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Design of Adiabatic Packed Bed Reactor for Styrene Production

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ABSTRACT

Design of reactor with large area and high cost of maintenance is a major problem for styrene production, this research work is aimed designing an adiabatic packed bed reactor with smaller area for dehydrogenation of ethyl benzene by the application of the principles of conservation of mass and energy. The research objectives are to develop functional and dimensional models for the reactor, by Incorporating the kinetic model of dehydrogenation of ethyl benzene into the performance equations of the reactor then Solving the developed functional and dimensional equations using Matlab program. Simulation of the functional and dimensional model using Matlab program was the method applied in this research work. The reactor was designed with a range of fractional conversion, XA = 0.90 to 0.95 and reactor diameter, Di = 0.05 to 0.1m. The analysis of the heat exchanger yielded a favourable steady state result for reactor operations of styrene production, the heat transfer coefficient was obtained as U_0= 72.58W/m^2.^{o}C with shell side pressure P_t= 38242.78atm, Area of the exchanger, A = 1.263m^2, tube length 6.10m, LMTD = 52.716K heat duty Q= 17289471.93kJ/hr and the steady state time was obtained to be 90 sec, the results obtained showed that the design models were correct, predicting the amount of heat transferred for the heat exchanger and the steady state time for the designed reactor compares favourably with the output of an industrial reactor. The results obtained provided information for the evaluation of the functional parameters of the reactor which include reactor volume, spacetime, space velocity, rate of heat generation per unit reactor volume, pressure drop and reactor length.

Key Words: Styrene, Design, Reactor, Matlab, Ethylbenzene, Mass, Energy.

1. INTRODUCTION

Styrene is essential and important hydrocarbon in the petrochemical industry; primarily the world demand for commercial production of styrene is increasing on a daily basis, the adiabatic dehydrogenation method is extensive used as a widely accepted method to produce styrene, 85% of commercial production utilizes this rout. (James etal., 1994) the process is more of catalytic reaction because the catalyst plays a large part in the production in the production process.

Styrene is the second principal monomer of the polymer class, the reaction mechanism for obtaining styrene from ethylbenzene involves an endothermic reversible reaction (Lee, 1973) Carried out a research in which the by-product was determined to be benzene and toluene.
The advancement of the society has made the utilization of styrene based plastic to be growing quickly (Akpa, 2012) .
Styrene is valuable commodities due to it demand by various polymer industry globally. The main method for styrene production is more of energy consuming because substantial amount of energy is needed for the process due to the use of high temperature gas, (Emad etal., 2018) was able to Study the energy requirement and recovery using exergy analysis method, and also applying heat integration (HI) based on pinch design method. The amount of gas plays an important role in the tradeoff between styrene yield and energy savings. Therefore, optimizing the working conditions for energy reduction is not possible. The heat connection shows an insufficient reduction in the average energy requirement and energy losses, but 24% and 34% in external heating and cooling respectively. When the required hydraulic power is created by recirculating the heat of the reactor energy, significant savings in total energy can be made with, around a reduction in energy dissipation.

Potassium is very Important for dehydrogenation process for ethylbenzene because it is a main promoter for Fe_20_3 due to its ability to enhance and increase selectivity (shibata et.al 1969) studied the unpromoted and was able to determine the activation energy with an increasing selectivity above one order of magnitude hence increasing the formation of the desired product and stabilising the catalyst, (coulter et.al 1995) also studied the kinetic of the reaction with unpromoted and K-promoted polycrystalline catalyst his observation show the unpromoted catalyst was able to yield an activation energy of 155.4KJ/mol which was also confirmed by (Addiego et.al 1981) the study proved that an increase in the initial loading of potassium decreased the activation energy of the reaction to 142.8KJ/mol

the following researchers (Addiego et.al 1981 (coulter et.al, 1995) and (shekhah et.al,2004) where able to conclude that the addition of potassium did not alter the assumption geometry and nature of the active site nevertheless a decrease in formation of by-product was observed
Most of the work reviewed had the following limitations:

(i) Most of the works done on styrene production has to do with just modeling, and simulation. (Akpa, 2012) actually did a good work on simulation of catalytic membrane reactor for the dehydrogenation of ethylebenzen most researcher do not consider the design of the reactor and heat exchanger unit for the operation other limitation includes,
(ii) Lack of evaluation of the specification of styrene monomers,
(iii) Adopting and using the standard test method,
(iv) Estimating the impurities in styrene monomers.
The aim of the current study is design an Adiabatic Packed Bed Reactor for Styrene Production. The following objectives were carried out in order to achieve the aim of the study:

(i) Develop the functional and dimensional models for the reactor by the application of the principles of conservation of mass and energy
(ii) Incorporate the kinetic model into the performance equation of the reactor
(iii) Solve the developed functional and dimensional equation using Matlab programming language
(iv) To simulate the functional and dimensional model using Matlab programming language

2. Materials and Methods

2.1 Materials

The materials adopted for this research are Principle of Conservation of Mass and Energy, Packed Bed Reactor design Equation, Energy balance equation. Heat exchanger design equation, Heat exchanger Energy balance equation, Space time, Space velocity and Literature data.

