Thermodynamic Modelling of the Gasification Process of Waste Tyres as A Feed Source into a Plasma arc Furnace Reactor

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***Abstract*---**In an attempt to alleviate the on-going waste accumulation problem that society faces, various technologies are being researched in order to convert waste materials into useful commodities. One suggestion is the use of a plasma arc gasification process to convert any kind of organic waste materials into an energy vector that would be useful for the society at large.

Studies have indicated that from known technologies such as incineration, pyrolysis, gasification and plasma arc gasification, the plasma technology has proven to be the cleanest due to the absence of an incineration or burning process [1].

Various thermodynamic models exist to predict the product gas composition delivered by gasification. These include, but are not limited to the Factsage model, the HSC Chemistry model, the Gasifiq model etc. [2-4], although a limited number of these models have been used to predict the yields of specifically a plasma arc gasification reactor.

This study aims to predict the syngas yields of a tyre-waste fed plasma arc gasification reactor using the known chemical thermodynamic modelling tool HSC Chemistry. Various scenarios corresponding to different operating conditions in the plasma arc reactor are being simulated in the modelling software for a laboratory scale plasma arc furnace with validation of the results on an actual laboratory scale reactor.

The various operating conditions that are being investigated in both the modelling and validation phases of this project include variations in (i) energy supply to the plasma arc torch (which is in direct relation to the temperature inside the furnace), (ii) the moisture addition to the reactor feed (which acts as additional source of both oxygen and hydrogen) and (iii) oxygen addition to the reactor.

***Index Terms*-**plasma arc gasification, syngas, HSC Chemistry, Tyre waste.

I. INTRODUCTION

In the last century waste management has become a critical issue as the sheer amount of it has risen immensely [5]. According to a draft of the National Waste Information Baseline Report South Africa produced roughly 108 million tons of waste in 2011 of which 59 million tons was general waste alone, waste tyres contributed 7.4 million tons to this general waste. It has also been found that merely 10% of this waste was recycled and the remaining 90% was landfilled. The recycling rate of tyres was at a dismal 4% for this year [6]. Almost 11 million waste tyres are added to this number annually. This imposes a great number of environmental and health risks because these tyres are often burnt for their scrap metal content or for heat generation, releasing toxic fumes and liquids in the process [7].

Currently there are a number of thermal applications for treating waste tyres. These include incineration, pyrolysis, gasification, geo-plasma and plasma-arc. The main focus will be on plasma-arc gasification. When considering an arc welding machine, an electrical arc is struck between two electrodes, a plasma arc reactor runs in a comparable way. Organic waste is converted into light organics and primary elements by the high temperatures that are created by the high energy arc. Organic waste material is fed to the plasma arc where it is enclosed in a chamber, the intense heat emitted from the arc breaks down organic molecules. The waste is completely dissociated by the high temperatures that are created by the tale flame. These atoms then recombine into stable gases for instance carbon monoxide and hydrogen in a carefully controlled process. With the plasma arc technology stable molten slag is produced and it does not involve incineration or burning [1].

The primary purpose of the gasification of waste tyres is to alleviate the pollution that tyre waste landfills bring about and to transfer the once considered waste into a usable energy source such as a syngas for the generation of electricity or the production of other fuel types.

Commercially, the operational procedure for plasma arc gasification includes feeding a carbonaceous feedstock into a plasma arc heated reactor. In an oxygen starved environment, the heat for the pyrolysis process reactions is generated when this material responds rapidly with the exposure to added oxygen. In equation (1) the carbonaceous material, depicted by C, produces a constrained combustion when it reacts with oxygen but it still contains the required energy for the syngas reactions which are equations (2) – (6). [5]

$$C + O_2 \rightarrow CO_2 \quad (1)$$

$$C + H_2O \leftrightarrow CO + H_2 \quad (2)$$

$$C + 2\,H_2 \leftrightarrow CH_4 \quad (3)$$

$$C + CO_2 \leftrightarrow 2\,CO \quad (4)$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \quad (5)$$

$$C_nH_m + nH_2O \leftrightarrow nCO + (n + \tfrac{1}{2}m)\,H_2 \quad (6)$$

For a specific syngas (CO/H_2) composition, steam or O_2 has to be added to the reactor. Exothermic combustion reactions

