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Simulation of the Combustion of Onyeama Coal in a Batch Reactor Using Comsol Multiphysics Model

Iortyer, H. A[1], Agabi, J. A[2] , Kucha, E.I.[1]
[1] University of Agriculture Makurdi, College of Engineering, Department of Mechanical Engineering.
[2]Council for Regulation of Engineering in Nigeria (COREN), 22 Addis Ababa Crescent, Wuse Zone 4, P.O. Box 8461, Abuja, Nigeria.
*Corresponding Author: * Iortyer, H. A*

Abstract: *The simulation of combustion of Onyeama coal in a batch reactor using COMSOL MULTIPHYSICS model was carried out in order to develop necessary baseline combustion reaction data and also to provide data for the assessment of coal combustion performance at high temperatures. The volatile matter component of Onyeama coal and some parameters from Illinois No.6 coal were used for the simulation. The volatile matter combustion reaction rates were converted into batch reactor space using air to fuel ratio at set tolerance levels and initial temperature of 800K. Key indices such as model volatile gas specie evolution rates, calorific value and gas temperature profiles were computed using three and thirty three reaction kinetic equations from a natural gas combustion model some of which had to be adapted to the COMSOL model. In order to predict the quantity of the volatile matter present at any time, the reaction time was divided into two zones (10^{-3} and 10^{-6}). The results showed that predicted energy released by the Onyeama coal was highest* (i.e $2.6258*10^3$ at 0.00s) *at the beginning of combustion and fluctuatd as the combustion progressed to a value of 0 J within a reaction time of at time $5.0 * 10^{-4}$s.. Maximum combustion temperature was 3130K. Carbon produced was 0.049 mol/m^3 while NO_2 amounted to 0.00001396 mol/$m^3$and the values for H_2O, CO_2, CH_4 and C_2H_6 at 0.001s were 0.2555 mol/m^3, 0.3999 mol/m^3, $2.95x10^{-15}$ mol/m^3 and $1.1x10^{-29}$ mol/m^3 respectively. It was concluded that the simulation of Onyeama coal has adequately shown the nature of its combustion in the model batch reactor. Experiments with Onyeama coal in a batch reactor of similar design are recommended for validation of this result.*

Keywords: *Simulation, Combustion, Onyeama Coal, Batch Reactor*

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I. Introduction

In recent years, increase in exploitation of crude oil and natural gas, concerns about their depletion and security of supply have turned attention to the possibility of obtaining fuel for power generation and feed stocks for chemical industry from the gasification of coal. Coal is a principal energy source that originated from vegetable matter which grew millions of years ago. Trees and plants falling into water decayed and later produced peat bogs. Huge geological upheavals buried these bogs under layers of silt. Subterranean heat, soil pressure and movement of earth crust distilled off some of the bogs moisture and hardened it to form brown coal or lignite (Okafor, 2009). The properties of coal of particular importance are its heating value, the amounts of fixed carbon and volatile material, and the amounts of moisture, sulfur, and ash (Roberts and Meyers, 1982). Coal is a solid and contains no volatile material. However, when it is heated above 400°C, some of the coal material decomposes and is given off as gas. This is referred to as the volatile material in the coal (Roberts and Meyers, 1982). The heating of coal is usually carried out in mechanical devices known as gasifiers using a process called gasification. Gasification is the reaction of coal with insufficient oxygen to produce syngas which can be used as fuel or a raw material for the synthesis of chemicals, liquid fuels or other gaseous fuels. Syngas is made up of carbon monoxide, hydrogen and light hydrocarbons (Rohan, 2014). The combustion process includes devolatilization (pyrolysis), homogeneous reactions (reactions of volatile components), heterogeneous reactions (surface reactions or char oxidation), swelling, cracking, etc. Many research workers such as Mohammed (2011), Chinh(1995), Hla(2007), Saxena (1990), etc., have attempted to simplify the process by dividing it into several sub-processes, such as devolatilization, char oxidation, etc. Coal gasification is undertaken in gasifiers. There are three main types of gasifiers namely; moving (also known as fixed) bed, fluidized bed and entrained flow (Rohan, 2014). One of the key enabling technologies fundamental to power generation through gasification is the integrated gasification combined cycle (IGCC) system. Gasification process in IGCC systems is largely influenced by coal type and operating conditions. In order to better understand the complex processes occurring in a gassifier, computational models in conjunction with plant data can be used to evaluate gasifier operation, solve problems, probe new designs and provide performance data for commercial scale up (Rohan, 2014). Many models exist for the modeling of coal gasification. These are broadly classified into; zero dimensional, one dimensional, two dimensional and three dimensional models. Specifically, models for pyrolysis, char oxidation, and a number of reactions for volatile oxidation have been proposed. Each model has several empirical constants which are found under certain conditions. These constants or models must be tested in different cases with different conditions. Smoot (1984, 1991) made a review of models for pulverized coal combustors/gasifiers; one-dimensional and multi-dimensional coal reactors, fixed bed and one-dimensional fluidized bed. In order to improve power supply from its current abysmal level, Nigeria is diversifying its power generation by looking at the possibility of using several energy resources such as oil and gas, coal and renewable energy resources. Nigeria has major coal resources that have not been well explored or exploited. The proven coal reserves so far in the country are in hundreds of millions of tons while estimated reserves are in billions of tons. It is essential that the behavior of Nigerian coals in new gasification technologies is fully understood in order to assist power utilities in their adoption of the new technologies and to help coal exporters to market Nigerian coals. The objective of this research was, therefore, to accurately simulate the combustion of Onyeama coal in a zero dimensional model batch reactor using the COMSOL multiphysics reactor software that can be used to generate data suitable for the design and construction of coal combustion chambers or equipment for a wide array of purposes.

