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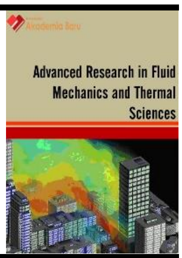

Mathematical Analysis and Thermal Modelling of a Pilot-Scale Pyrolysis Gas Furnace

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ABSTRACT

A numerical model for the thermal operations directly related to all significant heat and mass transfer within a designed furnace chamber was developed, taking into consideration the surface area of the internal structures and surrounding furnace walls of the furnace. Some specific sets of theories on the internal and external flow of heat energy in furnaces as well as boilers were adopted and modified to exhibit a steady-state condition model for the designed gas-fired pyrolytic furnace. Existing thermal models were selected and adjusted to arrive at a unique mathematical model that was used to analyse and verify the heat distribution at different regions of the built pyrolytic furnace with the aid of the basic principles of heat and mass transfer and the associated assumptions. The distinctive numerical model formed the basis for the MATLAB Simulink program used to validate the experimental data gotten from runs of heating and cooling of the pyrolytic furnace during operation. The result of the simulated behaviour of the furnace achieved a fit to the estimation of the data of 87.16% in correlation with the real experimental data. This established a thermal function that can be used as a model for potential optimisation of the pyrolysis process of the pilot furnace.

1. Introduction

To carry out scientifically oriented researches, it is always appropriate to build up a logical analysis. It is usually suitable to develop a scientific model to execute any meaningful analysis [1]. Scientific models are majorly divided into theoretical and experimental models. An experimental model can be defined as any form of imitation of a real system that can be examined for research purposes using a series of organised trials and methodologies [2]. While a theoretical model could be described as using mathematical equations and theorems to replicate and analyse a physical system

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[3]. Theoretical models can further be classified into either analytical models or mathematical models. The analytical model attempts to find an exact solution to a specific problem, while mathematical model endeavours to find an approximate solution limited to a satisfactory tolerance limit in terms of calculation time, as well as the precision of the result, obtained [4]. A mathematical model, also sometimes referred to as the numerical model, is a portrayal of a particular real system using mathematics [5]. The model enables logical inter-relationships and the phenomena occurring in a system to be expressed, which consequently makes it possible for the system to be analytically validated [6].

1.1 The Pyrolysis

Pyrolysis can be defined as the thermal decomposition of precursor materials at elevated temperatures in the absence of air [7]. Pyrolysis is irreversible, and it is an effective waste treatment method [8]. Products of pyrolysis: Carbon black and Graphite have critical engineering applications [9]. A furnace conceals the temperature of a heat source heat a material that must be subjected to high/controlled temperature [10]. The quality of the furnace depends on the quality of the distribution of the incubation temperature and how it can be controlled [11]. Pyrolysis can be fast or slow; fast pyrolysis, when the furnace rapidly raises the temperature to a predetermined temperature, and slow pyrolysis, when the heat increases over a very long time, both produce different types of materials [12-15]. The pyrolysis products can also be influenced by the type of the material being pyrolyzed [16,17] , temperature residency period [18], as well as the different types of catalysts present in the pyrolysis chamber [19-21].

