are feed air compression, double distillation column separation and product compression. Firstly, the ambient air is compressed using assumed multiple-stage compressor. After cooling the compressed air to 298 K, it goes through the multi-phase

heat exchangers (MHEX) to achieve cryogenic temperature around 100 K by exchanging the heat with product streams directly from the distillation column. Then it is split into two parts to complete the separation by sequentially making use of the High Pressure Column (HPC), the one with only condenser and Low Pressure Column (LPC), the one only with reboiler. They could be thermal coupled with each other using special heat exchanger. Finally, the product streams respectively from the top and bottom tray of LPC are compressed to satisfy the requirement from downstream device, such as GT combustor and gasifier.
When the air going through the Main Air Compressor (MAC), an isentropic process is assumed with taking the isentropic efficiency into consideration. The relationship physical properties between the inlet stream and the output stream is described by Eq(7).

$$T_{MAC,isen} = T_0 \left({P_{MAC}}/{P_0} \right)^{(r-1)/r} \tag{7}$$

Where $T_{MAC,isen}$ is the outlet temperature of compressor in K after the isentropic process? T_0 and P_0 are the inlet air temperature (298 K) and pressure (1 atm). P_{MAC} is the discharge pressure of the compressor in atm. And r means the isentropic index (1.4 for air). According to the process, P_{MAC} can be calculated as below:

$$P_{MAC} = P_{HPC} + dP \tag{8}$$

Where P_{HPC} is the operation pressure of HPC in the ASU in atm and dP is the pressure difference for downstream injection preventing the pressure loss in transportation. dP is set as the constant equals to 0.5 atm in this work. The isentropic efficiency of the MAC, which is assumed as 0.9.Then the compressed air is cooled down by MHEX. The output temperature of hot streams are settled as 296 K, which sets the approach temperature as 2 K based on the speciality of MHEX. After that, the cryogenic air stream is split into two parts to delivery to HPC and LPC. The split ratio is assumed as 0.95, which means 95 % of the cryogenic air is be injected to the HPC. For the simulation of the distillation columns, namely HPC and LPC, the rigorous calculation is applied through top to the bottom tray by tray with the assumption of not only ideal properties but also the phase equilibrium. The phase equilibrium for each tray is described in Eq(9):

$$y_i P = x_i P_i^{\theta} \tag{9}$$

Where y_i is the mole fraction in gas phase for i and x_i is its mole fraction in liquid phase. P is the pressure of the selected system, namely the column operation pressure. And P_i^{θ} is the saturated vapour pressure of i in the system temperature, which could be calculated by the Antoine equations in Eq(10):

$$\log(P_i^{\theta}) = A_i - {B_i}/{(T + C_i)} \tag{10}$$

Where T is the system temperature, namely the tray temperature, and A_i, B_i and C_i are the coefficients reported by Mallard. What should be emphasized is that the HPC doesn't have a reboiler while the LPC doesn't have the condenser. As a result, the HPC condenser and LPC reboiler have to exchange heat with each other, which is also an outstanding feature of double column cryogenic ASU configuration. The constraint for this heat exchanger is described as:

$$T_{HPC,con} - T_{LPC,reb} \geq 2\ K \tag{11}$$

Where $T_{HPC,con}$ and $T_{LPC,reb}$ are the temperature of HPC condenser and LPC reboiler respectively. While 2 K is approach temperature according to the real application. (Smith, 2001)

3.3 Gas turbine modelling

The simulation of the GT compressor is similar with the MAC in the ASU mentioned above. The high temperature (1,300 K to 1,600 K) and high pressure (10 atm to 20 atm) combustion gas is exhausted to the turbine for power generation. (Farmer, 2010) The modelling of the turbine also follows the principle of ideal isentropic process plus efficiency. Similar equations of the physical property's relationship and isentropic efficiency definition could be applied. The isentropic efficiency of turbine in this work is assumed as 0.9. After going through the turbine, the temperature is decreased to the range of 600 K to 800 K. The ratio of air cooling is set as 0.183 extracted from real industry practice. (Eldrid, 2001)The degree of air integration and nitrogen injection are generated with the simulation.

4. Case study

According to the detail process shown in Figure 1, a mathematical model of IGCC plant, is built in Microsoft Excel 2010 in equations considering the heat and mass balance. One base case is completed for not only the simulation validation but also for the further comparison with the improved case by simultaneous optimization and integration. In the base case, besides the assumption as mentioned above, the syngas compositions is settled as listed in Table 1.