II. Methods

2.1 Steps for gathering data for model input

The method involved is using the volatile component of the proximate analysis of Onyeama coal obtained from an experiment carried out at the national metallurgical development center (NMDC) by Mohammed (2011) and Illinois no.6 Coal (Chinh, 1995) for the simulation. The simulation was carried out using a batch digester in COMSOL MULTIPHYSICS software. Since information on some parameters needed for simulation of the combustion of Onyeama coal in the COMSOL MULTIPHYSIS software was not available from the laboratory experiments of the primary literature material, data from the Illinois #6 coal (Chinh, 1995) whose volatile mass fraction closely approximates that of Onyeama coal was used. To carry out this simulation in order to determine with respect to reaction time, the temperature, volatile specie evolution, energy release rate with Onyeama coal as feed, the following steps were undertaken;

- data from proximate analysis of onyeama coal was used to determine the mass fraction of species per unit mass of coal;
- volumetric mass fraction per unit mass of coal was determined;
- solid coal feed rate was transformed to its corresponding volumetric feed rate;
- the corresponding volume occupied by species was calculated;
- gaseous volumetric feed flow rates from all streams were derived at their initial temperatures;
- steady flow feed rate data for all coal and air reactions were reduced to batch samples;
- the sample volumes corresponding to the magnitudes of their volumetric feed rates were used for simulation of combustion of onyeama coal in a batch reactor model using the COMSOL reaction engineering lab software.
- These reaction rates were converted to suit the reactor model space using air to fuel ratio at a set tolerance level and initial temperature of 800K.
- lastly, time-based graphs of key indices such as combustion gas temperatures, specie concentrations and the calorific value of the coal with respect to time were plotted.

2.2 Development of Modelling Technique for a Batch Reactor

To model a batch reactor for this research work, the following assumptions were made. The rate constants used for the model were obtained from COMSOL software version 1.4, the number of kinetic constants and reaction pathways were obtained from Gri-Mech reaction scheme 2000.

2.3 Assumptions for a Zero Dimensional Model Batch Reactor

The following assumptions were made for the sample material and batch reactor in order for COMSOL software to process the combustion reaction:

- The gas mixture was perfectly mixed and behaved as an ideal gas
- The system was assumed to be an adiabatic one.
- The coal particles were assumed to be composed of ash, moisture, volatile matter and char.
- Particles were spherical in shape.
- The temperature of solid was uniform throughout the particles (i.e negligible temperature gradients)
- Pulverized carbon was in a near atomized state allowing for close approximation to a fluid state.

- Momentum balance was neglected.
- Gas phase oxidation reaction rates were determined by Arrhenius expressions.
- In the char particle oxidation model, char (carbon) was not included in the mass balance, hence, its consumption was not considered.
- To determine the composition of volatile gases, all of the non-carbon elements were assumed to be released during devolatilisation.
- Heat of pyrolysis was neglected.

