NUMERICAL DESIGN MODEL OF FURNACE REACTOR FOR ETHANE CRACKING

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Abstract

Appropriate design models for typical furnace reactor for cracking of 100% ethane feed has been developed. The research considers the radiation, convective, pressure drop effect and composite heat balance on the convective and radiation zones of the reactor operations. Principles of material and energy balances and pressure effects from the flow of feed material from the convective section to the radiation zone were incorporated into lumped-design model equations. The models were resolved applying numerical ode 45 to generate the profiles on conversion along the length of reactor, pressure drop effects and energy balance which were compared with plant data of Indorama Eleme petrochemicals complex to validate the dynamics in the reactor in figures 1,2,3, 4,5,6,7,and 8.The pressure effects profile of the reactor operation at steady states showed a quasi-flat shape at 30-45% conversion to constant pressure drop as depletion process progressed to 65% upwards.

Keywords: *Furnace Reactor, Radiation-Convection Sections, Cracking, Heat Balance Radiation-Convection, Design Model, Numerical.*

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1. INTRODUCTION

In Petrochemical industry, furnace reactor is the fundamental equipment for the cracking of ethane to yield ethylene. Ethylene production is one of the largest sectors and is the building blocks in manufacturing of petrochemicals. Notably among the olefins produced is ethylene whose worldwide production in 2012 (109 million tons in 2008) exceeds that of any other organic compound. Ethylene can also be synthesized by dehydrogenation of ethane. It is worthy to note that the dehydrogenation processes of ethane are expected to play a large role in the future production of ethylene since ethane is an abundant component in natural gas which is an alternate resource to traditional petroleum [3]. The furnace reactor consists of long coiled radiant tubes placed vertically inside a rectangular gas-fired furnace. The tubes are hung vertically to allow for expansion and to avoid sagging, consequently lengthening tube life. The furnace reactor system consists of the convection and radiation zones. The feedstock which is usually light hydrocarbons like ethane, ethane-propane mixtures or naphtha first enters the convection zone where it is pre-heated to about 500-800^{0}c and any liquid vaporized before it enters the radiation zone where pyrolytic reactions takes place, inducing numerous free radical reactions. The products from the reactor are immediately quenched to stop these reactions. First, pyrolysis of ethane gives rise to some carbon (coke) formation. This coke deposition increases pressure drop and inhibits heat transfer up to a point where stops for mechanical cleaning are mandatory.

Furthermore, the energy change associated with the process is endothermic and consequently, requires huge energy. However, once started the energy efficiency is high as heat energy recovered from the cracked gas is used to make high pressure stream. This steam is in turn used to drive the turbines for compressing the cracked gas, propylene refrigeration compressor and the ethylene refrigeration compressor [8].
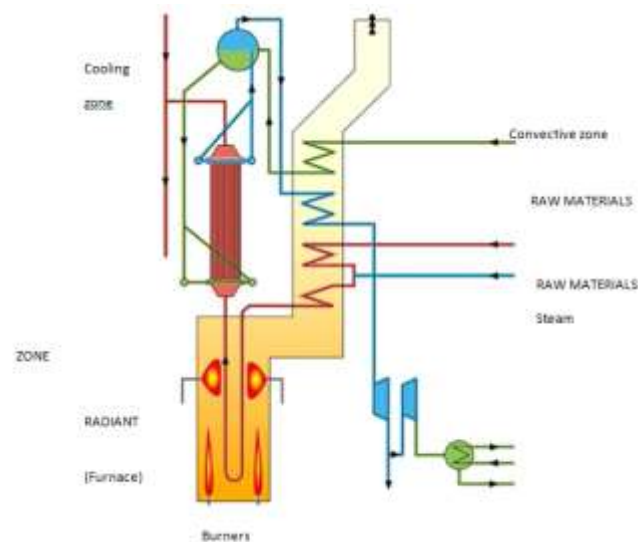

Fig 1: Schematics of atypical ethane furnace reactor

1.1 Process Concept of Furnace Reactor

The reactor is identified to comprise of two major sections of cracking reactions, radiation and convective zones. The kinetics and convective forces of ethane cracking process is essentially coupled in the numerical computer model for investigative study. Literature have shown that research

have been carried out on the radiation section [1], but did not consider convective section forces on the cracking process and the pressure drop along the reactor. The observed gap in the previous research forms the main frame-work of the present research.

2. MATERIALS AND METHOD

The furnace reactor is modeled as a tubular reactor. Design equations for predicting material and energy interchange in the reaction zone of the reactor as well as equation accounting for pressure drop along the reactor length were developed. Radiation and convective heat transfer equations were established to account for temperature effects in the convective zone of the reactor and then coupled with the overall energy balance of the reactor system.

2.1 Process Chemistry

Pyrolysis of ethane is represented essentially by the irreversible first order chemical reaction equation in the temperature range of 900 to 1200K.

The stoichiometric balanced equation for ethane cracking process in furnace reactor is kinetically stated as [7]

$$C_2H_{6(g)} \rightarrow C_2H_{4(g)} + H_{2(g)} \qquad (1)$$
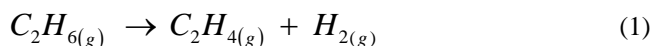
A pure ethane is fed at known inlet temperature and pressure to a steel tube contained in an ethane pyrolysis furnace. Heat is supplied by the furnace to the reactor. At temperatures of about 980–1200°C, C-H bonds of ethane molecules dissociates such that ethylene and hydrogen are produced as major products. Conversion of ethane to ethylene can be as high as 65-70%. Thermodynamic properties such as standard heat of formation (ΔH^0_{298}), Specific heat capacity (Cp) and related kinetic data for chemical species associated with the reaction equation (1) above is as shown in table (1) below [6]

Table1. Physical Properties and data for ethane pyrolysis reaction

Component	ΔH^0_{298} (KJ/Kgmol)	C_p (KJ/kgmolk)
A = C_2H_6	- 83820	14.1504+7.549x10^{-2} T-1.799 x 10^{-5} T^2
B = C_2H_4	52510	1.839 + 1.19167 x 10^{-1} T – 3.6515 x10^{-5} T^2
C = H_2	0.00	27.012 + 3.5085 x 10^{-3}T + 6.9 x 10^{4}T^{-1}
Reaction rate constant: $$k = 4.717 \, x \, 10^{14} \, Exp(\frac{-36354.6}{T})$$ Atomic weights: C = 12, H = 1 Gas Constant (R): $$8.314 Kpa.m^3 / kgmol.K$$		

2.2 Material Balance

The furnace reactor is modeled as a plug flow reactor. The approach involves establishing the steady state material balance over a differential volume element (dV$_R$) of reactor length (dz), as shown in figure (1) below. Basis is a mole of ethane.
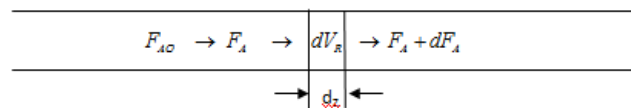