Table 1: syngas product compositions

Components	Mole fraction
H_2	0.26
CO	0.50
CH_4	0.01
CO_2	0.05
N_2	0.03
H_2O	0.15

At the same time, according to the gasification condition, the supplied oxygen should in almost pure, 99 %. Also following the requirement of further nitrogen injection, the nitrogen product should also be in the purity of more than 99 %. If there is no product treatment, the work consumption of ASU is calculated as 0.287 kWh/ kgO_2, which is quite similar with an example Seltzer reported in 2006 as 0.290 kWh/ kgO_2. The performance of GT is also validated using the data of frame F gas turbine. The key input and output information of the GT in the base case are listed in Table 2.

Table 2: results of the base case

Items	Values
GT Combustion temperature	1,545 K
GT Combustion pressure	15 atm
Mole flow rate of syngas	2,000 kmol/h
Net power output	44,761.9 kW
Thermal efficiency	38.72 %

Compared the calculation results with the literature data, the thermal efficiency of the base case is in the range of the frame F GT design, which is 37 % to 45 %. (Eldrid, 2001) In order to have a better comparison with literature example, the integration is not taken into the consideration in the base case.

If only mass integration is added into the problem, based on the problem statement above, the constraints of air integration, nitrogen injection and steam injection are all included. The ratio of air integration and nitrogen injection are treated as variable, while the related constraints are also added. In this case, the simultaneous optimization and mass integration of ASU and GT could be achieve by mathematical modelling and solved directly using Microsoft Excel solver. What's need to mentioned before is the operation pressure of HPC in ASU. If it is assumed as 10 atm, the maximize power output could be 48,912.1 kWh, which is about 10 % higher than the base case. Actually the reasons why mass integration constraints could be easily included into the mathematical optimization modelling are the pressures in the ASU and GT process playing the signification and unique role of deciding the objective.

For the simultaneous optimization and integration in both heat and mass aspect, the example is taken following the framework developed in previous chapter. In Figure 2, the composite curve of the case when HPC is operated in 6.5 atm is drawn. And if the HPC pressure is changed, the composite curve will be changed like the dash line described at the same time. Another curve shows the trend for the work assumption of the MAC in different HPC pressure conditions.

5. Conclusions

In this work, simultaneous optimization and integration of ASU and GT system is achieved step by step. Firstly, a mathematical simulation has been built in Microsoft Excel 2010. In the base case, the model validation shows good consistency with the literature data, such as ASU work consumption and GT efficiency. The optimisation target is set as net power output maximisation. The simultaneous optimisation and mass integration including nitrogen injection, steam injection and air integration, is achieved. A graphical approach is proposed to achieve the aim of simultaneous optimisation and integration, both of Mass and Heat Integration.

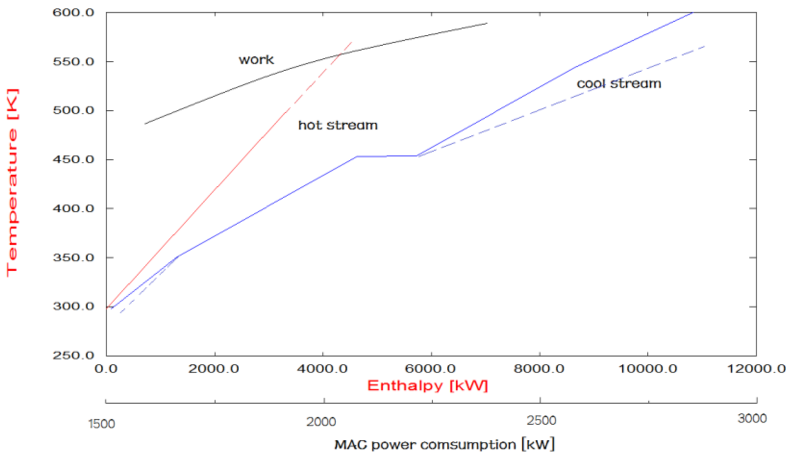

Figure 2: Simultaneous optimisation and integration of improved case

The good performance can be demonstrated in the additional power output of 10 % for the improved case compared with the base case. At the same time, the superiority of simultaneous optimization and integration compared with sequential one can be clarified.

Acknowledgments

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