III. Results and Discussion

3.1 The Effect of Reaction Time on Temperature

The result of temperature versus reaction time is shown in Fig. 1. It is evident that the reacting mixture through an exothermic process raises the temperature sharply and steadily from a temperature of 800K at 0.00s to a temperature of 3128.439K at 0.000199 s and a maximum of 3130K at 0.0004 s. It then experiences a slight drop to 3126.4K at 0.000199 s before proceeding at steady state conditions. The reason is probably due to the dominance of the endothermic reactions which absorb energy and, consequently, cause a drop in temperature (Hla *et al.,* 2009).

Both solid and gas phase temperatures increase when combustion of the volatiles and char takes place (Shen *et al*., 2006). Here, it has to be noted that gas phase combustion rates are determined by finite chemical reaction rates alone. Chemical reaction rates of gas phase oxidation are exponential so that rise of temperature and depletion of oxygen is very rapid. When all oxygen is consumed and exothermic oxidation reactions cease, the particle temperature starts to decrease (Shen *et al.,* 2006).

Therefore, it is necessary that materials that can withstand temperatures well over 3500K should be used for the design and construction of the model batch reactor to avoid material failure during the coal combustion process as the maximum temperature encountered in the combustion of Onyeama coal is 3130K.

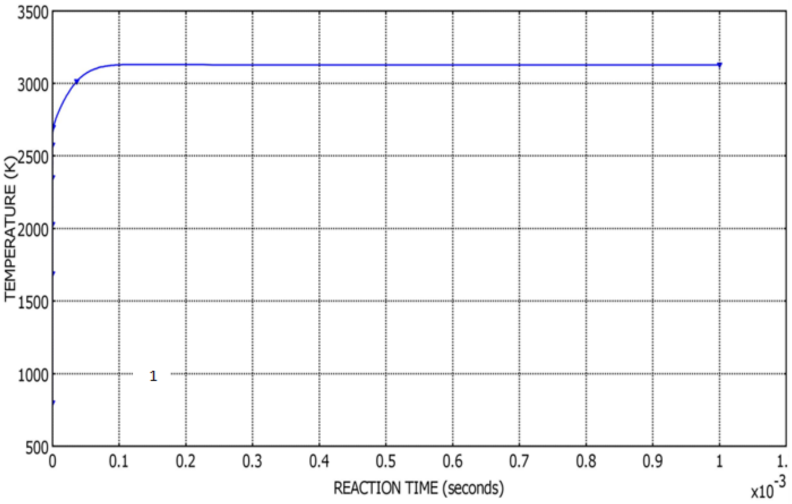


Fig. 1. Effect of Reaction time on temperature

3.2 The Effect of Reaction Time on Oxygen Depletion

The result of oxygen depletion versus reaction time is shown Fig. 2. The oxygen concentration drops from about 1.75 mol/m^3 at 0.00 s to about 0.67 mol/m^3 at 0.0001s. The sharp drop at the beginning of the reaction observed could be due to the high consumption of oxygen during the volatile species combustion and carbon combustion. The excess oxygen at the beginning shows that the oxygen was well in excess for this reaction.

When the coal feed rate is increased with the same gas flow rate, the amount of combustible volatile gas released during the pyrolysis process also increases. Therefore, the oxygen depletion rate is faster in the case of a lower stoichiometry as gas combustion processes are much faster than char combustion. CO and H_2 appear at the end of the combustion zone; consequently the point of depletion of O_2 is a measure of the start of the gasification zone.

In testing the oxygen concentrations in the batch reactor, more CO_2 is produced with higher oxygen concentration in the batch reactor. The CO_2 comes partly from the pyrolysis, partly from the char oxidation and partly from the oxidation of CO in the gas phase. The CO concentration was also high but it was quickly oxidized in the gas phase. The CO concentration is high with a low oxygen concentration in the batch reactor. The heat generation by char oxidation depends on the oxygen concentration in the batch reactor.

It was observed that, the greater the oxygen concentration in the batch reactor, the greater the char oxidation and the more the energy generated.

