Application Of Computer-Aided Modeling In Thermochemical Processes: A Review

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ABSTRACT

The purpose of this study is to review the literature on implementation of software-aided thermochemical modelling depending on thermodynamic principles with the Aspen Plus software program. With rapid urbanization, population increase, and world's energy consumption is on the rise due to global economic developments. To meet this increasing demand, thermal processes and technologies are rapidly gaining value in the world today. For thermal plants to achieve maximum efficiency, software like Aspen Plus has been used for years. For this purpose, computer software used in thermochemical process implementations is examined due to the literature survey. Gasification that converts organic matter into valuable and highly energetic syngas needs pre-application steps due to its complexity. Besides energy and/or raw material production opportunities, gasification is known to be an environmentally benign technology. Using thermodynamic equilibrium principles, gasification systems are modified and optimized in order to achieve the highest conversion efficiencies with the help of software. The literature survey showed that gasification system parameters can easily and accurately be determined in a short period of time with high accuracy. The application of Aspen Plus can prevent the running of expensive and time-consuming gasification laboratory experiments since both experiment and Aspen Plus software results correspond. Therefore, the application of Aspen Plus in new thermochemical models can accelerate energy production.

Keywords: Aspen Plus; Gasification; Modelling; Thermal Process.

INTRODUCTION

With increasing urbanization, population growth, and economic development, energy consumption in the world is on the rise—thus a demand for searching new energy sources. One of the processes that has gained value in the world is heat technology. Among the heat treatment technologies, gasification process stands out as a clean and environmentally friendly technology with low emissions and least amount of waste generation. For thermal systems to obtain maximum efficiency, computer-aided programs such as Aspen Plus have been employed. Therefore, the aim of this review is to examine thermochemical models created by Aspen Plus software. In this review, results obtained using computer aided modelling are examined and interpreted.

Gasification process and reaction

Gasification is a partial oxidation process whereby a carbon source such as coal, natural gas or biomass, is broken down into carbon monoxide (CO) and hydrogen (H_2), plus carbon dioxide (CO_2) and possibly hydrocarbon molecules such as methane (CH_4). And other bi-products like syngas, tar and ash are also formed. Another important source of raw material for gasification process is industrial waste which can be an alternative to fossil fuels as it ensures sustainable global energy (Özek and Öngen, 2016, Öngen et al.,2017). The generated gas is used in engines and turbines to produce heat and power. Gasification process has been known since the late C18th. As a general rule of any thermal process, gasification involves the conversion of hydrocarbon fuels such as carbon, petroleum, biomass and solid wastes into gases, like CO, H_2, CO_2 and CH_4, in a process known as partial oxidation that involves a series of chemical reactions (Öngen, 2016; Öngen et al.,2017). Between solid fuel and solid waste based electricity generation technologies, gasification process stands out as a clean and environmentally friendly technology with the lowest emissions, solid and liquid waste values. In addition, in gasification process, less CO_2, SO_2 and NO_x are formed than in any other combustion technologies (Olgun et al., 1999, URL 1). Thus, the use of gasification technology in meeting the increased energy need is of utmost importance in ensuring energy security in a sustainable development (Öngen et al.,2017)

Until today, it is predicted that coal which has the largest share in the heat, steam and electricity production in the thermal process, will continue to have an important place even in the near future. In the gasification mechanism, the raw material first passes through the drying process followed by pyrolysis, oxidation and finally gasification. In the gasifier, the transfer of the raw material within these stages is provided by air movements. The gasification of the fuel in the gasifier is carried out in four separate processes; Drying> 150ºC, Pyrolysis: 150-700ºC, Burning: 700-1500ºC, Reduction: 800-1100ºC (Öngen and Arayıcı, 2014; Öngen and Arayıcı, 2015).

An Overview of Computer Aided Aspen Software Used in Thermal Processes

Aspen Plus computer-aided software program is widely used by researchers in the modelling of gasification systems. In the program system, the gasification system model is created by entering the necessary date into the system. The process consists of consecutive modules where results emerging from one module become the inputs of the other module. The results obtained are retrieved from the program as a table or diagram. The Aspen Plus program facilitates the design of complex processes, which provides researchers with the development of large systems. This program ensures that the outputs of the designed system are foreseen for accuracy and optimum operating conditions under different operating conditions. It establishes mass and energy balances and provides foresight about the dimensions of system's equipment. Simulation results are obtained much faster than

laboratory experiments when the test systems are installed and operated for a long time. In addition, it is possible to obtain data for high pressure and temperature conditions which are difficult to be realized in the test systems (Nayır, 2012).
Using Aspen software, optimum and most efficient system of more than one design system under varying environmental conditions can be determined without doing laboratory work. The Aspen program, a process simulation program, first appeared in 1981 with a research project jointly developed by Massachusetts Institute of Technology (MIT) and the United States Department of Energy (DOE). This was developed by AspenTech, a joint venture company. The name Aspen comes from the first letters of the words "Advanced System for Process Engineering (ASPEN)". With this program, it is possible to carry out chemical engineering and chemical process simulation for steady state condition, and it is possible to reach all kinds of information sought with 23,000 pure substances, 30,000 binary mixtures and more than 4 million total experimental data in the database. Aspen is capable of the following; calculation of the material and energy balance for any kind of chemical process equipment, calculation of thermodynamics for any chemical pure substance or mixture, calculation of substance and energy balance by forming a chemical process complete flow diagram, calculations for increasing the efficiency of chemical process, investment in any equipment or whole process and calculation of operating cost (Kupecki, 2009).