Fig 2: Differential Element Of Tubular Reactor

Taking a balance for 1 mole of fresh feed of ethane A over the differential reactor volume (dv$_R$); rate of inflow of feed into differential volume element F$_A$ equal to rate of outflow of feed from differential volume element $F_A + dF_A$ minus rate of depletion of feed due to chemical reaction within differential volume element $(-r_A)dv_R$ and rate of accumulation of feed within volume element at steady state process gives equation (2),

$$F_A = (F_A + dF_A) + - r_A \, dv_R + 0 \qquad (2)$$

$$\therefore F_A + r_A \, dv_R = F_A + dF_A$$

$$\therefore r_A \, dv_R = dF_A \qquad (3)$$

The differential reactor volume element (dv$_R$) is related to the differential reactor length by;

$$dv_R = Adz \qquad (4)$$

By substituting equation (4) into (3) and rearranging, we obtain;

$$\therefore r_A = \frac{dF_A}{dv_R} = \frac{d[F_{AO}(1-\alpha_A)]}{Adz}$$

$$\therefore r_A = - \frac{F_{A0}}{Adz} d\alpha_A \qquad (5)$$

For a first-order irreversible reaction, the kinetic rate equation is given mathematically;

$$-r_A = K_1 C_A \qquad (6)$$

At low pressure (P < 5 bar) of the reacting gas mixture, the gas law

$$P_A V_A = n_A R T_R \qquad (7)$$

$$\frac{n_A}{V_R} = C_A = \frac{P_A}{R T_R} \qquad (8)$$

$$\therefore \quad C_A = \frac{P_A}{RT_R} \qquad (9)$$

From Daltons' Law;

$$P_A = y_A P_{TOt.} \qquad (10)$$

By substituting equation (9) into (8) we obtain;

$$C_A = \frac{y_A P_{Tot.}}{RT_R} \qquad (11)$$

Substituting (10) into (6) we obtain the rate equation

$$r_A = -K \frac{y_A P_{Tot.}}{RT_R} \qquad (12)$$

Hence, determine the mole fraction of ethane (y_A), mole balance of the reacting species with respect to differential volume element figure 1 is shown in table 2 below;

Table 3. Mole balance for the reacting species

Component	Inlet molar flow rate	Outlet molar flow rate at conversion x
A = C_2H_6	F_{AO}	$F_{AO}(1-\alpha_A)$
B = C_2H_4	0	$F_{AO}\alpha_A$
C = H_2	0	$F_{AO}\alpha_A$
TOTAL	$F_{TO} = F_{AO}$	$F_T = F_{AO} + F_{AO}\alpha_A = F_{AO}(1+\alpha_A)$

Hence, mole fraction of ethane (y_A) is given by;

$$y_A = \frac{molar\ flow\ of\ ethane}{Total\ molar\ flow\ of\ gas} \qquad (13)$$

$$y_A = \frac{1-\alpha_A}{1+\alpha_A} \qquad (14)$$

By substituting equation (13) into (10), we have:

$$r_A = -K\left(\frac{1-\alpha_A}{1+\alpha_A}\right)\frac{P_{Tot.}}{RT_R} \qquad (15)$$

By equating (5) and (14) we obtain;

$$r_A = -\frac{F_{AO}}{A}\frac{d_X}{dz} = -K\left(\frac{1-\alpha_A}{1+\alpha_A}\right)\frac{P_{Tot.}}{RT_R}$$

$$\therefore \quad \frac{d\alpha_A}{dz} = K\left(\frac{1-\alpha_A}{1+\alpha_A}\right)\frac{P_{Tot.}}{F_{AO}RT_R} \qquad (16)$$

Hence the conversion X_A as a function of reactor length z is defined by the solution of the first order ordinary differential equation (15).

From the Arrhenius Equation;

$$K_1 = A_1 Exp\left(\frac{E}{RT_R}\right) \qquad (17)$$

and by using data from table (1) we have;

$$K_1 = 4.717\ x\ 10^{14}\ Exp(-\frac{363546}{T}) \qquad (18)$$

Substituting equation (17) into (15) yields;

$$\frac{d\alpha_A}{dZ} = \left[\frac{4.717\ x\ 10^{14}\ AP_{Tot.}}{F_{AO}R}\right]\left[\frac{Exp(-\frac{363546}{T_R})}{T_R}\right]\left(\frac{1-\alpha_A}{1+\alpha_A}\right)$$

$$(19)$$

For a given tube internal diameter, reactor pressure, and inlet ethane flow rate the term $\frac{4.717\ x\ 10^{14}\ AP_{Tot.}}{F_{AO}R}$ is constant and the other term $\frac{Exp\left(-\frac{363546}{T_R}\right)}{T_R}$ is dependent on temperature.

3. ENERGY BALANCE

The energy balance over the differential volume (dv_R) element accounts for heat of reaction, heat transfer from furnace to the tube wall and sensible heat effects in the following gas stream.

The overall energy balance with respect to the differential volume element of the reactor is given by the fundamental equation below [5], [2].

$$\begin{bmatrix} Rate\,of\ Inflow\ of\ energy \\ Into\ differential \\ volume\ element \end{bmatrix} = \begin{bmatrix} Rate\ of\ outflow\ of \\ energy\ from \\ differential\ volume \\ element \end{bmatrix} - \begin{bmatrix} Rate\ of\ generation\,of \\ energy\,due\,to\ chemical\ reaction \\ within\ differential \\ Volume\ Element \end{bmatrix} + \begin{bmatrix} Rate\ of\ accumulation' \\ of\ energy\ within \\ differential \\ Volume\ element \end{bmatrix} \quad (20)$$

Where;

(i) Rate of inflow of energy into differential volume element is given by; qdz

(ii). Rate of outflow of energy from differential volume element is given by;

$$\Delta H_{T_R} = \left[F_A C_{PA} + F_B C_{PB} + F_C C_{PC} \right] dT_R \qquad (21)$$

Where:

A	C_2H_6
B	C_2H_4
C	H_2

But,

F_A = $F_{AO}(1-\alpha_A)$

F_B = $F_{AO}\,\alpha_A$

F_C = $F_{AO}\,\alpha_A$

Substituting into equation (21) gives

$$\Delta H_{T_R} = \left[F_{A0}(1-\alpha_A)C_{PA} + F_{AO}\alpha_A(C_{PB}) + F_{AO}\alpha_A C_{PC} \right] dT_R$$

$$\Delta H_{T_R} = \left[F_{A0}(1-\alpha_A)C_{PA} + F_{AO}\alpha_A(C_{PB}+C_{PC}) \right] dT_R$$

$$\therefore \Delta H_{T_R} = F_{AO} \left[(1-\alpha_A)C_{PA} + \alpha_A(C_{PB}+C_{PC}) \right] dT_R \qquad (22)$$