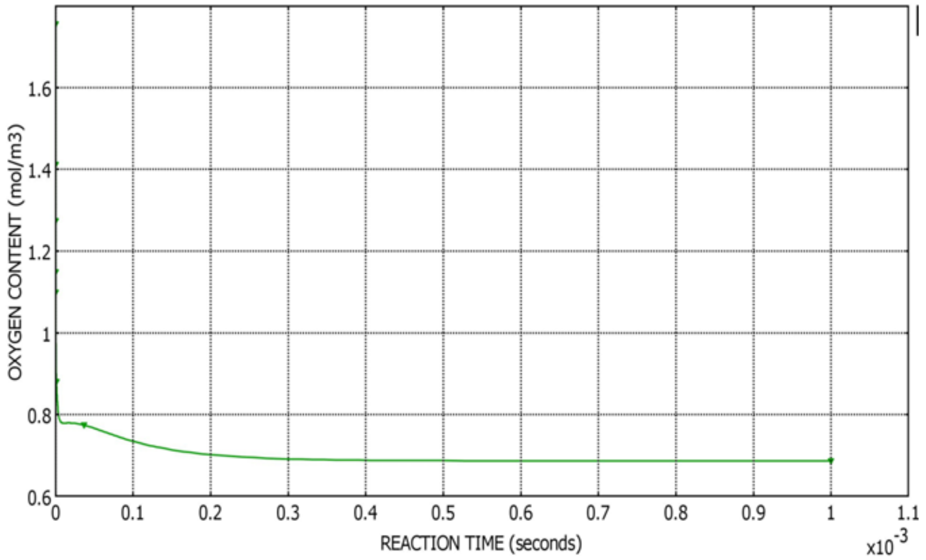


Fig. 2: Effect of Reaction Time on Oxygen Content

4.3 The Effect of Reaction Time on CO, NO_2, H_2O, CO_2, CH_4, and C_2H_6

The graph in Fig. 3 shows the effect of reaction time on volatile species and it is observed from it that the concentration of the NO_2 rises steadily to a maximum of $1.2 * 10^{-4}$ mol/m^3 out of a maximum total molar concentration of 8.354 mol/m^3. This translates to a 14,364 ppm concentration of NO_2 in the flue gas. This ratio remains at that level for steady state. This is well above the EPA (Environmental Protection Agency, USA) safe limits of ambient atmospheric concentrations for health and public safety of 0.053 ppm.

It can be seen from the graph in Fig. 3 that the concentration of CO reaches a maximum of 0.5 mol/m^3 out of a maximum total molar concentration of 8.354 mol/m^3. This translates into a 59,851 ppm concentration of CO in the flue gas. This ratio remains at that level for steady state. This is well above the EPA (Environmental Protection Agency, USA) safe limits of ambient atmospheric concentrations for health and public safety of 100 ppm.

The effect of the reaction time on the pollutants as the combustion progresses indicates that at 0.00 s, no pollutant is produced but as the combustion progresses to 0.001s (Fig.4), NO_2 amounted to 0.00001396 mol/m^3 (Fig. 5) while CO produced amounted to 0.491 mol/m^3 (Fig. 6). This indicates that more CO is produced at the early stage of the combustion. The values for H_2O, CO_2, CH_4 and C_2H_6 at 0.001 s are 0.2555 mol/m^3, 0.3999 mol/m^3, $2.95*10^{-15}$ mol/m^3 and $1.11*10^{-29}$ mol/m^3 respectively.