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supplies some heat supplemented by the plasma arc torch. Endothermic pyrolysis reactions requires all of the process heat to be supplied by the plasma arc torch.[5]

It is found that plasma gasification also utilizes a supply of heat externally, in order to convert the waste into gas, culminating in limited combustion. A large portion of the carbon present is transformed into fuel gas. When it comes to pure gasification, plasma gasification is the most convenient innovation. Mostly on account of the high temperatures concerned, the dioxins, tars and char are completely broken down. No ash can be found at the bottom of the reactor due to this and the exiting gas is also proven to be much cleaner.[4]

The primary objective for this article is to investigate (i) whether for a specific feed rate of waste tyres the yields of the syngas achieved by a plasma arc furnace reactor can be predicted by using a thermodynamic model. (ii) Validating this theoretical data with experimental data collected on a laboratory scale plasma arc furnace reactor. As a secondary objective ways on how the received yields can be improved based on the thermodynamic model will be suggested

II. Experimental

A. Feed preparation

The waste tyres used in the experiments were stored, prepared and provided by Necsa (The South African Nuclear Energy Corporation SOC Ltd). The feed was prepared by passing it through a heavy duty shredder numerous times in order for the feed to reach an optimal size in which it can be fed to the gasification reactor.

An ultimate analysis was done on a representative sample of the waste tyres, by grinding some of the feed further to achieve a fine powder which is optimum for this analysis. This yielded the chemical composition, moisture content, ash content and other properties of the tyre feed material.

1) Feeder calibration

It is necessary to calibrate the screw feeder for the specific feed material that will be used during the experimentation e.g. the shredded waste tyres. The calibration was done by first filling the hopper with 5 kilograms of waste tyres and feeding it through the feeder at intervals of 5 min at different speed settings. A plastic container was used to collect the delivered material where after it was weighed. The procedure was repeated 3 times for each speed setting to obtain an average mass flow per hour at that particular speed setting. The system operates at roughly 1 kg feed per hour. Table 1 shows the average mass flow at each speed setting. Figure 1 shows the Feeder calibration graph with a 5 percentile error margin that was determined.

TABLE I
AVERAGE MASS FLOW PER HOUR AT SPECIFIC SPEED SETTING

Rpm	Average Mass flow (kg/h)
40	0.735
50	0.894
60	1.062
70	1.217

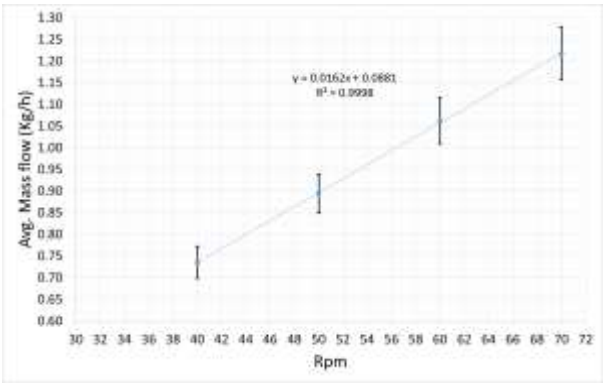

Fig. 1 Feeder calibration graph with 5% percentage error margins

B. Experimental procedure

1) Experimental setup

The experimental study was conducted on a laboratory scale plasma gasification process which is depicted by the following figure.

