

Introducing novel graphical techniques to assess gasification

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ABSTRACT

Due to its complexity, coal gasification is perhaps one industry's least understood processes. This is despite the fact that this process is critical to countries such as South Africa, as it is responsible for producing a large portion of the country's fuel needs through the Fischer–Tropsch process. Worldwide, this process has also become critical for applications such as IGCC, for the production of electricity. It is because of this importance that it is necessary to better understand this process. Another motivating factor is that gasifiers are very expensive and are big energy consumers as well as being large carbon dioxide producers.

Much experimental work has been done in the area of gasification, but this can be very expensive and is time consuming. It is with this in mind, that we have developed a quick, relatively simple and yet very powerful graphical tool to assess and better understand gasification and to use this tool to look for opportunities to improve efficiencies of process and to reduce carbon dioxide emissions.

The approach used here is to make a few reasonable assumptions to set up mass balances; the energy balance and reaction equilibria around a coal gasifier. This paper deals with how these balances can be set up; it also looks at what effect the feed composition and choice of reaction conditions (temperature and pressure), may have on the possible gasifier product.

The result of this approach shows that we can work in a stoichiometric subspace defined by the energy and mass balance. Furthermore we can show that gasification is energy and not work limited which has implications for the design and operation of these units.

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1. Introduction

A common factor in models that look at predicting or analysing gasification is that they usually require some kind of experimental result or access to thermodynamic databases to accurately predict the behaviour of a gasifier. Also common among these is that they all make assumptions regarding the reactions that occur in a gasifier.

Zainal et al. [2] have selected one reaction resulting from the combination of the Boudouard equilibrium and heterogeneous water gas shift reaction and the hydrogenating gasification as the main gasification reactions, while Schuster et al. [3] have selected the water gas shift reaction along with the methane decomposition reaction.

According to the thermodynamic theory of independent reaction selection, there is no significant difference between the above reported models [5]. The only point that differentiates the equilibrium reactions is that the methane decomposition reaction is favoured in the case of steam gasification (high feed moisture content) and not in the case of the conventional gasification pro-

cess. This paper uses a similar approach in selecting independent reactions that can occur in a coal gasifier.

Various people have developed models for gasification and one of the more significant ones is the GasifEq equilibrium model developed by Mountouris et al. [11,12] and applied to the plasma gasification of sewage sludge. The model includes the energy supplied to the main section of the plasma gasification process (electricity), the formation of the basic gasification gaseous products and the possibility of some remaining solid carbon.

The model also uses the mass balance and energy balance around a gasifier, which is a concept that has been used extensively in this paper. Crucial to their model is the use of recent thermodynamic data which also considers the possibility for soot formation, as a solid carbon by-product. The GasifEq model also has the capability of energy and exergy calculations that are required for the optimization of such processes. Instead of exergy, in this paper we use the idea of a work balance as developed by Patel et al. [1] to better understand the energetic performance of a gasifier.

Prins [4] chooses three main reactions in the gasifier and these are the methane decomposition reaction, the Boudouard reaction and the heterogeneous gasification reaction. The energy conversion process studied is shown in a triangular C–H–O diagram as shown in Fig. 1 below.

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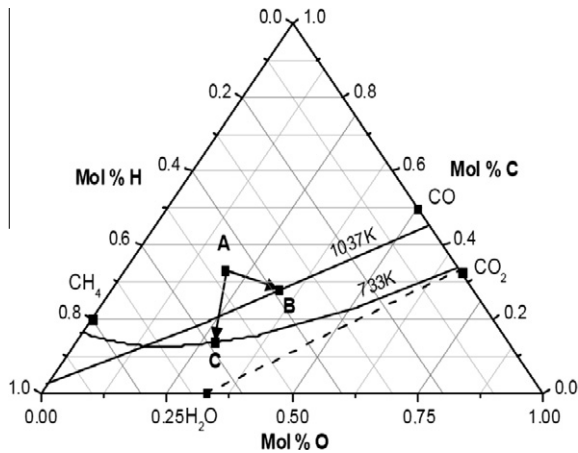


Fig. 1. Molar triangular diagram indicating (A) biomass feed, (B) biomass in equilibrium with air at carbon boundary and (C) biomass in equilibrium with steam of 500 K at carbon boundary.

The composition at any point in the diagram can be computed at a given temperature and pressure by calculation of the gas phase compositions in equilibrium with solid carbon (graphite).