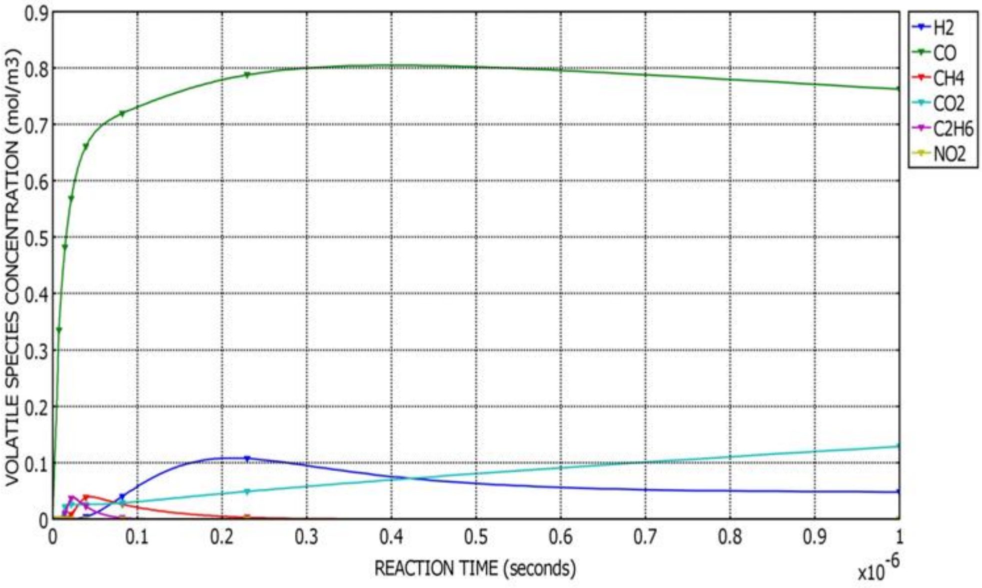


Fig.3:Effect of Reaction Time on Volatile Species from 0 to 10^{-6} s

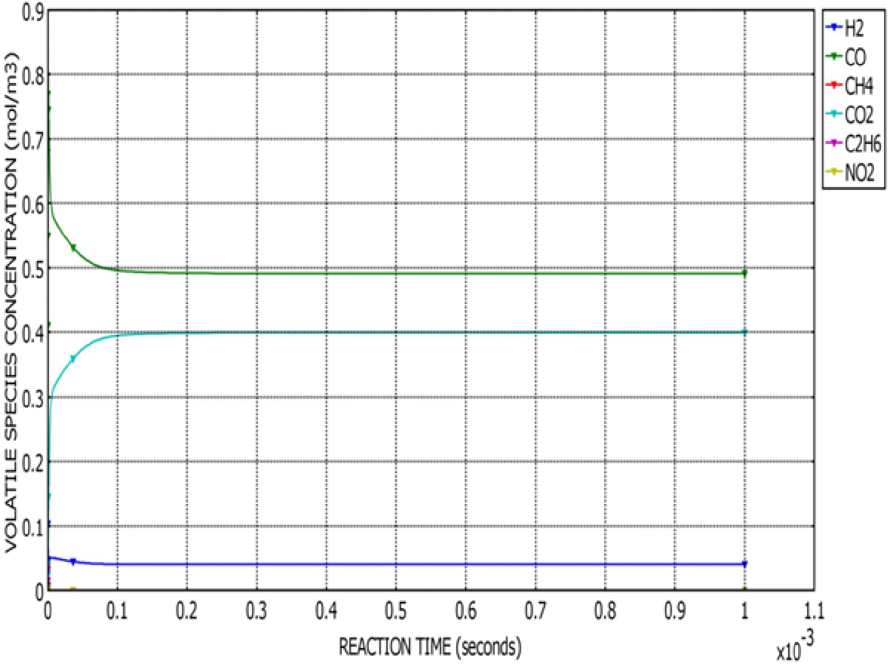


Fig.4: Effect of Reaction Time on Volatile Species from 0 to 10^{-3} s

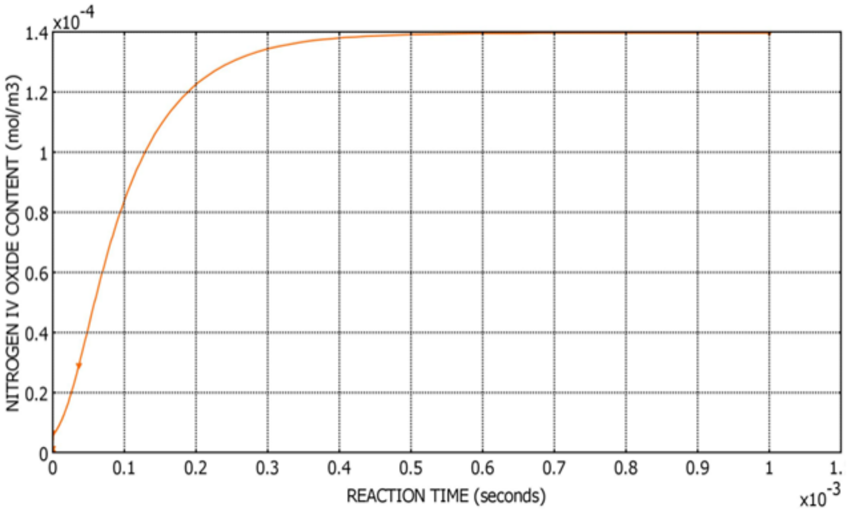