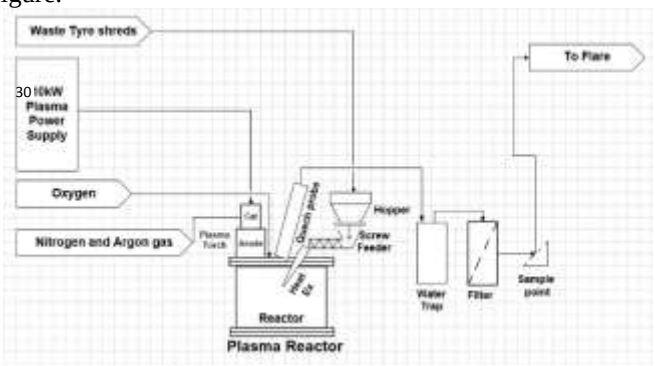

Fig. 2 Process flow diagram of plasma arc gasification system

The heat generated by the plasma torch allows the reactor enclosure to reach temperatures up to 1200 ºC. The gas mixture formed inside the reactor as waste tyre shreds are fed through the screw feeder, is rapidly cooled in a water-cooled quench probe. It then travels through a liquid trap to remove condensable species. Ash and soot is removed as the gas passes through a cartridge filter. Hereafter a point is located where samples can be taken by means of U-tubes to be analysed by various techniques, such as GC analyses, to determine the composition of the product gas.

Initially argon is used to establish the plasma where after nitrogen is used to sustain the plasma throughout experimentation.

2) Manipulative variables for experiments

Eleven experimental runs where executed. Both the base case where no parameters where changed, and the stoichiometric oxygen experiments were repeated twice for the experimental error determination. The other variables involved (i) changing the current settings as this has a direct correlation to the reactor temperature, (ii) feeding of additional oxygen to the system at half stoichiometric and two times stoichiometric levels and (iii) varying the moisture added to the feed at initially zero percent for the base case and oxygen experiments and then at 5 wt% and 10 wt%. Table 2 shows a comprehensive summary of the different conditions for each experimental run.

TABLE II
MANIPULATED VARIABLES FOR DIFFERENT CASES

Variables	Run	Repeat	Current (A)	Oxygen (stoich)	Oxygen (%)	Moisture (wt. %)
Base Case	1	2	90	0	0	0
	2		90	0	0	0
	3		90	0	0	0
Current Case	1	1	100	0	0	0
	2		110	0	0	0
	3		120	0	0	0
Oxygen Case	1	2	90	0.5	11.50	0
	2		90	1	24.42	0
	3		90	2	50.25	0
Moisture Case	1	1	90	0	0	5
	2		90	0	0	10

The experimental error was calculated to be 27.4 percent which is acceptable for the proof-of-concept experiments performed.

C. Model development

1) Gasification reactions

In the model moisture and oxygen is added separately in different proportions in order to convert the carbon content to CO. The following table contains a summary of the modelling inputs for the manipulated variables oxygen and moisture content. Because HSC Chemistry does not provide a sound input for the energy supplied to the system except for the temperature, the manipulated variable concerning the current supplied had to be evaluated elsewhere.

TABLE III
MODELLING INPUTS INTO HSC CHEMISTRY CONCERNING DIFFERENT SCENARIOS

Input			
Feed rate	Oxygen		
kg/h	Stoichiometric	kmole/h	kg/h
1.00	2.00	0.0678	2.1710
1.00	1.00	0.0330	1.0548
1.00	0.50	0.0155	0.4967
	Moisture		
kg/h	% mass	kmole/h	kg/h
1.00	0.05	0.0030	0.0538
1.00	0.10	0.0058	0.1038

The partial combustion of the tyres with oxygen delivers the CO gas needed as seen in the equation below.

$$C + \tfrac{1}{2} O_2 (g) = CO (g) \quad (7)$$

This equation was used to calculate the necessary oxygen that needed to be supplied to the system for stoichiometric combustion and in addition the amounts needed for sub- and super-stoichiometric. The following table shows the calculated values. The units are converted into g/s and from there it is adapted to the flow meter setting for the plasma gasification system in percentage.

TABLE IV
STOICHIOMETRIC VALUES FOR OXYGEN

C + 1/2 O2 = CO	Kmole/h	g/s
C	0.0698	
CO	0.0698	
O2(stoichiometric)	0.0349	
O2(supply)	0.0330	0.3
Flow meter setting (%)		24
O2(1/2 stoichiometric)	0.0174	
O2(supply)	0.0155	0.1
Flow meter setting (%)		11
O2(2 stoichiometric)	0.0698	
O2(supply)	0.0678	0.6
Flow meter setting (%)		50

The subsequent table shows the calculated values for the water supply that are necessary to test the influence moisture has on the product gas delivered.