1.2 The Physical and operational features of the Pilot Pyrolysis Furnace

The floor plan of the furnace has an auxiliary measurement of 0.8 m by 0.8 m, as shown in Figure 1. The pyrolysis furnace has a rectangular combustion chamber with a 0.3 m by 0.3 m square openings that cut the length of the furnace (i.e. 0.8 m) and is surrounded by 0.125 m thick refractory bricks. In the middle of the cubic space is a barrel-shaped chamber that is closed at both ends as an anaerobic chamber or a pyrolysis chamber [22]. The pyrolysis chamber is 1.2 m long and 0.17 m wide with a 3 mm carbon steel tube [22]. Two burners were placed along the length of the two-chamber. The use of oxygen enriched burners was ensured to attain excess air above stoichiometric air-fuel ratio, hence complete combustion leading to higher heating temperature and better the energy savings [23]. With the ultimate goal of limiting the rate of heat loss and thus ensuring optimum efficiency, heat-resistant kaolin bricks, about 12.5 cm thick, have been formed around the combustion chamber. Different types of furnaces that depend on the energy source: natural gas, electricity and liquid fuel, with emphasis on the means expected to reach the required temperature for the pyrolysis process. It is imperative to take into account the type of fuel to use [24]. The gas fire is generally a clean, affordable, accessible and efficient choice [25]. The furnace is controlled by regulating the combustion of the fuel. The choice of methane was guided by availability and competitive econometrics advantages. Ignition at the entry points of the gas serves as a source for the transition of the heat flow, then heat transfer takes place throughout the furnace with motions ranging from the end of heat concentration in the smallest area to 'to attain a state of equilibrium, provided that the limitation of heat is sufficient [26]. The thick layers of refractory blocks in the vicinity of the combustion chamber prevent heat loss to the environment along with the medium thus causing the heat to be retained and accumulated in the furnace [27].

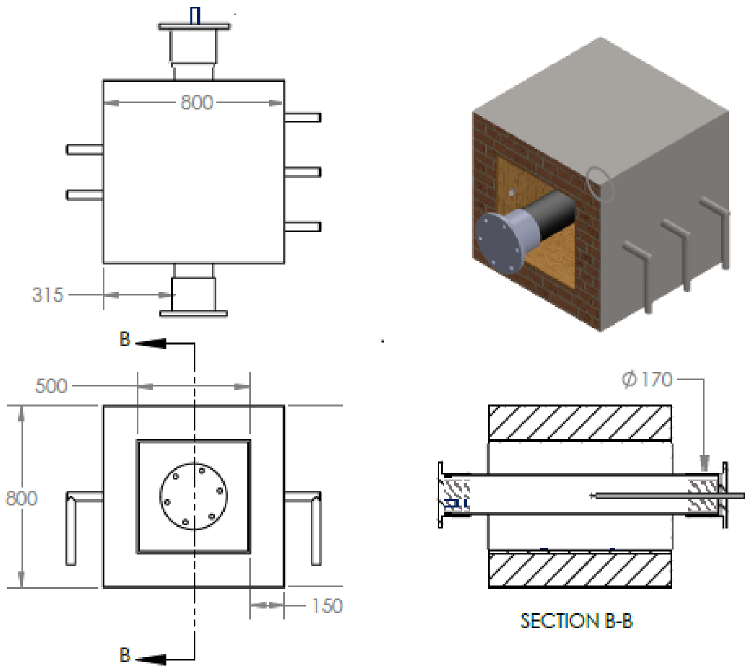

Fig. 1. Technical drawing of the model pyrolysis furnace [22]

2. Methods of Operation for the Pilot Pyrolysis Furnace

The principles of operation for the designed pyrolysis furnace (Figure 2) are conduction, convection, and radiation relating together at a level of complex interactions [28]. Thermal energy transfer in molecules due to energy gradient from more energetic to the less active region is usually referred to as conduction. The relation governing the phenomenon is Fourier's law and Navier stokes equation to inculcate momentum and continuity of conduction that leads to an exchange of energy from the high-temperature area to the low temperature [29]. Convection can be described as the energy transfer in fluid or gas due to the macroscopic motion. It is a combination of conduction and advection subject to an empirical relationship known as Newton's Law of Cooling. Convection occurs when the liquid molecules pass or flow through a physically solid body or channel due to temperature differences between the fluid phase and the body surface [28]. Thermal radiation can be summarised as an energy emission of a material due to changes in the configuration of the electron, the energy changing through photons. Radiation takes place without medium and it is being governed by Stefan Boltzmann [30]. This mode of heat transfer (radiation) is particularly pronounced in the pyrolysis chamber because the flame generated in the combustion chamber is fed into the container housing the precursors [31].

