Contents lists available at ScienceDirect

Chemical Engineering Research and Design

journal homepage: www.elsevier.com/locate/cherd

Simultaneous optimization of a heat integrated coal gasification process

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ARTICLE INFO

Article history:
Received 13 October 2014
Received in revised form 5 March 2015
Accepted 23 April 2015
Available online 28 April 2015

Keywords:
Gasification
Simultaneous optimization
Heat integration

ABSTRACT

This study develops a novel mathematical model which simultaneously optimizes the key operating parameters of a heat integrated coal gasification process to achieve maximum economic profit. It has been proved that, at above 1400 K, the operating conditions that maximize the profit automatically lead to minimized Gibbs free energy of products. Thus, the complicated bi-level problem of profit optimization (CGE maximization and Gibbs free energy minimization) is simplified to a single level problem of profit maximization, and the model can be developed accordingly. The model consists of several constraints including the heat balance, elemental balances and feasible heat exchange. Optimum conditions for the maximum profit can be determined from the model using a generalized reduced gradients nonlinear solver. Case studies have been conducted to illustrate the effectiveness and efficiency of the profit optimization using this single level model. The results of the case studies also indicates that by assigning part of the sensible heat to preheat the reactants, the profit can be increased by 40% compared with that of using sensible heat for HP steam production indifferently.

1. Introduction

Despite of the call for low-carbon economy all over the world, the global annual primary energy consumption was estimated to be 12,700 million tonnes of oil equivalent in 2013 (British Petroleum, 2014). Fossil fuels accounted for 86.4% of the primary energy consumption, with oil (32.9%), coal (29.9%) and natural gas (23.6%) as the major fuels (British Petroleum, 2014). Massive utilization of fossil fuels has increased the threat of global warming and energy crises. Therefore, cleaner and more efficient fuel conversion technologies are urged. Among them, gasification has received increasing attention due to its great potentials of reducing the environmental footprint in fossil fuel utilization (Childress et al., 2007).

Gasification is a process that converts carbonaceous feedstock into syngas, primarily composed of carbon monoxide (CO) and hydrogen (H_2), which can be directly used as fuels in a combined cycle power plant, converted into transportation fuels, or utilized as chemical feedstock. In the gasification process, the carbonaceous feedstock is decomposed in the presence of controlled amounts of oxygen and gasification feed water (GFW) at high temperatures. The production of syngas via gasification is a complex process that is strongly affected by the composition of feedstock, the gasification temperature and pressure, the amount of fed water and oxygen, etc. (Abuadala et al., 2010).

To quantitatively evaluate how the key parameters of a gasification process affect its efficiency, kinetic or thermodynamic equilibrium models are often used. A kinetic model basically investigates the reaction rates and mechanisms in correlation to the reaction conditions, amounts of reactants, geometric coefficients of the gasifier, etc. (Hameed et al., 2014;

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http://dx.doi.org/10.1016/j.cherd.2015.04.025

Nomenclature

G_{sys}	Gibbs free energy of system, kJ
n_i	molar flow rate of species i, kmol/h
$\Delta G^0_{f,i}$	standard Gibbs free energy of formation for species i, kJ/kmol
P,T	total pressure and temperature of the system, bar and K
R	universal gas constant, 8.314 kJ/kmol K
y_i	mole fraction of species i
$\Delta H^0_{f,i}$	standard enthalpy of formation of ith compound, kJ/kmol
$H_{f,fuel}$	enthalpy of formation of fuel, kJ/kmol
H_p	preheating heat and sensible heat of syngas, kJ/kmol
$H_{f,i}$	enthalpy of formation of ith species, kJ/kmol fuel
$H_{fa,i}$	apparent enthalpy of formation, kJ/kmol
C_p	constant pressure heat capacity, kJ/kmol K
S	entropy, kJ/(kmol K)
$a_{i,k}$	the number of atoms of the kth element present in each molecule of chemical species i
K	equilibrium constant
v_i	stoichiometric number of species i in the reaction
T_p	temperature of pinch candidate
δT_m	minimum temperature approach
H_{hd}	minimum heating demand
H_{cd}	minimum cooling demand
H^p_{ha}	heat source above the pinch candidate
H^p_{ca}	cooling source above the pinch candidate
H^p_{hb}	heat source below the pinch candidate
H^p_{cb}	cooling source below the pinch candidate
H_h	heat content of hot process streams
H_c	heat content of cold process streams
H^p_{canv}	cooling source without vaporization above the pinch candidate
H^p_{cav}	cooling source with vaporization above the pinch candidate
H^p_{hanc}	heat source without condensation above the pinch candidate
O_{O_2}	oxygen atom from oxygen gas
O_{H_2O}	oxygen atom from H_2O
CGE	cold gas efficiency
GFW	gasification feed water
HP	high pressure
LHV	lower heating value, kJ/kmol
HHV	higher heating value, kJ/kmol
W_e	electricity power, kWh
C	unit price, $/kWh for electricity and $/t for other process streams
η_e	combined cycle efficiency