(iii) Rate of generation of energy due to chemical reaction within differential volume element is given by;

$$F_{AO} \left(-\Delta H_R \right) d\alpha_A \qquad (23)$$

Substituting F_A, F_B, and F_C values into (19), we obtain;

$$F_{A0} d\alpha_A \left(1-\Delta H_R \right) + qdZ = F_{AO} \left[(1-\alpha_A)C_{PA} + \alpha_A(Cp_B+C_{PC}) \right] dT_R \qquad (24)$$

By dividing through equation (21) by dz and F_{AO}, then the change in temperature as a function of length is described by the first order ordinary differential equation.

$$\frac{(-\Delta H_R)d\alpha_A}{dZ} + \left(\frac{q}{F_{AO}} \right) = \left[(1-\alpha_A)C_{PA} + \alpha_A(C_{PB}+C_{PC}) \right] \frac{dT_R}{dZ} \qquad (25)$$

Making $\dfrac{dT_R}{dZ}$ subject of equation;

$$\frac{dT_R}{dZ} = \frac{\left[\dfrac{q}{F_{AO}} \right] + \dfrac{(-\Delta H_R)d\alpha_A}{dZ}}{(1-\alpha_A)C_{PA} + \alpha_A(C_{PB}+C_{PC})} \qquad (26)$$

Where:

$$q = q_{c} + q_R \qquad (27)$$

The convective zone of the reactor preheats the feed to a temperature T_C. Heat from the flue gas of the furnace is transferred to the feed in two stages;

(1) Conductive heat transfer of heat from flue gas to internal surface of convective tube described by the equation;

$$\frac{dq}{dA} = \frac{K}{\Delta d} \left[T_{FG} - T_i \right] \qquad (28)$$

(2) Convective heat transfer of heat from internal surface of tube to the feed gas described by the equation;

$$\frac{dq}{dA} = hi \left[T_C - T_i \right] \qquad (29)$$

At steady state, heat transferred by conduction from flue gas to convective tube wall equals convective heat transferred from the tube wall to the flowing gas stream. Hence, by equating equation **(28)** to **(29)** we obtain;

$$\frac{dq}{dA} = \frac{K}{\Delta d} \left[T_{FG} - T_i \right] = hi \left(T_C - T_i \right) \qquad (30)$$

From which we obtain;

$$\therefore \; T_C \;=\; \frac{K}{\Delta d}\left[T_{FG}-T_i\right]+T_i \qquad (31)$$

But, convective heat flux can be expressed by the equation;

$$q_c \;=\; GC_{PA}\left(T_C-T_i\right) \qquad (32)$$

Substituting equation **(31)** into **(32),** we obtain **(33)** as;

$$q_c \;=\; GC_{PA}\left(\frac{K}{h_i\Delta d}\right)\left(T_{FG}-T_i\right) \qquad (33)$$

For most applications, the heat flux (q_R) to the tubes in the radiant section ranges between 20 to 40 KW/M^2. For this work, a literature value of 20 KW/M^2 is used. Hence, the total heat flux is given as;

$$q \;=\; 20 + GC_{PA}\left(\frac{K}{h_i\Delta d}\right)\left(T_{FG}-T_i\right) \qquad (34)$$

Also, the heat capacity relationships in table 1 are applied directly in determining the heat of reaction $\left(-\Delta H_R\right)$ in equation **(26)** as shown in equation **(35)**;

$$\Delta H_R \;=\; \Delta H^0{}_{298} \;+\; \int_{298}^{T}\left[C_{PB}+C_{PC}-C_{PA}\right]dT_R \qquad (35)$$

The heat of reaction at 298k ($\Delta H^0{}_{298}$) can be calculated from the heats of formation of Table 3.1 using the equation [6];

$$\Delta H^0{}_{298} \;=\; C^0_{P_B} + C^0_{P_C} - C^0_{P_A} \qquad (36)$$
$$= 52510 + 0.0 - (-83820)$$
$$= 52510 + 83820$$

$$\Delta H_{298}{}^0 = 136{,}330\, KJ\ per\ Kgmol.K$$

Introducing the heat capacity relationships of table 1 and the calculated value for the heat of reaction at standard state (298K) into equation **(35)** and integrating yields the heat of reaction $\left(\Delta H_R\right)$ at any reactor temperature T_R (k) as shown;

$$\Delta H_R \;=\; 136{,}330 + \left[24.701\left(T_R-298\right)+0.02384\left(T_R{}^2-298\right)-6.177\,x\,10^{-5}\left(T_R{}^3-298^3\right)-\left(\frac{6.9\,x\,10^4}{T_R-298}\right)\right] \qquad (37)$$

3.1 Pressure Drop

For flow of fluids in pipes, the pressure drop along the length of the pipe [5]

$$\frac{dp_{Tot.}}{dZ} \;=\; -\,\frac{2fG^2}{1000\rho d} \qquad (38)$$

3.2 Solution Technique

Equations (19) and (26) are nonlinear equations developed and are subjected to iterative simultaneous numerical process to obtain the profiles as in figures 1, 2 and 3

4. MODEL RESULTS

Summary of simulation results obtained by linear interpolation is as shown in table1 below;

Table 1: Simulation Results

X_A	d(m)	Z(m)	T_R(k)	Δp (Kpa)	τ (S)
0.30	0.0508	133.1250	1100.00	0.5990	4.6945
0.35	0.0635	136.8750	1185.00	0.6085	8.0480
0.40	0.0762	140.6250	1460.00	0.6011	10.7430
0.45	0.0890	141.2500	1460.10	0.6000	12.4190
0.50	0.1016	145.0000	1460.50	0.5842	14.0950
0.55	0.1270	148.7500	146.72	0.5789	15.7590
0.60	0.1400	153.1250	1460.80	0.5730	17.4540
0.65	0.1524	155.000	1461.00	0.5700	19.1780