2.1 The Heat Transfer Model

As with the case with the present study involving a gas-powered pyrolysis furnace, any gas or fossil fuel furnaces usually undergo four independent but interactive processes, namely

i. The flow of fuel.
ii. Combustion taking place as a result of combusting fuel.
iii. Generation of heat energy: radiation, convection, conduction as a result of combustion.
iv. Mass Transfer; which involves processes like absorption of the heat by the host material, evaporation of liquid and gaseous components during the pyrolysis process and either deflection or absorption of heat by the refractory material.

The heat transfer in the furnaces can only occur if all these interactive processes are evident [28]. Each of these processes has some governing equations. It should be noted that full implementation of these theoretical analyses is complex and therefore probably inaccurate, as many assumptions can be made to represent the real-life conditions. Some underlying assumptions include uniformity in temperature of the interacting surfaces, an isothermal condition of operation, a uniform thermal conductivity and homogeneity of materials [15]. According to Li and Zhou, heat transfer in a combustion chamber can be expressed as

$$Q = k\Delta TA \quad (1)$$

where *k* is the heat transfer per square meter of a heating surface area *A* at which a temperature rise of one unit, i.e. 1°C, is present. This determines the intensity of the heat transfer process. ΔT represents the temperature difference.

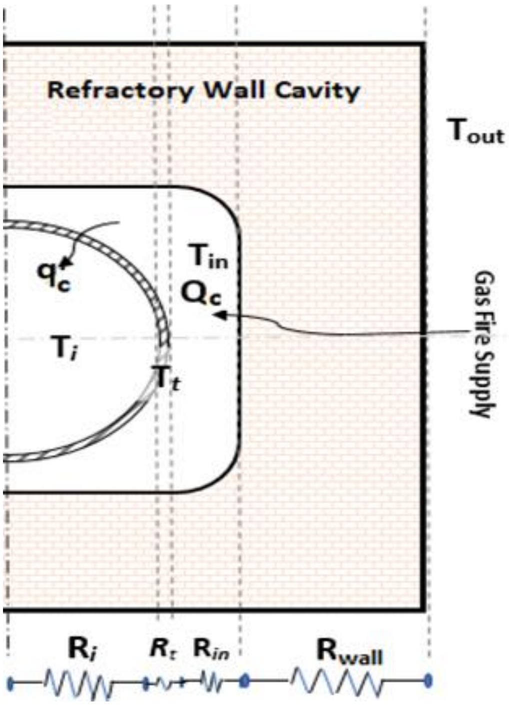

Fig. 2. Schematic representation of the Pyrolysis Furnace [22]

However, heat from a combusting gas to the furnace combustion chamber per kg of fuel is given as

$$Q_c = \frac{k\Delta TA}{B_{Cal}} \quad (2)$$

where B_{cal} = Burnt Fuel, where Q_c is the Heat as a result of the combusting gasses and the heat is meant to be transferred by convection to the precursor per Kg of the surface being heated by a unit of fuel; thus, the effect of Qc on the precursor is given by convection heating Surface for a unit surface

$$q_c = \frac{Q_c}{A} = k\Delta T \quad (3)$$

q_c = surface heat flux as a result of a particular mode of heat transfer. The higher the heat transfer coefficient, the more efficient the heat transfer process.

2.2 Heat Transfer Co-efficient (K)

For the designed pyrolysis furnace, the heat transfer coefficient is very similar to a convection process going on in a boiler. The heat is being transferred from hot gas to the target medium through the tube wall. The same principle applied to the model pyrolysis furnace is in a combination of three (3) significant processes.

i. Heat disbursed from the combusting gas dissipates into the combustion chamber.
ii. The heat is transmitted by conduction from the outer surface of the cylinder/capsule through the shell to the inner surface of the cylinder.
iii. The heat released from the inner surface of the capsule to the target matter.

The process is in the form of a general serial heat transfer method by which the released heat from the combusting gas outlet to the outer shell of the pyrolysis capsule (through the combustion chamber) includes convection and radiation. In the same vein, the transferred heat from the capsule's outer shell to the inner surface is purely conductive, and finally, the transferred heat from the inner shell of the cylinder to the precursor is purely convective nature [32].