TABLE V
WATER SUPPLY TO SYSTEM AND MODEL

	ml/kg water	kmole water	Input into HSC kmole/h
H2O in feed			0.0002
5 weight %	50	0.0028	0.0030
10 weight %	100	0.0056	0.0058

2) Feed stock chemical composition

The composition of the waste tyres used for modelling can be seen in Table 6 below.

TABLE VI
ULTIMATE ANALYSIS DATA

Component	Mass%	Mass%
	Dry Ash Free	As received
C	85.90	83.72
N	0.70	0.68
N2		
S	0.35	0.34
H	6.75	6.58
H2		
O	6.30	6.14
O2		
Total	100	97.46
Ash		2.23
Moisture		0.38
Total (as received)		100.07

3) Equilibrium composition calculations

In the Equilibrium Composition module of HSC a new Input file is created where the five elements are selected (H, C, O, N, and S). Hereafter, based on sound chemical knowledge, irrelevant species are eliminated.

The ash does not take part in the gasification process and is therefore not included in the calculations.

The molar required amounts for N_2 and O_2 are then entered. Calculations are done at 1 bar pressure and in the temperature range of 25 °C to 1600 °C.

After the equilibrium calculations are made an equilibrium diagram is obtained, the "Table" tab is selected and the data

received is then copied into excel where further calculation can be made.

III. Results and Discussion

A. Evaluation of model and experimental results

1) Assessment of various cases

a) Base case

The following figure shows the correlation between the results predicted by HSC Chemistry and that of the results received from experimentation in kilograms for the base case where no parameters were changed e.g. Amps at 90 with no added oxygen or moisture.

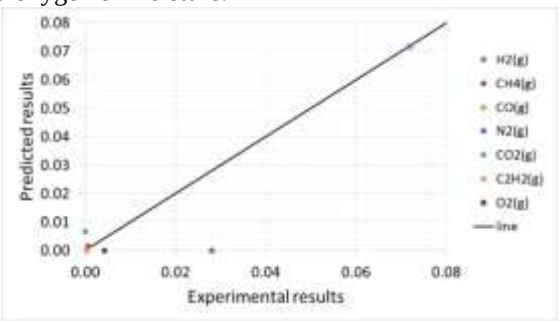

Fig. 3 Correlation between predicted results and experimental results for the base case

From the figure it can be seen that for H_2 and C_2H_2 the model prediction was very accurate, the predicted results for CO_2 were slightly higher than what was actually received and the obtained values for O_2 and N_2 were higher than what was predicted. In general except for two data points namely H_2 and C_2H_2 the models prediction capability is poor.

b) Additional oxygen added case

The figure below shows the relationship between the predicted yields from HSC chemistry and that which were determined experimentally in kilograms for the case when oxygen was additionally added at different stoichiometric scenarios. A circle marker indicates a component at half stoichiometric level, a square marker indicates a component at stoichiometric level and a triangle marker indicates a component at double stoichiometric level.

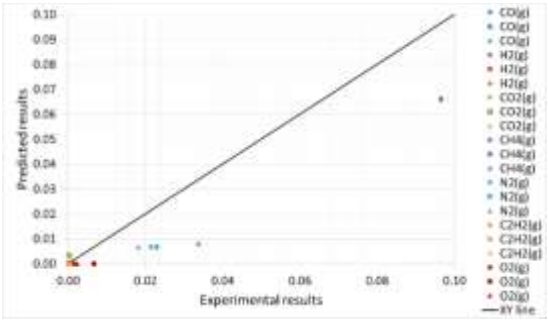

Fig. 4 Correlation between predicted results and experimental results for the different oxygen cases

This shows that for oxygen added at different stoichiometric levels the HSC model did not accurately predict the yields of the product gas however, a good prediction for CH4 could be made. For all the other components the experimental yields were higher than that which was predicted.

Due to scaling reasons the comparison of CO was left out of the figure but the values obtained from the model and experiments can be seen in the subsequent table.