The simulation results is obtained by using Runge-Kutta numerical method for solving simultaneous differential equation on computer program mat lab ODE 45 for the three lumped equations (19), (26) and (38) generated from the design model.
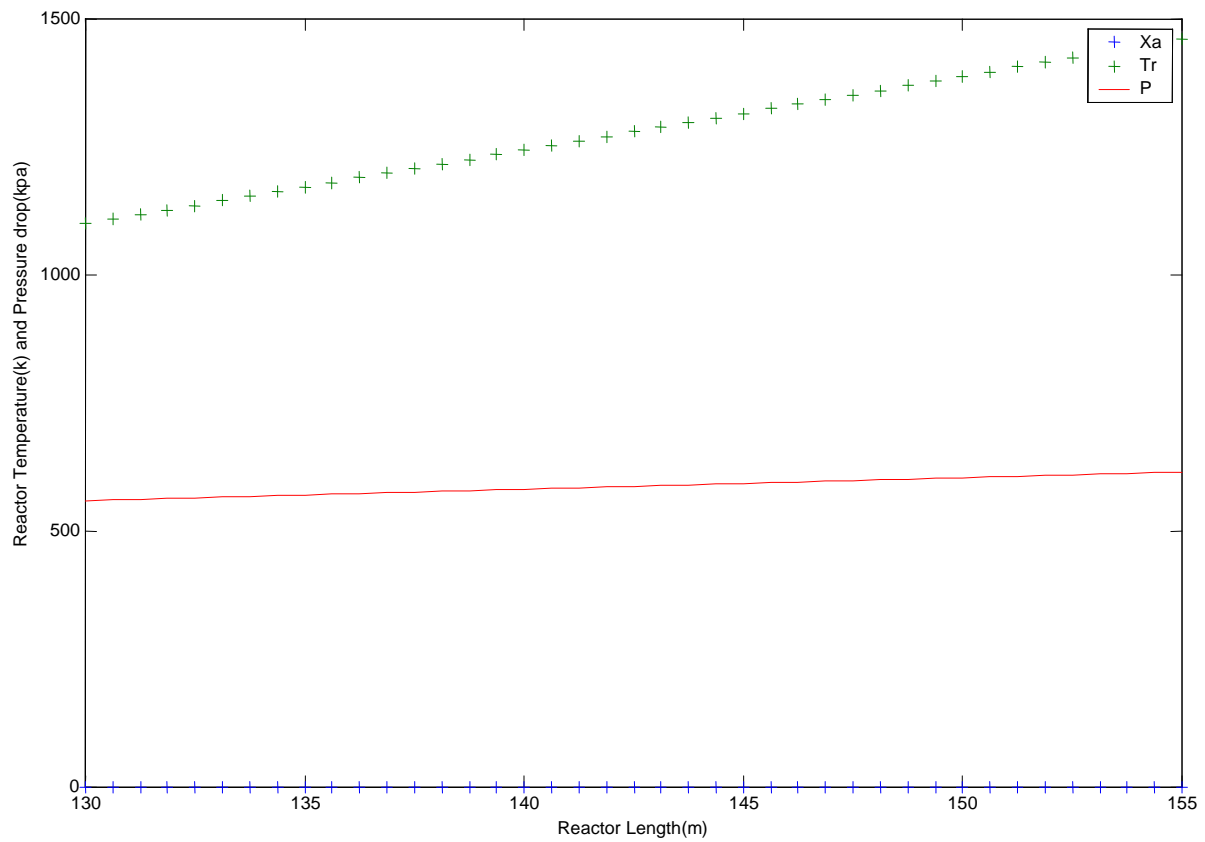
5. DISCUSSION

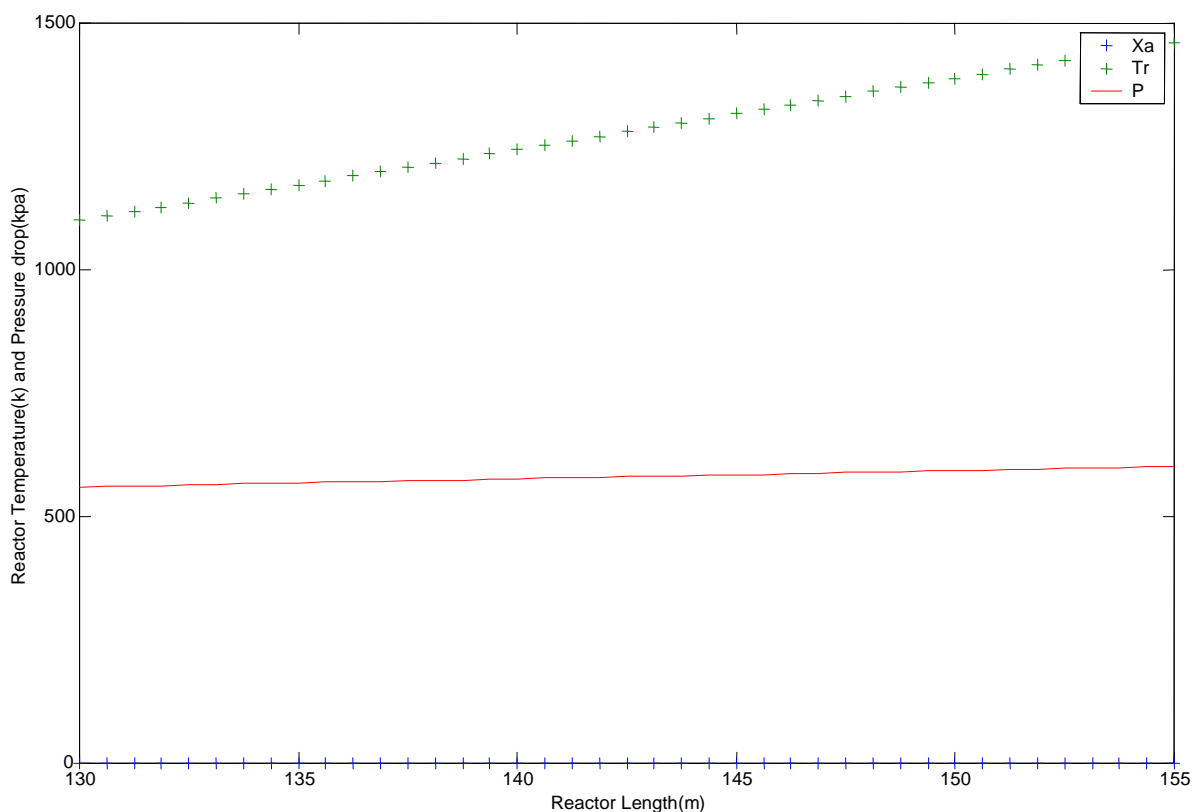**Fig 1:** Plot of reactor Temperature and Pressure Drop for $\alpha_A = 0.35, d = 0.0635m$