3. Heat Flow Through the Refractory Material of the Furnace

For a 1D conduction occurring in a flat wall, the heat transfer occurs in x-coordinate direction only. From Figure 3, heat transfer by convection is from a hot region of temperature, $T_{\infty 1}$ to the inner surface of the wall to drop to a lower temperature, T_{S1}.

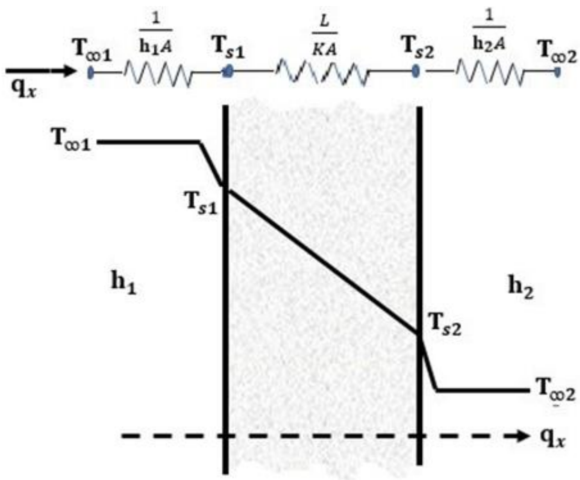

Fig. 3. 1D Heat transfer model prediction through the pilot furnace refractory wall; showing both the temperature profile and the equivalent thermal circuit [32]

The heat again is being transferred through the solid wall to emerge at the opposite surface at a further lower temperature, T_{S2} only by conduction and finally, the heat at the inner surface of the furnace wall emerges to the environment at another temperature $T_{\infty 2}$ of much lower magnitude by convection. It can be deduced that the progressive decrease of the temperature through the subsystems are due to either energy lost to enthalpy or energy retained in such subsystem [33].

3.1 Assumptions

i. Heat flux is constant and independent of x.
ii. The thermal conductivity of the subsystems is constant,
iii. No generation of heat within the media [32].

According to Incropera *et al.,* the appropriate form of the heat equation Eq. (3) can be integrated twice to obtain a general solution

$$\mathrm{T}_{(x)} = \mathrm{C}_1 x + \mathrm{C}_2 \tag{4}$$

Boundary Conditions: Taking x = L, i.e. length at which the q_x (energy) travelled $\mathrm{T}_{(0)} = \mathrm{T}_{s1}$ and $\mathrm{T}_{(x=L)} = \mathrm{T}_{s2}$

Temperature distribution

$$\mathrm{T}_{(x)} = (\mathrm{T}_{s2} + \mathrm{T}_{s1})\frac{x}{L} + \mathrm{T}_{s2} \tag{5}$$

Now using Fourier's Law, heat rate is

$$\mathrm{q}_x = -\, k\mathrm{A}_w \frac{dt}{dx} \tag{6}$$

$$\mathrm{q}_x = \frac{K\mathrm{A}_w}{L}(\mathrm{T}_{s1} + \mathrm{T}_{s2}) \tag{7}$$

Given: A_w as the plane wall's area, normal to the heat Transfer direction and of course it is constant and independent of x. For x = 0 and x = L as boundary conditions. The heat flux becomes

$$\mathrm{q}_x{}^n = \frac{\mathrm{q}_s}{L} = \frac{K}{L}(\mathrm{T}_{s1} + \mathrm{T}_{s2}) \tag{8}$$

Some other considerations are as listed
i. Fourier equation is valid for all matter at any state of solid, liquid or gas.
ii. The vector expression indicating that heat flow rate is normal to an isotherm and is usually in the direction of decreasing temperature.
iii. It cannot be derived from the first principle.
iv. It helps to define the 'k' [34].