TABLE VII
COMPARISON BETWEEN HSC AND EXPERIMENTAL RESULTS FOR CO IN THE CASE OF ADDED OXYGEN

	Predicted by HSC	Received by experiments
CO(g) at 0.5 Stoich	0.9798	0.0084
CO(g) at Stoich	1.9499	0.0084
CO(g) at double Stoich	0.8043	0.0160

The highest yield for CO was predicted at a stoichiometric level fed to the system and the lowest yield at double stoichiometric because it is expected that at double stoichiometric levels the CO will start to convert to CO_2. However, the opposite is experimentally observed and the highest CO yield is received at double stoichiometric oxygen level fed.

c) Additional moisture added case

From the following figure the relationship between the predicted and experimentally received results for the different moisture content added to the system at 5 wt. % and 10 wt. % respectively. A circle marker indicates a component at 5 wt. % added moisture to the feed and a square marker indicates a component at 10 wt. % added moisture to the feed.

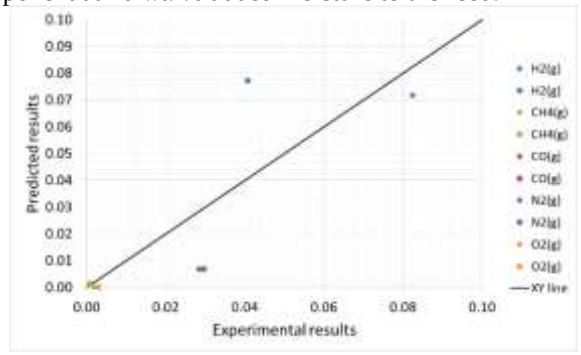

Fig. 5 Correlation between predicted results and experimental results for the different moisture cases

The preceding figure shows that for the added moisture content the HSC model did not accurately predict the yields of the product gas. The closest predicted value to that obtained from experiments is that of H_2 at 5 wt. % moisture added. N_2, specifically for this case yielded significantly more experimentally for each amount added than that which was predicted.

Because of scaling reasons the comparison of CO was left out of the figure but the values obtained from the model and experiments can be seen in the following table.

TABLE VIII
COMPARISON BETWEEN HSC AND EXPERIMENTAL RESULTS FOR CO IN THE CASE OF ADDED MOISTURE

	Predicted by HSC	Received by experiments
CO(g) at 5 wt. %	0.1905	0.0005
CO(g) at 10 wt. %	0.2680	0.0008

Here, it is noticeable that the predicted values for CO is a lot higher than which was ultimately received experimentally. Therefore, it is safe to say that the added moisture has little to no effect on the composition of the product gas especially at 5 wt. % and 10 wt. % added moisture.

2) Assessment of component yields

The following section is dedicated to describing how each component in the product gas was successfully or unsuccessfully predicted by HSC. This is done by using one of Excels linear regression outputs namely the correlation coefficient (R^2) which shows the reliability of the linear relationship between the experimental results and the predicted results. Along with this, the root mean square error (RMSE) is also calculated where a small value indicates a good model predictability. This is calculated by using the equation below.

$$RMSE = \sqrt{\frac{\sum_{i=n}^{n}(Y_l - Y_i)^2}{n}} \quad (8)$$

$Y_l = experimental\ result$
$Y_i = predicted\ result$
$n = number\ of\ variables$

It is also important to keep in mind that these correlations are only done for the additional oxygen and moisture cases as HSC is not able to predict the composition of the product gas when current is set as a variable.

a) CO

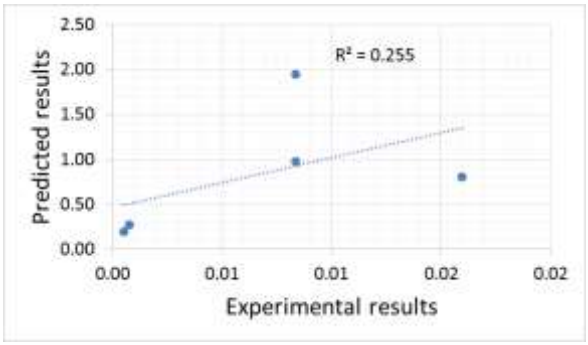

Fig. 6 Comparison between predicted and experimental results for CO

A correlation of 25 percent is achieved by the model when predicting the yield of CO. A RMSE of 1.04 was attained; this value is relatively high which means that for the component CO the HSC model does not give a reliable estimation.