Fig.5: Effect of Reaction Time on Nitrogen IV Oxide Content

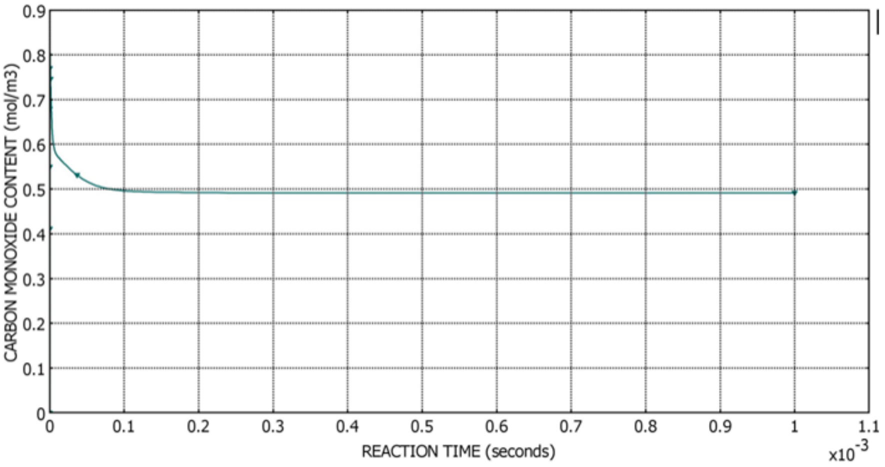
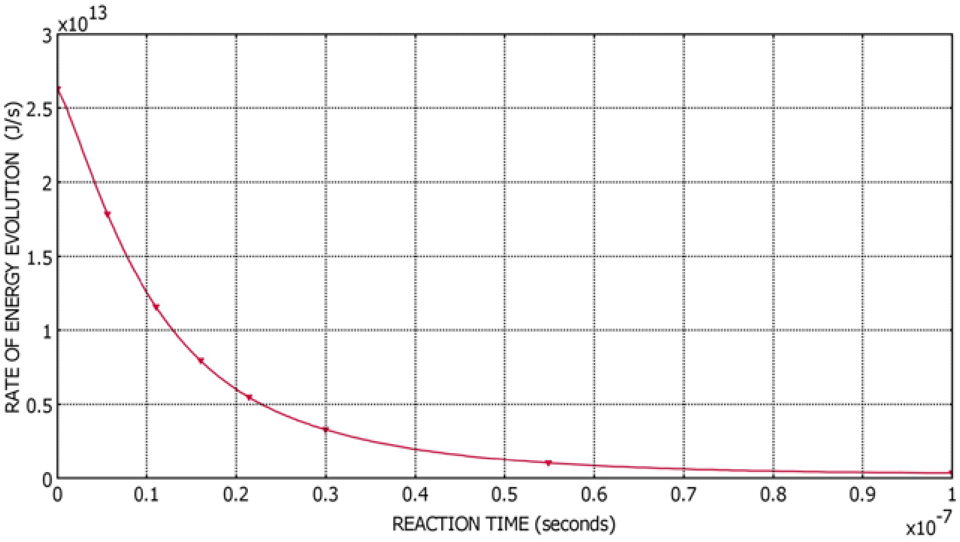


Fig.6: Effect of Reaction Time on Carbon Monoxide Content

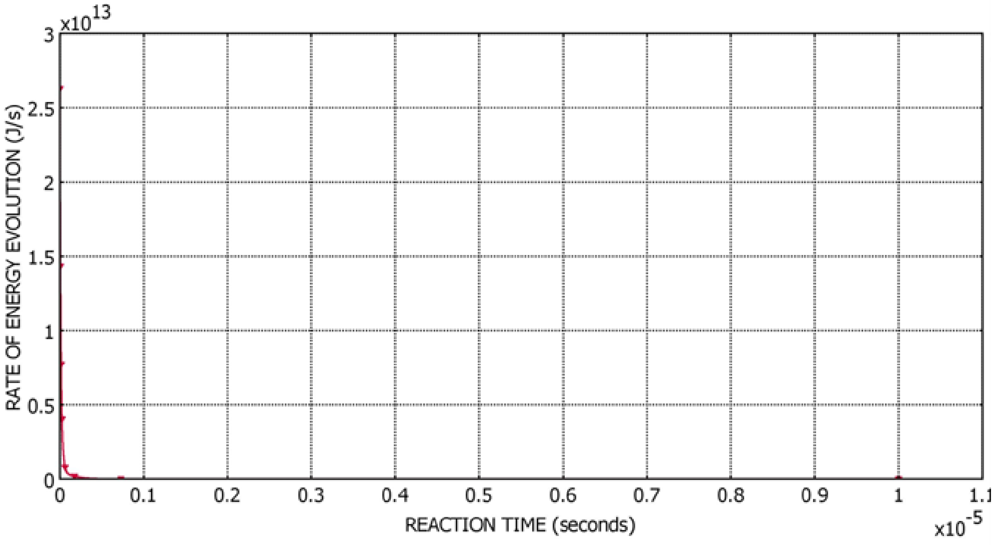
34 Effect of Reaction Time on Rate of Energy Evolution