3.2 Heat Conservation Process of the Furnace Refractory

Resistance is the ratio of driving potential to the corresponding rate of transfer. Thermal resistance is similar to an electric resistance in behaviour. Therefore, the principle of Ohm's law is applicable. Thermal resistance for conduction going on in a plane body can be given as

$$\mathrm{R}_{tCond.} = \frac{(\mathrm{T}_{s2} - \mathrm{T}_{s1})}{q} = \frac{L}{KA} \tag{9}$$

By Ohm's law

$$R_e = \frac{(E_{s1} - E_{s2})}{I} = \frac{L}{\delta A} \tag{10}$$

From Newton's law of cooling

$$q = hA\,(T_{s1} + T_{s2}) \tag{11}$$

Then thermal Resistance for connection 0 is then

$$R_{tConv.} = \frac{(T_s - T_\infty)}{q} = \frac{1}{hA} \tag{12}$$

The heat transfer rate is now defined from separate considerations of each element in the network. q_x is a constant

$$q_x = \frac{(T_{\infty 1} - T_{s1})}{\frac{1}{h_1 / A}} \tag{13}$$

$$q_x = \frac{(T_{s1} - T_{s2})}{\frac{L}{KA}} \tag{14}$$

$$q_x = \frac{(T_{s2} - T_{\infty 2})}{\frac{1}{h_2 A}} \tag{15}$$

In terms of overall thermal different; $T_{\infty 1} - T_{\infty 2}$ moreover, total thermal resistance.

$$R_{Total} = \frac{(T_{\infty 1} - T_{\infty 2})}{q_x} \tag{16}$$

4. Heat Transfer Rate

The expected temperature distribution of any thermal system, in this case, the pyrolysis furnace, can be determined from the energy balance equation i. e "The rate of thermal conduction on all sides + the rate of heat generation inside = heat transfer rate." Because Conductive and Convective Resistances are established to be in series, it follows that

$$R_{Total} = \frac{1}{h_1 A} + \frac{L}{KA} + \frac{1}{h_2 A} \tag{17}$$

If the Conventional coefficient of the Heat Transfer is relatively small, then the Radiation heat exchange between the surface and the surroundings will become very significant. For natural convection in a gas, the coefficient of the Heat Transfer is usually small. A thermal Resistance in a radiation process may be defined as

$$R_{t,rad} = \frac{(T_\infty - T_{sur})}{q_{rad}} = \frac{1}{h_r A} \tag{18}$$

For radiation process taking place between a vast surrounding, h_r, and surface radiation. Surface radiation and convection resistance act in parallel to each other and if $T_\infty = T_{sur}$; then they combine to become a single and active surface resistance [31]. Figure 4 shows the test-running the model pyrolysis furnace.

Fig. 4. Test-Running the model pyrolysis furnace [35]

5. Model Analysis

Simulation is an exercise that follows a technique or set of techniques to study a particular dynamic behaviour of models [36]. A simulation package was contracted to investigate and validate the mathematical model that had been developed in this study. MATLAB/Simulink is one of the most efficient software for designing thermal models [37]. Inference from the principle of heat and mass transfer as itemised earlier indicated that the design of the components of the pyrolysis furnace has effects on energy loss due to the convection, conduction, and radiation, which also resultantly has effects on the effectiveness and efficiency of the pilot-scale pyrolysis model. The temperature profiles inside the pyrolysis furnace are solved using finite difference Simulink in a MATLAB programming by entering the necessary boundary conditions as highlighted in Figure 5. The details of the conditions are as enumerated in Table 1 below.

The analytical analysis based on the MATLAB Simulink output showed the disparity and similarity in the thermal generation and retention of the furnace. The results in graphical form (Figure 6) represents the thermal behaviour of the model furnace. The transient conduction graphical user interface (GUI) an installed widget was utilised by loading the experimental data into the interphase to provide a solution to the transient heat transfer problem and graphically presenting salient features as shown in Figure 6 and 7.