Fig 2: Plot of Reactor Temperature and Pressure drop against Reactor Length For $\alpha_A = 0.40, d = 0.0762m$
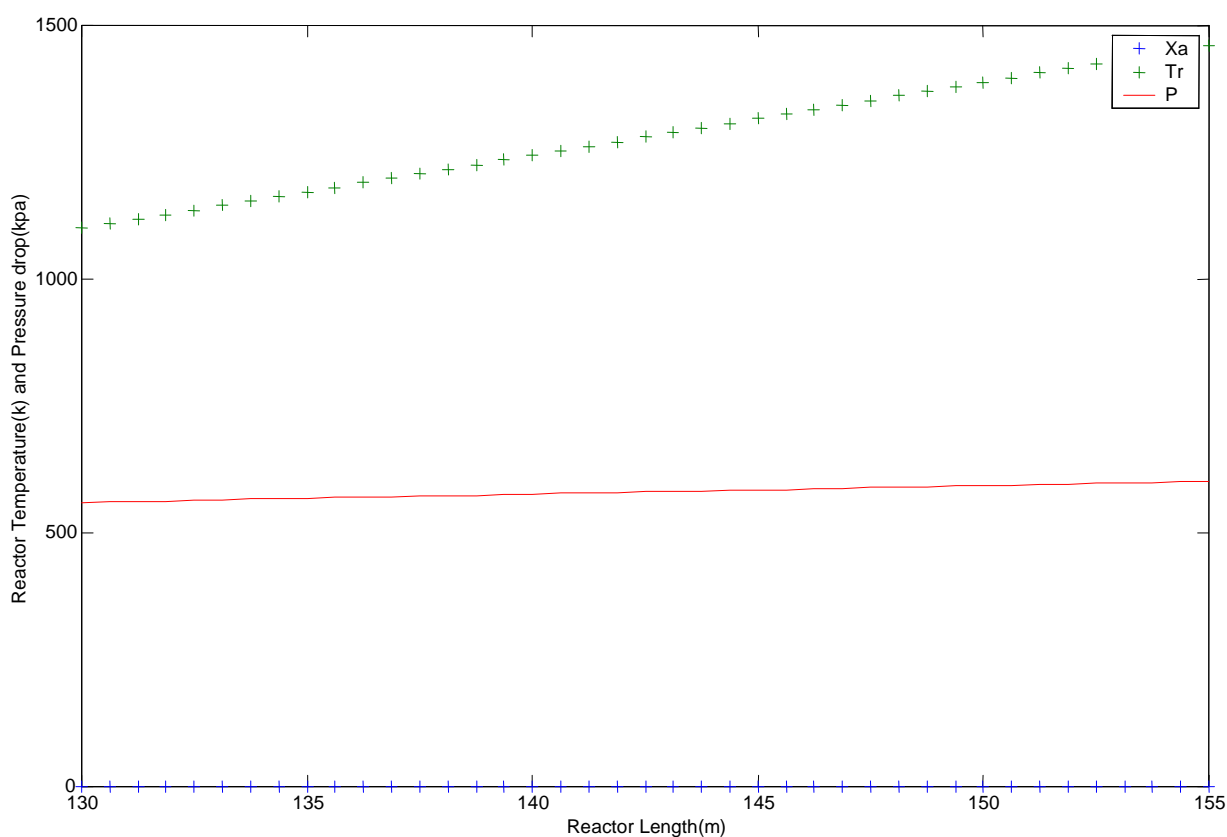

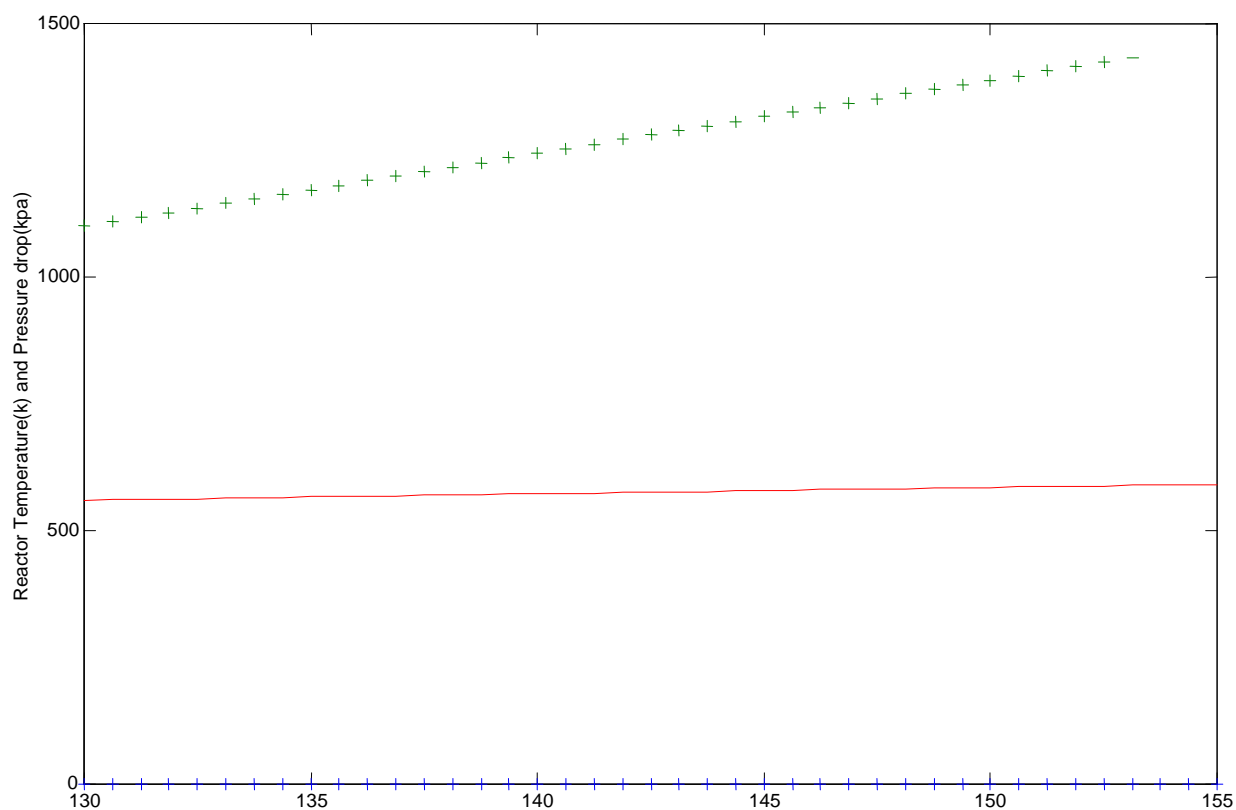**Fig 3:** Plot of reactor temperature and pressure drop for $\alpha_A = 0.4$ and d = 0.0762m