2.2 Methods

The method applied in this research work is to develop the design equation of packed bed reactor and formulating the appropriate kinetic model for ethyl benzene dehydrogenation.

2.2.1 Model equation

The design equation of chemical engineering system is obtained by modeling the system. Modeling is done in two approaches namely experimental approach (physical) and mathematical (theoretical) approach.

Physical approach is the use of physical equipment to test for the system required before modeling. It is capital intensive and time consuming. Mathematical approach is the use of differential or integral equations whose solution is equivalent to the dynamic behavior of the system. Mathematical approach will be used in this work to obtain the characteristics of the Fixed Bed Catalytic Reactor.

In developing model equation for fixed bed reactor, certain assumptions are made:

1. The reactor is assumed to operate at a steady state condition.
2. The composition of the fluid (reactants) varies from point to point along the flow path.
3. There is no conversion of reactants before being charged into the reactor.
4. The flow of the reactants into the reactor are orderly and hence, no mixing with any other element.

The starting point for all design is the material or mass balance which is expressed or either reactant or product. [Octave (2005)].

2.2.2 Material Balance

Material balance is nothing more than the application of the conservation law for mass: “matter is neither created nor destroyed” [Ogunda, 2006]. Thus, illustrated below as:

$$\begin{bmatrix} Rate\ of\ reac\tan t \\ flow\ \text{int}\ o\ element \\ of\ volume \end{bmatrix} = \begin{bmatrix} rate\ of\ reac\tan t \\ flowout\ of\ element \\ of\ volume \end{bmatrix} + \begin{bmatrix} rate\ of\ reac\tan t \\ loss\ due\ to\ chemical \\ reaction\ within\ the \\ element\ of\ volume \end{bmatrix} + \begin{bmatrix} rate\ of\ accumulation \\ of\ reac\tan t\ in \\ element\ of\ volume \end{bmatrix} \quad (1)$$

2.2.3 Component Mass Balance for the Reactor

The component balance will consider first the area in which the catalyst is acting.

Consider a schematic representation of a fixed bed reactor with feeds and products shown. The feed (reactant) to be considered is for reactant A.

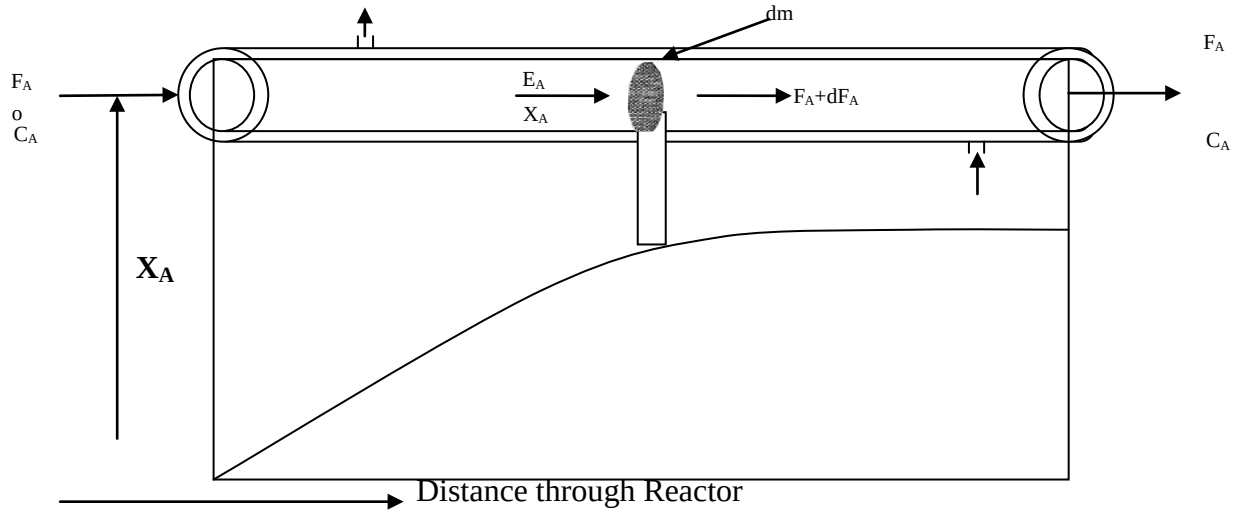
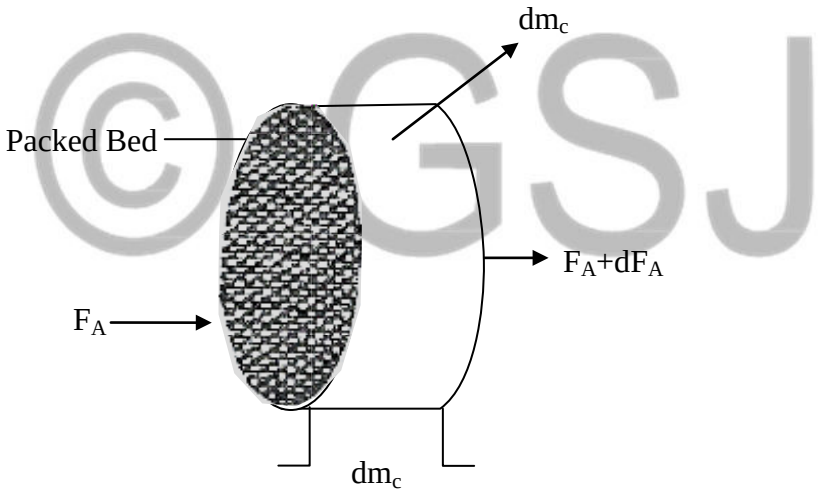