Table 1
MATLAB/Simulink parameters

Boundary Conditions	Geometry	Time-Convergence	Computation
L/R/T/B 700/700/800/600 Celsius Temp. Init. 40 degree Celsius (Initial Temperature) Temp. Opt. 480 degree Celsius (Optimum Heating Temperature)	x/y/dx/dy .225/.225/.02/.02 m	Dt/total time/ convergence criteria 1/3600/Ie-4	Air Medium Compared with Real life scenario

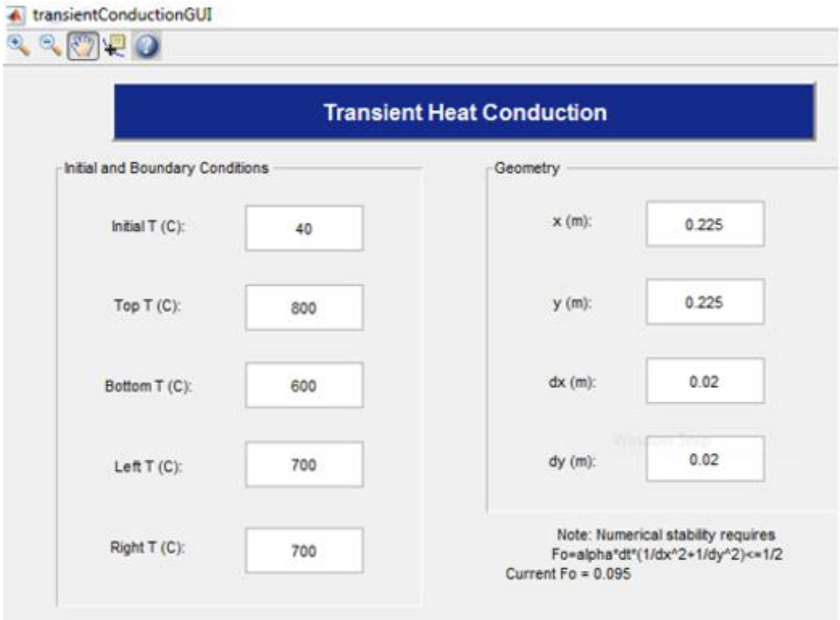

Fig. 5. GUI for setting boundary conditions transient heat conduction of the pyrolysis furnace

Figure 6 displays the graph of a cumulative of Input U1 (T1) and Output Y1 (T2) Signal over four runs of fast Pyrolysis process against Pyrolysis Time (t), heating up to 480°C within 60 mins. The input (U1) shows in the graph the pattern of heat supplied into the furnace through the heat source using the propane gas combustion. While the Output (Y1) graph is the accumulated temperature in the pyrolysis chamber as a result of energy gained from Input (U1). Figure 7 is the graph displaying the measured Output Y1 (T2) plotted against Pyrolysis Time (t). Also, on the same graph is represented two different types of simulated Output; one using State Space Models 1 (SS1) and the other using one using State Space Models 2 (SS2). Both SS1 and SS2 are continuous-time identified state-space model but with different transfer functions. The transfer function characteristics of the model are as highlighted below.

- From input "u 1" to output "y 1":
  - (0.02 z^- 1)/ (1 – 1.488 z^ - 1 + 0.5057 Z^ - 2)
    - Discrete-time identified transfer function
    - Sample time: 1 second.
- Parameterisation
  - Number of poles: 2 Number of Zeros
  - Number of free coefficients: 3
  - Number of iterations: 12
  - Number of function evaluations: 25
- Estimated using TFEST on time domain data "furnacedata".
    - Fit to estimation data: 87.16%