b) H_2

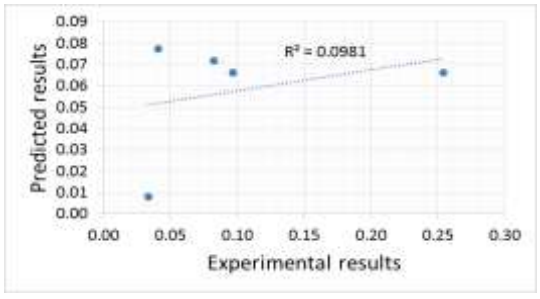

Fig. 7 Comparison between predicted and experimental results for H_2

The correlation between the predicted and experimental values is here at 10 percent and a RMSE of 0.09 is calculated. The RMSE is low which is ideal but this is because the values for H_2 are very low and thus this just means that the error between the predicted and experimental yields for H_2 are very low. If it was not for the outlier an almost horizontal line would have been a result thus meaning that the model is not very accurate.

c) CO_2

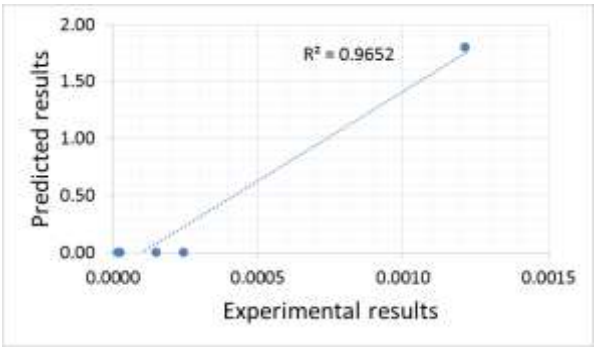

Fig. 8 Comparison between predicted and experimental results for CO_2

A 96 percent correlation is achieved when the model predicted the values for CO_2 at the different parameters, and a RMSE of 0.81 is calculated. Statistics suggest that the model concerning CO_2 predicted the yields well, but some data points are not considered due to the fact that none were predicted but experimentally produced and lies therefore on the axis.

d) CH_4

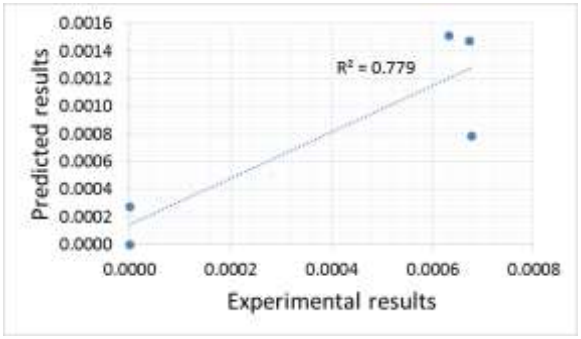

Fig. 9 Comparison between predicted and experimental results for CH_4

The CH_4 correlation is at 78 percent and the RMSE is at 0.0005, thus meaning that for CH_4 the model predictability is very good, except again when considering that some data points lie on the axis.

e) N_2

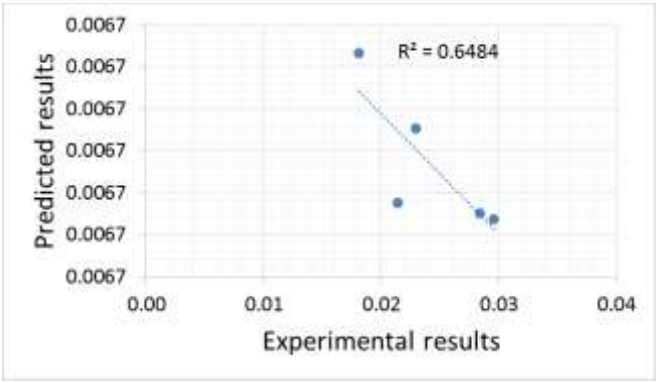

Fig. 10 Comparison between predicted and experimental results for N_2

For N_2 a correlation of 65 percent is achieved and a RMSE of 0.02. Even though these are good approximations the slope of the tredline is negative indicating that the model predicts the opposite of what is seen experimentally.