The values in Fig. 7a,b and c show the effect of reaction time on energy content. The graphs show the effect of reaction time on energy content at different intervals and it can be seen that energy released is highest (i.e $2.6258*10^3$ at 0.00s) at the beginning of combustion and fluctuates as the combustion progresses. The rate of energy released drops slightly into the negative before the reaction reaches a steady state toward the end of the combustion. The reason for this negative value is because towards the end of the reaction as oxygen is being consumed and temperatures increase, the gasification reactions which are endothermic begin to dominate and hence keep absorbing energy (though relatively small amounts) from the reacting mixture(Hla *et al.*,2009).

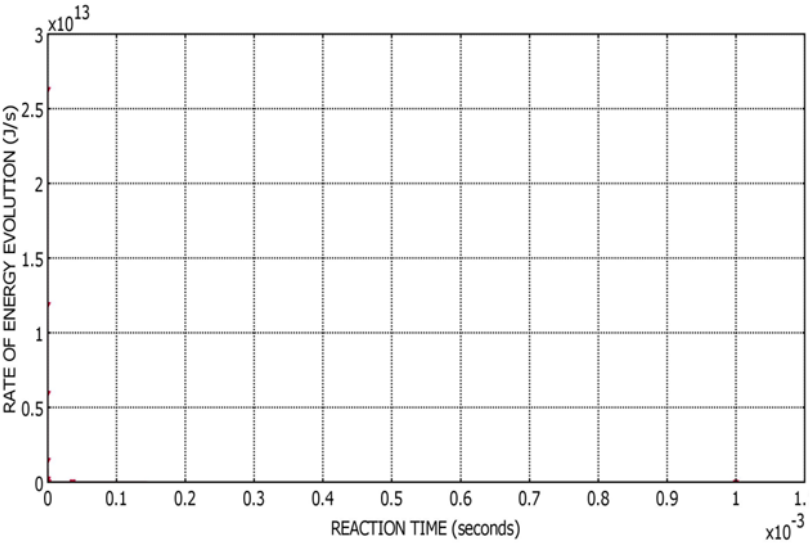
Hence there is a need to know when reaction should be stopped, which ultimately is a direct consequence of residence time. This will assist during design and operation that parameters used are adequate for maximum energy release. The graphs show a value of zero energy produced is reached at t = $1.44 *10^{-4}$s. Also that at $5.0 * 10^{-4}$s, energy produced had fallen to 0 J. Hence, total combustion is completed in $5 * 10^{-4}$s.



(a)



(b)



(c)

Fig.7: Effect of Reaction Time on Rate of Energy Evolution

IV. Conclusion

The simulation of combustion of Onyeama coal in a batch reactor using COMSOL MULTIPHYSICS model was carried out. From the maximum values of parameters such as temperature, reaction time and total energy released for Onyeama coal, it can be seen that the model has accurately predicted the maximum parameters of the Onyeama coal as:

- Energy released was highest (i.e $2.6258*10^3$ at 0.00s) at the beginning of combustion and fluctuates as the combustion progressed..
- At the reaction time of $5.0 * 10^{-4}$s, energy produced had fallen to 0 J. Hence, total combustion was completed in $5 * 10^{-4}$ s.
- Maximum combustion temperature was 3130K.
- At the end of reaction, CO produced amounted to 0.491 mol/m^3 while NO_2 amounted to 0.00001396 mol/m^3

The values for H_2O, CO_2, CH_4 and C_2H_6 at 0.0001s are 0.2555 mol/m^3, 0.3999mol/m^3, $2.95*10^{-15}$mol/m^3 and $1.11*10^{-29}$ mol/m^3 respectively

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