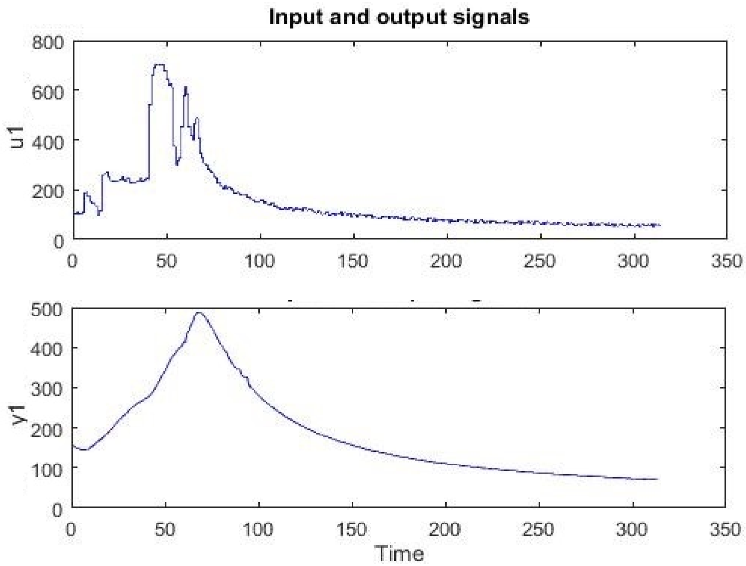

Fig. 6. Graph Showing a cumulative of Input U1 (T1) and Output Y1 (T2) Signal over four runs of fast Pyrolysis process against Pyrolysis Time (t)

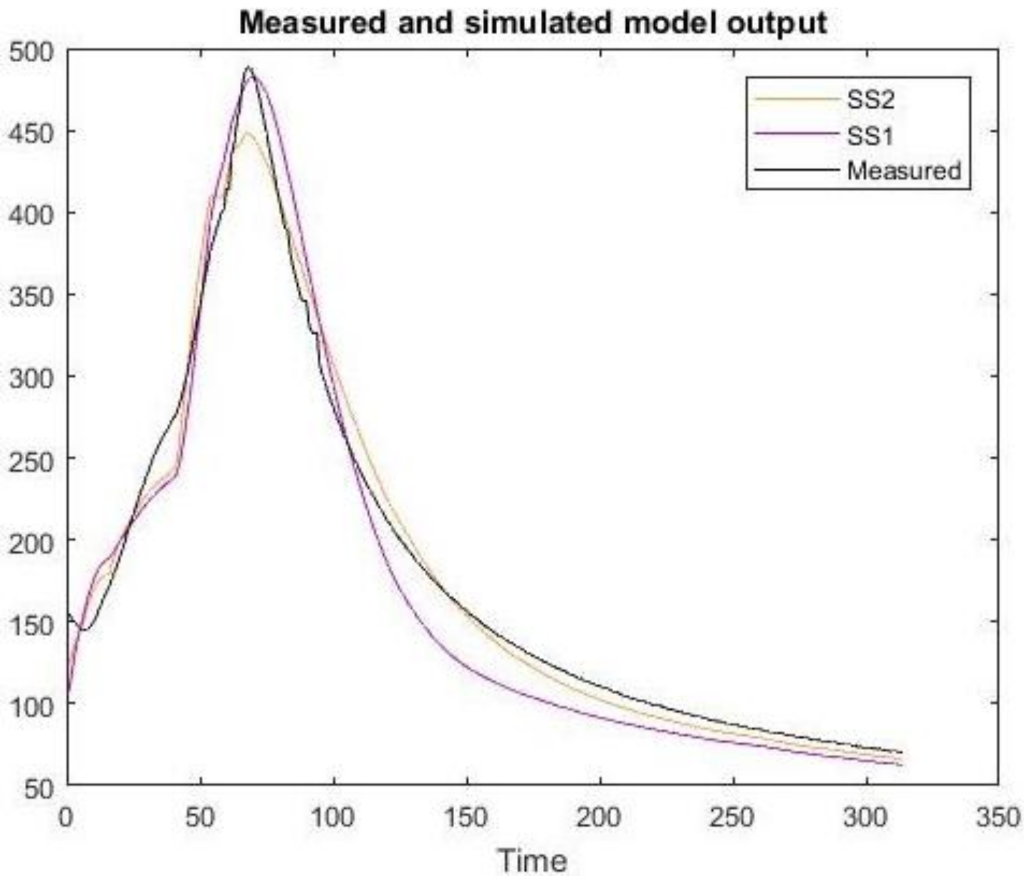

Fig. 7. Graph Showing the measured Output Y1 (T2) plotted with the Simulated Output using State Space Models 1 (SS1) and 2 (SS2) against Pyrolysis Time (t)