f) C_2H_2

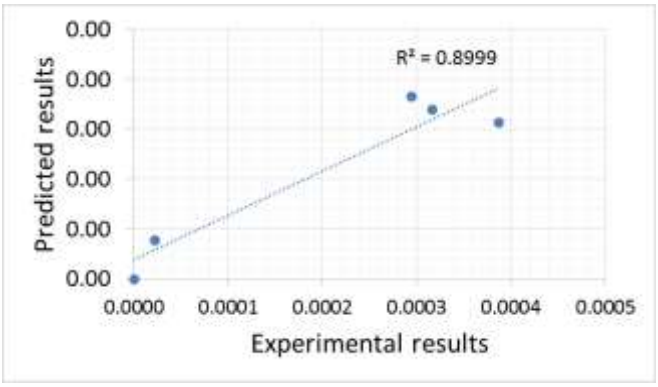

Fig. 11 Comparison between predicted and experimental results for C_2H_2

Again here for C_2H_2 the model gives relatively accurate predictions with a correlation of 90 percent and a RMSE of 0.0003.

g) O_2

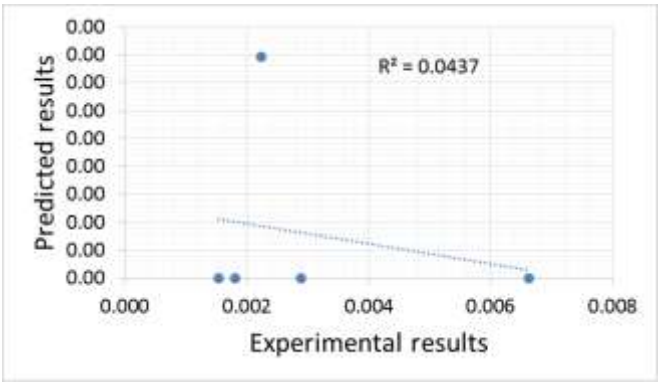

Fig. 12 Comparison between predicted and experimental results for O_2

For O_2 it can again be seen that a negative trend is observed thus meaning that the model predicts the opposite of what is achieved experimentally. This is reflected with a correlation of 4 percent. However, the RMSE is 0.0035 which is again a very low value this is mostly due to the extremely low predicted yields with orders of up to minus 19.

B. Discussion

When regarding the data predicted by HSC Chemistry and the received experimental results, it can be seen that there are somewhat similarities but also some outliers. It is noticeable that the Carbon monoxide and the Nitrogen gas are frequent components that stand out and do not particularly fit the models predictions, no matter what variable was changed.

HSC Chemistry does not have the capabilities to directly compare the composition of the predicted syngas to that of experimental data when the energy supplied to the system is varied.

IV. CONCLUSION

It was found that the HSC Chemistry model created helped assist in the predictions of the syngas compositions to some extent for the additional oxygen fed and moisture content added scenarios, however it could not predict the composition of the syngas when energy input acted as manipulative variable.

The model predicted H_2, CH_4 and C_2H_2 to some extent but not the other species. N_2, cannot be predicted by HSC and should not be considered in this approach.

In general, HSC is considered unsuitable for predicting plasma arc reactor yields, and other known models should be considered for future studies.

It is found that for the complete gasification of the carbon present in the feed material the oxygen content is insufficient and therefore additional oxygen is necessary to transfer the carbon to CO and H_2 at temperatures above 800 ºC. From the data it can be seen that at stoichiometric levels the highest outcomes for these components can be expected, in practice the stoichiometric amount of O_2 will vary with the moisture content of the feed. Therefore, gasification under conditions which will deliver the maximum amount of syngas is when O_2 and moisture content is added in stoichiometric ratios. If too much O_2 is added the syngas gradually converts to CO_2 and H_2O.

ACKNOWLEDGMENT

The author is grateful to Necsa and the contributions of Mr A.A. Jansen as his guidance was really appreciated.

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