In the triangular diagram, several lines are shown, the so-called carbon deposition boundaries. Above the solid carbon boundary, solid carbon exists in heterogeneous equilibrium with gaseous components, while below the carbon boundary no solid carbon is present. Most hydrocarbon fuels are located above the carbon boundary, which means that if these fuels are brought to chemical equilibrium, solid carbon is formed. This implies that in order to avoid solid carbon formation and achieve complete gasification, oxygen and/or hydrogen must be added. Oxygen and hydrogen sources are H_2 , H_2O , O_2 , air or CO_2 .

Mountouris et al. also present a ternary map that represents the carbon deposition in a gasifier; we represent this in a stoichiometric subspace defined by the energy and mass balance.

An important point in the modelling procedure of gasifiers is whether equilibrium is reached in the gasification process, i.e. whether the operating conditions allow the chemical reactions to reach an equilibrium state. As far as the gasification temperature is concerned, it is stated that equilibrium is not achieved when the gasification temperature is sufficiently below 800 °C (common gasifiers), while it is reached for higher temperatures like those of plasma gasification [6,7].

Regarding the other crucial factor relevant to an equilibrium state, that is the residence time, Prins et al. [8] reported that for air gasification, the residence time is sufficiently long and equilibrium is well verified, while for steam gasification, equilibrium may not be reached due to the lower operating temperatures.

In addition, Calaminus and Stahlberg [9], based on experimental facts, stated that during gasification in the Thermostelect plant, the residence times for the gas phase and also for the molten phases are sufficient for equilibrium to be attained, i.e. for the solids it is about 1–2 h and for the gas phase 2–4 s at about 1200 °C.

Chen et al. [10] presented that in such processes, a significant increase of gas yield is noted between 2 and 3 s (as a result of a tar cracking reaction), and after that time period, equilibrium is assumed to be attained.

Consequently, in this work we have studied gasification based on equilibrium terms in order to describe the process and to present its energetic performance in relevance to the main operational parameters, e.g. moisture, oxygen, pressure and temperature.

The heart of this work lies in the use of fundamental mass balances, energy balance and thermodynamic properties to define a

stoichiometric space, within which we can attempt to better understand, operate and optimize gasification processes.

The approach that we follow in this paper is to initially simplify the description of the fundamental processes occurring in gasification as far as possible and to later add other phenomena and variables to cater for a more detailed description where and when necessary.

2. The mass balance

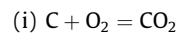
2.1. Degrees of freedom for the mass balance: defining the independent mass balances

It is known that there are a large number of reactions that can occur in a gasifier but we will look at the most important of these in terms of mass, heat and work flows.

In terms of the mass balance, the major species in the gasifier in the feed stream are C, O_2 and H_2O , while the major species in the product streams are CO_2 , CO, H_2 and H_2O . If we analyse the system we see that we have three degrees of freedom and thus we require three independent mass balances to relate the gasifier inputs and outputs.

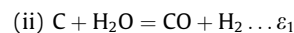
These three mass balances do not need to describe the actual chemistry or reactions occurring in the gasifier but are merely mathematical descriptions. In essence the mass balances we choose are independent dimensions of the stoichiometric subspace and are a convenient way of relating inputs and outputs from the gasifier.

The first independent mass balance we consider is the combustion reaction, namely:



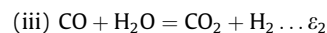
We assume that coal is pure carbon (which is a not particularly good assumption), but we can adapt this description if we have a chemical analysis of a specific coal. We can reasonably assume that this reaction goes nearly to completion and provides the energy necessary for the other gasification reactions. Thus the extent of this reaction is essentially equal to the amount of O_2 that is fed to the gasifier.

The second independent mass balance we use is a gasification reaction, that is:



This reaction may not occur to completion and we define the extent of the reaction/mass balance to be ε_1 .

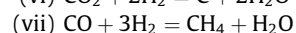
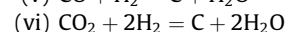
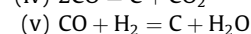
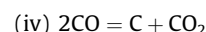
The third and final independent mass balance is the water gas shift reaction or:



This reaction will also not occur to completion and we define the extent of this reaction to be ε_2 .

Although we have three independent reactions and hence a three dimensional mass balance space, we have by the assumption that the first reaction, the combustion reaction, goes to completion; effectively reduced the dimension of the space that we work into a two dimensional space.

The other reactions that will be considered are:



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