The efficiency of a furnace is mainly determined by its ability to minimize heat loss. keeping in mind that the quantified loss is considered as heat that escapes from the surface of the furnace body into its immediate environment by natural convection and radiation [38]. From the result of the MATLAB simulation displayed above, the transfer function was given as

(0.02 z^- 1)/ (1 – 1.488 z^ - 1 + 0.5057 Z^ - 2)

Likewise, a T-test was conducted on the data fed into the software. The statistical T-test result carried out was output as TFEST which is equal to 87.16% fit to the estimation. Figure 8 shows the simulated temperature gradient over x and y directions of the furnace from the outer wall of the furnace to the centre of the furnace which is usually the hottest as a result of heat transfer in the pyrolysis furnace at a pyrolysis time, t = 1450seconds.

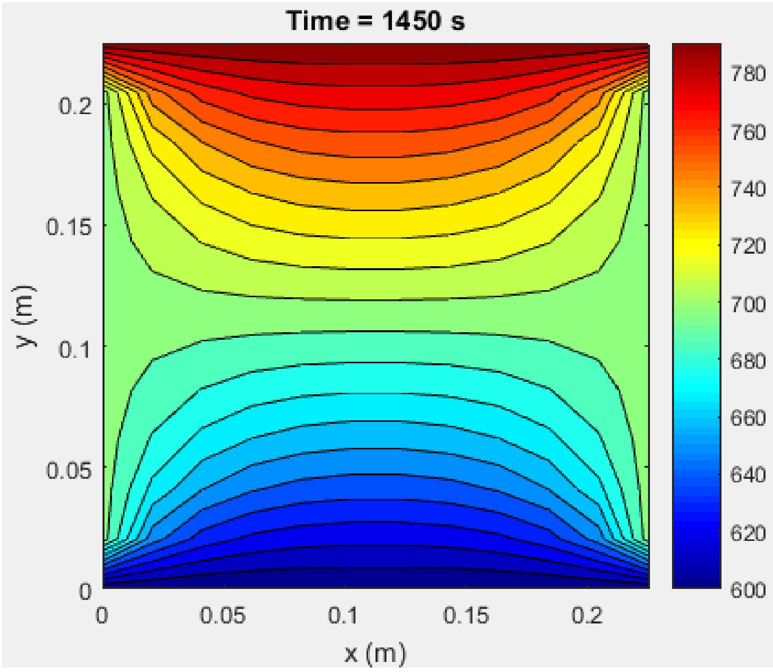

Fig. 8. Graph Showing the snapshot of heat transfer over x and y directions representing a specific temperature distribution pattern in the pyrolysis furnace at a pyrolysis time, t= 1450 seconds

6. Conclusions

The study produced a thermal model for the heat transfer and temperature distribution profile for a batch loading operation in the pilot pyrolysis furnace constructed for the production of an intended product from all of the precursors of carbon. The mathematics of thermal modelling had been used to develop a model that describes the heat distribution in different regions of the pyrolytic furnace with the aid of the basic principles of heat and mass transfer. Although the thermal model expressed an approximate solution that is limited to an adequate margin of tolerance in terms of computation time and accuracy of the result obtained. Some certain assumptions were made to be able to surmount the complex nature of the real-life model of the pyrolysis furnace. MATLAB Simulink, simulation software was used to analyse, validate and verify the heat distribution at different regions of the pyrolytic furnace using the experimental data gotten from runs of heating and cooling of the pyrolytic furnace during operation. The fit to the estimation of the data achieved was 87.16% which shows that the result of the model can be used to facilitate the monitoring of temperature at the required interval to ensure optimisation of the operational conditions of the furnace and consequently optimising the control over the quality of the products.

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Conflict of Interest
The authors declare no conflict of interest.

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