A Software Applications in Thermal Processes

Aspen Plus is an important design tool in many industries with the ability to simulate a variety of steady-state processes, from simple to complex processes involving multiple units. Studies on Aspen Plus, a computer-aided software program, have been going on for the past decades, and they are increasing day by day. This is attributed to the fact that experimental studies take a lot of time and their costs are high. Thus field computer-aided software programs are widely used by both researchers and commercial companies in the design of gasification processes. Albeit the generated models may not give coinciding results with real systems, when system inputs and reactions overlap thermodynamic and hydrodynamic conditions are used to build the systems, the results obtained approach real systems (Zheng and Furinsky, 2005; Ordarica-Garcia et al., 2006; Dai et al., 2008; Nathen et al., 2008; Robinson and Luyben, 2008, URL2). There are different approaches to modelling gasification systems. In some studies, the chemical equilibrium of exit gas composition is taken into account, while in some models the complex mechanisms that occur along the gasifier are examined by separating them into at least two distinct regions (Arnavat et al., 2010).

Generally, the modelling can be classified as; kinetic models, chemical equilibrium models, artificial neural networks, or computational fluid dynamics models. Thermodynamic equilibrium models are divided into the stoichiometric method and non-stoichiometric method. While all the reaction mechanisms and reactions are defined in the stoichiometric approach, the non-stoichiometric method works on the basis of the minimization of the Gibbs free energy value (Kupecki, 2009). Melgar et al. (2005) studied the downstream gasification systems with thermochemical equilibrium model. The established model was confirmed by experimental data and simulation data in the literature. When the literature was compared with the model, it was determined that the predicted results were very close to the experimental system. Li et al. (2003) examined the gasification of various biomass samples at different temperatures and temperatures in an air-circulating fluidized bed system. In order to predict the performance of the system, the working model with the principle of minimizing the Gibbs free energy was established and compared with the data obtained from the model experiments. Due to various constraints in the system, the deviation of the gas composition from the real equilibrium model was determined. Using the data obtained from the experiment, a corrected model was generated using untransformed carbon and CH_4 data; it was found that when the corrected model was used, the gas composition and the thermal value obtained in the corrected model overlapped with the data obtained from the experiments.

Nathen et al. (2008) examined the gasification of New Zealand lignite and bituminous coals using a computer-aided software program. The Peng Robinson model was used for the simulation of the system and the drag-flow type Shell type reactor suitable for low-temperature lignite was preferred as the gasifier. The similarity model was established and the published data obtained with different types of coal were compared. The error rate between the upper-temperature value of the synthesis gas obtained from the simulation and the actual value of the synthesis gas was found to be 11.3%. In another model study (Mahinpey and Nikoo, 2008), the gasification of biomass in a bubbling fluidized bed system operating at atmospheric pressure was investigated using the Aspen Plus program. In order to verify the model formed, experimental data was used in laboratory scale gasifier by using the yellow pine chip. The model created in Aspen Plus program was defined in the system according to biomass elemental analysis. The effects of factors such as air-fuel ratio and particle size change on the gas composition were investigated in the model.

Fortes et al. (2008) investigated the design of an integrated gasification combined cycle (IGCC) system using a computer-aided software program in the study of gasification effects of biomass added to coal. The aim of the work done was to investigate the feasibility of gasification with solid wastes. As a result of the affinity study, it was determined that the coal is the most efficient fuel for IGCC systems, with lower CO_2 emissions values obtained when solid wastes are gasified with coal. Duan et al. (2015) modelled the coal gasification system using heat recovery from steam and high-temperature furnace slag waste with the Aspen Plus modelling program. The model based on mass and energy balance was based on the Gibbs free energy minimization approach and the chemical equilibrium system used to recover the heat of the high-temperature furnace slag. Carbon gasification yield exceeded 90 % and the cold gas efficiency, synthesis product efficiency, and the heat value reached the maximum. Clean synthesis gas conversion was made with the coal gasification reaction and the slag waste heat was efficiently recovered (83.08 %).

Ramzan et al. (2011) developed a gasification simulation model in steady state using Aspen Plus. Simulation results were compared with experimental results. The effects of various parameters on the gasification system were investigated. Doherty et al. (2013) used the Aspen Plus program to create a gasification model based on the lowest reduction of Gibbs free energy. In this model, which was studied at the industrial scale, the experimental data were compared to determine the validity of the model. Until now, various working parameters have been studied under different conditions. Niu et al. (2013) created a model of solid waste gasification in a fluid bed reactor with a computer-aided software program. The effects on the gassing efficiency of operating parameters including gasification temperature, equivalence ratio, oxygen percentage, solid waste moisture content were analyzed. Sedghkerdar et al. (2015), the simulation results of the kinetic model were studied with the Aspen Plus simulation program and the results were in good agreement with the experimental data.

CONCLUSIONS

The aim of this review is to examine the application of models created by Aspen Plus computer software used in thermochemical applications. For this purpose, studies done with Aspen Plus computer-aided software program for the last two decades have been examined, and the results and studies have been compiled. In this context, the findings of this review can be listed as follows:

- The error margin is very low when the Aspen Plus simulation program is compared with the experimental data and the fit between the model and the test results is good.
- Aspen Plus, a computer-aided modelling program, has been found to be usable in thermochemical applications without the need for laboratory work. Given the compliance rates, Aspen Plus is predicted to be the perfect design tool for modelling gasification systems.
- Aspen Plus simulation program has the capacity to design a given process that can help the researcher to improve and develop large systems.
- In experimental systems that are difficult, risky and time consuming to run, it can be possible to acquire data with Aspen Plus program efficiently.

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