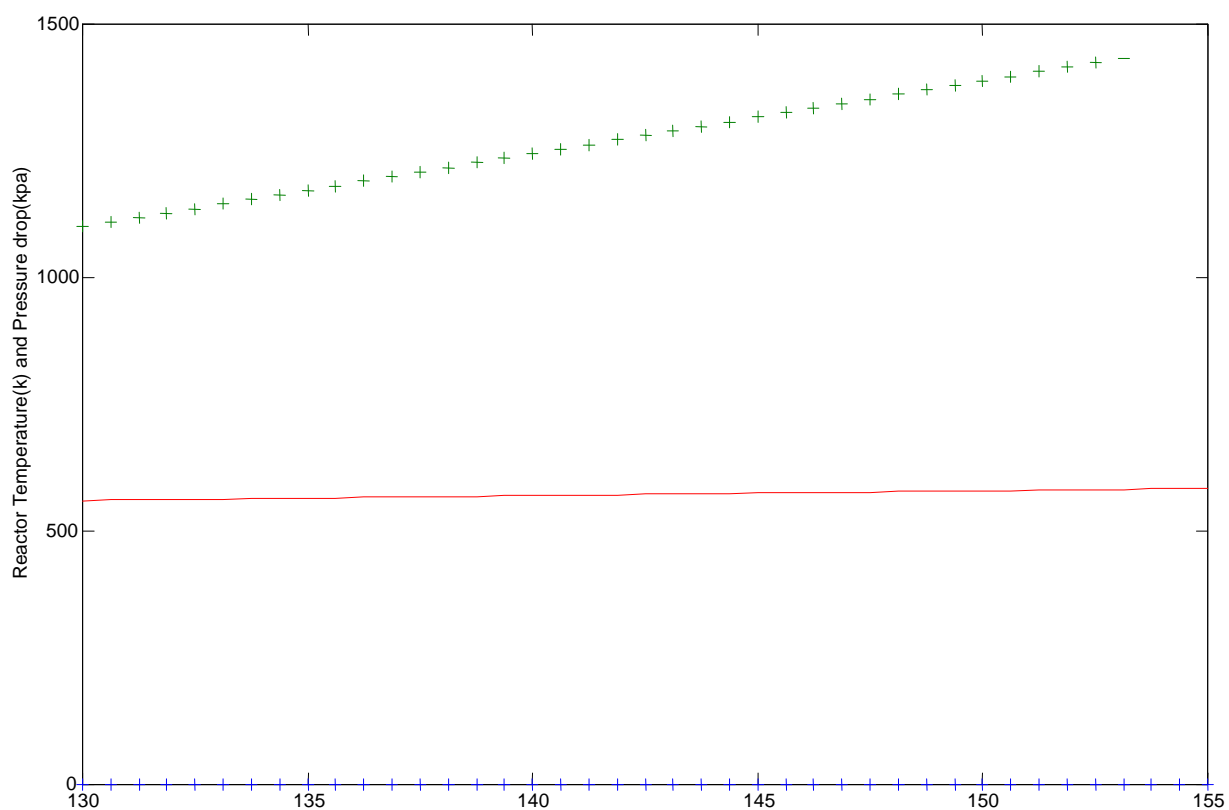**Fig 4**: Plot of reactor temperature and pressure drop for α_A = 0.45 and d = 0.0890m

Fig 5: Graph of reactor temperature and pressure drop for α_A = 0.5 and d = 0.1016m

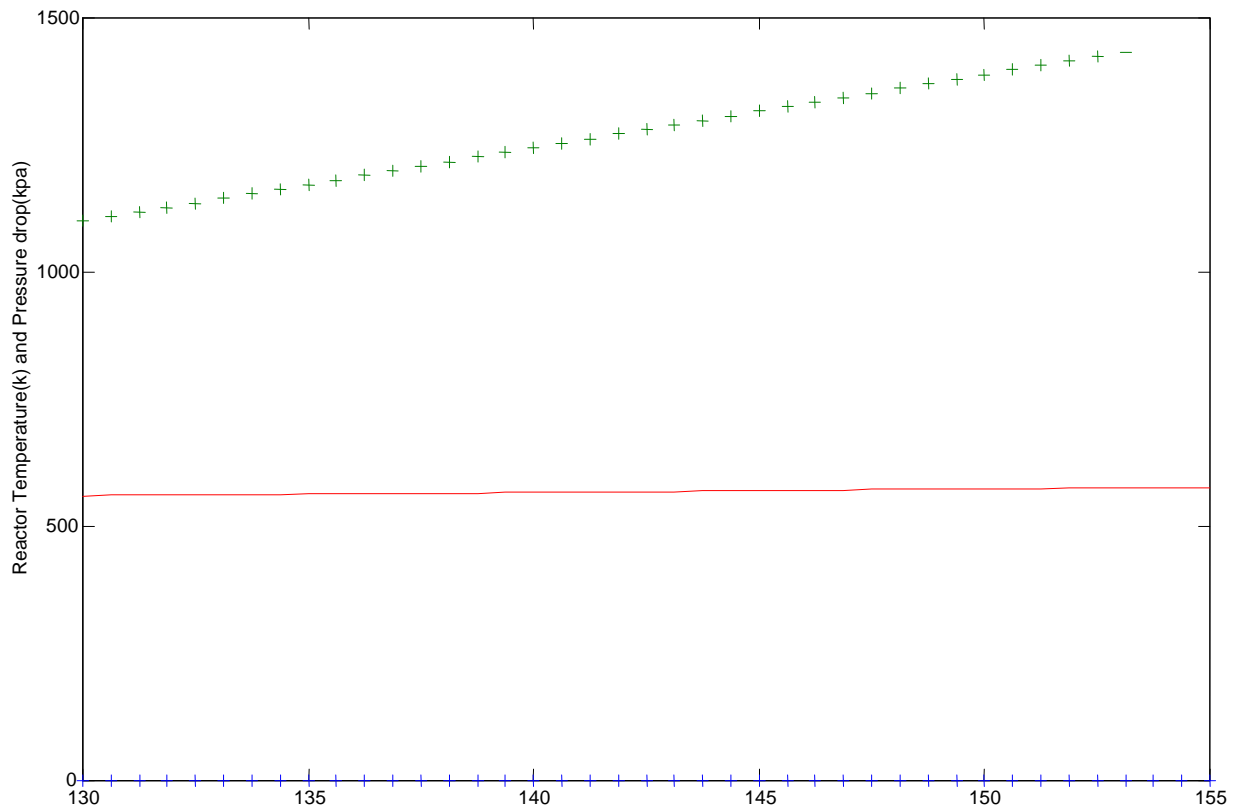**Fig 6:** Graph of reactor temperature and pressure drop for $\alpha_A = 0.55$ and d = 0.1270m