Subscripts

e	electricity
i	ith component species
j	jth constituent chemical substance
k	kth chemical element
l	temperature of a process stream at lth location

Edreis et al., 2014; Bhat et al., 2001; Wang and Kinoshita, 1993; Fiaschi and Michelini, 2001), A thermodynamic equilibrium model, also referred to as equilibrium model, on the other hand, studies the gasification products under different reaction conditions based on the second law of thermodynamics as well as the energy and material balances (Nguyen et al., 2012; Mathieu and Dubuisson, 2002; Baratieri et al., 2008; Tang and Kitagawa, 2005; Shabbar and Janajreh, 2013; Kamath, 2012). Between the two types of models, kinetic models are usually used to compare the reaction mechanisms and rates, while thermodynamic models focus on the gasification products and their thermodynamic status.

So far, many equilibrium models have been developed. Baratieri et al. used an equilibrium model based on the minimization of the Gibbs free energy to estimate the theoretical yield and the equilibrium reaction products (Baratieri et al., 2008). Tang et al. developed a thermodynamic model with direct Gibbs free energy minimization to estimate equilibrium composition for supercritical water gasification (SCWG) of glucose, cellulose and real biomass (Tang and Kitagawa, 2005). Shabbar et al. evaluated RTC-coal gasification using Gibbs free energy minimization model under different operating conditions including air, air-steam and solar heat (under standard pressure) (Shabbar and Janajreh, 2013). Further, Kamath et al. embedded Gibbs model as an inner minimization problem within an outer optimization problem (to minimize the cost) (Kamath, 2012). By solving this as a bi-level optimization problem, Kamath et al. was able to minimize Gibbs free energy on one hand and obtain the optimum gasification conditions resulting in maximum profitability on the other hand.

Although the existing equilibrium models have offered an iterative approach to optimize the operating parameters of gasification for maximized cold gas efficiency (CGE), the optimization process involves special modelling techniques and huge amounts of calculation (Kamath, 2012). Also, the process can be easily trapped at a local optimum, which requires an additional step to differentiate the global optimum from the local optimums. To solve this problem, a novel mathematical model has been developed in this work, which converts the bi-level problem (Gibbs free energy minimization and CGE maximization) into a single level profit maximization problem. Thus, in this model, the reactant (carbonaceous feedstock, GFW and O_2) supply, the reaction temperature, and the heat integration of a coal gasification process can be simultaneously optimized for maximum economic profit in a selected way of syngas utilization, instead of using an iterative approach. In addition, heat integration is considered by including a set of linear constraints (Linnhoff and Hindmarsh, 1983; Duran and Grossmann, 1986; Hui, 2014) to ensure the feasibility of heat exchange among the hot product gases, feed streams and steam boiler. Case studies have been conducted utilizing this model to optimize a heat integrated coal gasification process. Results obtained using the simplified single level model has been validated using ASPEN Plus simulation.

2. Equilibrium gasification model

2.1. *Gibbs free energy of gasification products*

An equilibrium state of gasification reactions is achieved when the total Gibbs free energy of the products is minimized. The major assumptions in this principle are (Puig-Arnavat et al., 2010):