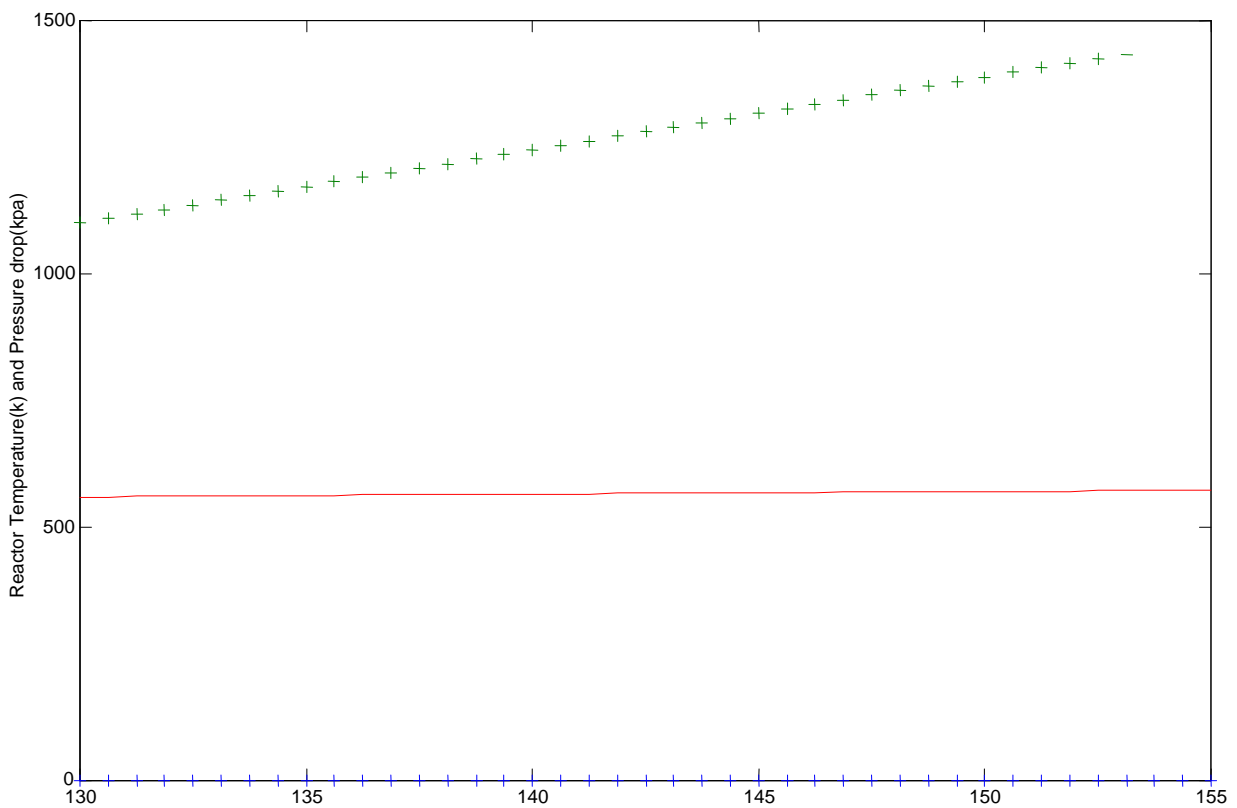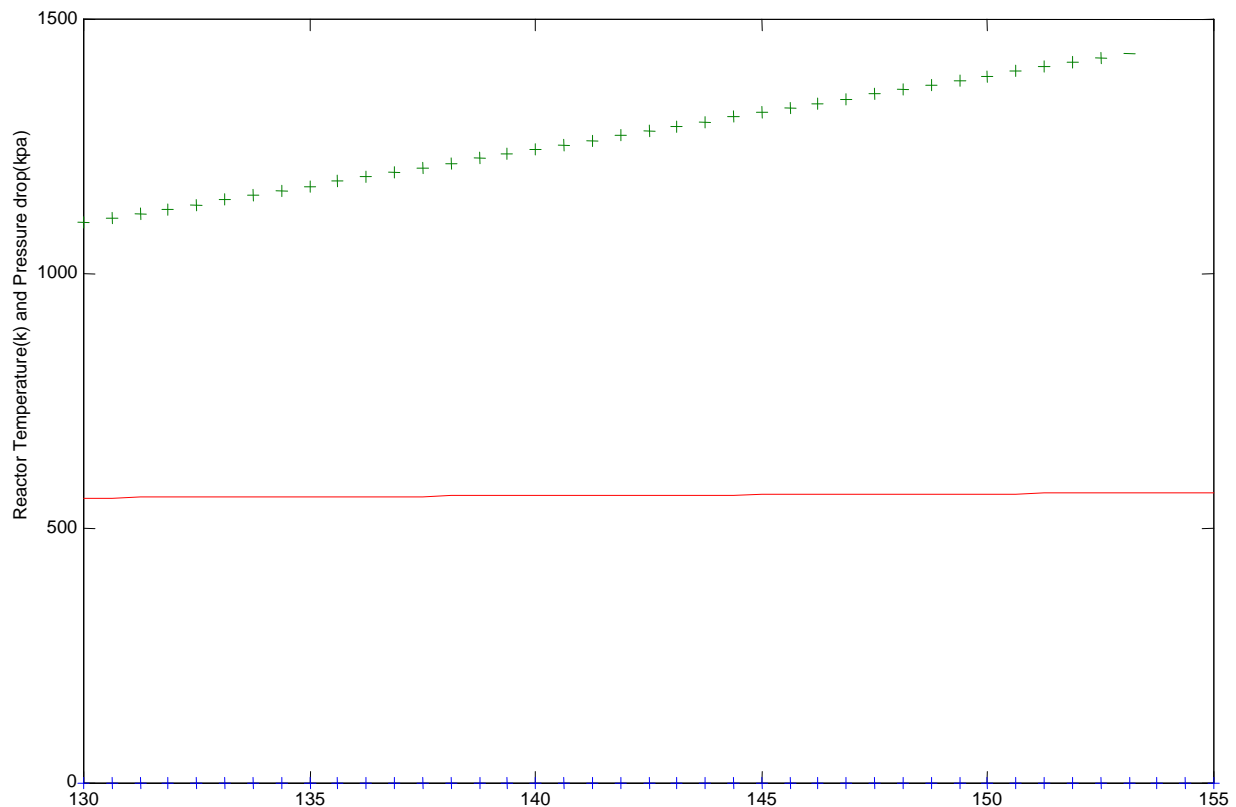**Fig 7:** Graph of reactor temperature and pressure drop for $\alpha_A = 0.6$ and d = 0.14m

Fig 8: Graph of reactor temperature and pressure drop for α_A = 0.65 and d = 0.1524m

From the graphs on figures 1 - 8, the reactor temperature increases along the length of the reactor from the convective zone to the radiation zone. This is expected because the heat flux to the radiation zone is greater than that of the convective zone as radiation zone is heated directly by the furnace and the convective zone is heated by the rising flue gas emanating from the furnace. The pressure drop increases steeply from the convective zone to the radiation zone at low conversion. At an optimum conversion of 65% as predicted by the model, the pressure drop maintains a constant flat shape along the length of the reactor and this is what is expected. For effective design, the pressure drop should remain constant as predicted by the model.
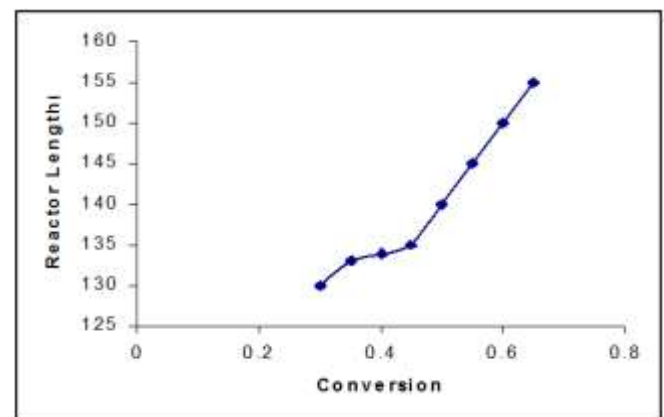

Figure 9 shows the conversion profile along the length of the reactor. There is only about 30% to 45% conversion of an ethane for the first 5 meters of the reaction zone. But as reactor temperature increases along the reactor length, the reaction conversion increases rapidly, and up to about 65-68% conversion for the remaining 20 meter of the reactor.
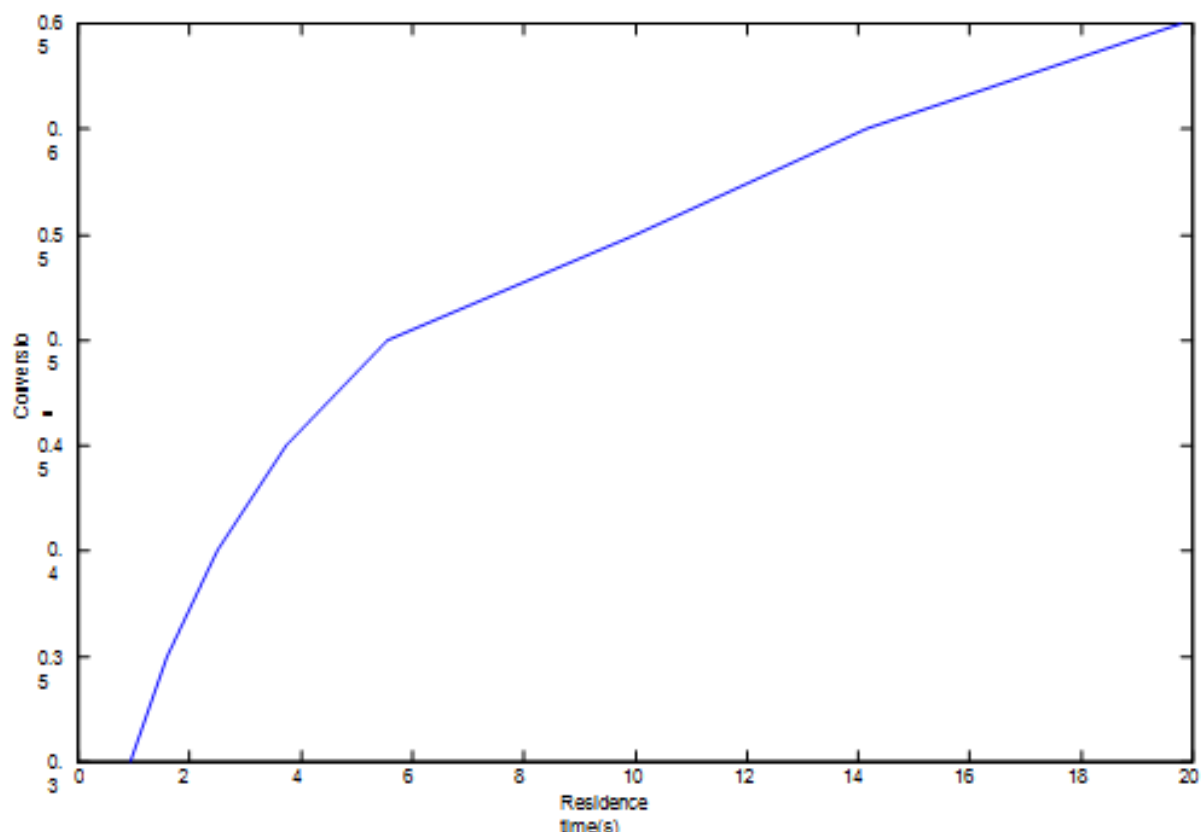
Fig 10: Graph of Conversion against residence time in sec.

From figure 10 above it is evident that conversion increases with residence time and this is what is expected for a plug flow reaction. The residence time for the reaction at 65% conversion is about 20 seconds.

The main criterion for the furnace reactor design depends on the selection of the proper dimension that provide the lowest value of pressure drop and residence time to prevent any explosion and coking of the hydrocarbons throughout the reactor.

From the plots presented, it is evident that the lowest and stable value for pressure drop is obtainable from figure 8. Design parameters deduced from model results are compared with actual plant specification as shown in table 2 below:

Table 2: Comparison of model prediction with actual plant specification for design parameters at 65% conversion

S/N	Parameter	Model prediction	Plant Specification	Absolute relative error (%)
1.	Tube diameter d(m)	0.1524	0.1600	4.75
2.	Tube thickness $\Delta d(m)$	0.0095	0.0100	5.00
3.	Pressure drop $\Delta p(Kpa)$	0.57	0.45	21.10
4.	Reactor Temperature, $T_R(k)$	1461	1373	6.41
5.	Reactor Length Z(m)	155.0	152.0	1.97
6.	Residence time $\tau, (s)$	19.1780	15.20	26.17

Where: From table 2, the deviation of model predictions with respect to actual plant design specification represented as absolute relative error, it can be deduced that the accuracy of the design model is sufficient for predicting design specification of a furnace reactor for cracking 100% ethane feed.

6. CONCLUSION

The presented numerical design model of ethane cracking in a furnace reactor is evaluated and found suitable in determining the reactor specification for effective design. An adequate reactor dimension is required to achieve the optimum conversion of the feed. Hence this model was found to be accurate for predicting a 65% ethane conversion to ethylene for a feed of 100% ethane.

NOMENCLATURE

A = Cross- sectional area of the reactor tube, (m^2)
C_i = Concentration of species i , $(kmol/m^3)$
C_{Pi} = Specific heat capacity of component i, (KJ/Kmol)
d = Pipe internal diameter, (m)
F_{AO} = Inlet molar fined rate of ethane, (Kmol/sec)
F_i = Molar flow rate of species i at any point, (Kmol/sec)

F_T = Total molar flow rate of gas mixture at any point, (Kmol/sec)

F_{TO} = Total inlet molar flow rate (Kmol/sec)

f = Fanning friction factor

G = Mass flux, (Kg/m^{2}S)

ΔH_{298}° = Heat of formation, (Kg/Kmol)

ΔH_R = Heat of pyrolysis reaction, (KJ/Kmol)

h_i = Heat transfer coefficient of reactor tube inner surface

K_1 = Reaction rate constant (S^{-1})

M_{wt} = Molecular weight of ethane (Kg/Kmol)

n_i = Number of moles of species i

P_O = Inlet total Pressure, (KPa)

P_{Tot} = Total pressure of gas mixture in reactor (KPa)

q = Heat input from furnace (KJ/s-m (of reactor length))

q_c = Heat input from furnace to convection zone (KJ/s-m)

q_R = Heat input from furnace to radiation zone (KJ/s-m)

R = Universal gas constant (KPam^3/Kmol)

Re = Reynolds number

r_A = Specific reaction rate (Kmol/m^{3}s)

T_i = Inlet feed Temperature, (K)

T_{out} = Outlet- temperature, (K)

T_R = Absolute reactor temperature, (K)

V_R = Reactor volume, (m^3)

V = Superficial velocity,(m/s)

y_A = Mole fraction of ethane

Z = Length of reactor tube, (m)

GREEK SYMBOLS

α_A = Mole fraction of ethane converted to products

α_i = range of 0.0-0.65

ρ = Density of the mixture at any point in the reactor (Kg/m^3)

τ = Residence time, (S)

μ = Viscosity of ethane at inlet condition (Kg/ms)

Δp = Pressure drop along the reactor (KPa)

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BIOGRAPHY

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