Fig 3.1 Hypothetical Tubular Reactor Unit

Considering the elemental path gives. (Richardson, 2006)



Considering the material balance equation

Input of A = Output of A + disappearance of A **(2)**

Input of A = F_A

Output = $F_A + dF_A$

Rate of disappearance = $(-r_A)\, dM_c$

Accumulation = O = because nothing accumulated

Substituting the terms into equation 3.1

$$F_A = F_A + dF_A + (-r_A)\, dM_c \quad \textbf{(3)}$$

But

$$F_A = F_{AO}\,(1 - X_A) \quad \textbf{(4)}$$

Differentiating, we have

$$dF_A = F_{AO}\,dx_A \quad \textbf{(5)}$$

Substituting 3.3 and 3.4 into 3.2 gives

$$F_{AO}(1 - X_A) = F_{AO}\,(1 - X_A) + (-F_{AO}dX_A) + (-r_A)dM_c$$

Collecting like terms gives

$$F_{AO}dX_A = (-r_A)dM_c$$

Re-arranging

$$\frac{dM_c}{F_{AO}} = \frac{dX_A}{(-r_A)}$$

Integrating

$$\int \frac{dM_c}{F_{AO}} = \int_0^{XA} \frac{dX_A}{(-r_A)}$$

$$Mc = F_{AO} \int_0^{XA} \frac{dX_A}{(-r_A)} \quad \textbf{(6)}$$

But

$$Mc = \rho_c V_{RC} \quad \textbf{(7)}$$

Because the weight of the catalyst and reactor volume are related by the catalyst bulk density

Substitute 3.5 into 3.6 gives

$$\rho_c V_{RC} = F_{AO} \int_0^{XA} \frac{dX_A}{(-r_A)}$$

Divide through by ρ_c

$$V_{RC} = \frac{F_{AO}}{\rho_C} \int_0^{XA} \frac{dX_A}{(-r_A)} \quad \textbf{(8)}$$

Equation 8 is the volume of reactor occupied by catalyst which is equivalent to volume of reactor since it is related m terms of the catalyst bulk density. Where:

C_{AO} = Molar concentration of reactant A in the reactor

F_{AO} = Molar flow rate of A in the reactor

V_{AO} = Volumetric flow rate of reactant A in the reactor

V_{RC} = Volume of reactor occupied by catalyst

X_A = Fractional conversion of reactant A

Mc = Mass of catalyst

ρ_c = Density of catalyst

K_1 = Rate constant

K_e = Equilibrium constant

2.2.4 Kinetics equation

(Elnashaie *etal.*, 2000) described the dehydrogenation reaction occurring in the reactor for the production of styrene and also incorporating a conclusions from the observations of Sheppard and Maier (1986) adopted this reaction paths for the dehydrogenation process with their respective rate expressions as follows:

$$C_6H_5CH_2CH_3 \xleftrightarrow{K1} C_6H_5C_2H_3 + H_2 \quad \Delta H_R = 124.9\text{KJ/mol} \qquad \textbf{(9)}$$

Side reactions:

$$C_6H_5C_2H_5 + H_2 \xrightarrow{k2} C_6H_5CH_3 + CH_4 \qquad \textbf{(10)}$$

$$C_6H_5C_2H_5 \xrightarrow{k3} C_6H_6 + C_2CH_4 \qquad \textbf{(11)}$$

$$H_2O + \frac{1}{2}C_2H_4 \xrightarrow{k4} CO + 2H_2 \qquad \textbf{(12)}$$

$$H_2O + CH_4 \xrightarrow{k5} CO + 3H_2 \qquad \textbf{(13)}$$

$$H_2O + CO \xrightarrow{k6} CO_2 + H_2 \qquad \textbf{(14)}$$

The rate equations for equations (9) - (14) are given below;

$$r_1 = K_1(P_{eb} - \frac{P_{st}P_{H2}}{K_{peb}}) \quad \textbf{(15)}$$

$$r_2 = K_2\ (P_{eb}\ P_{H2}) \quad \textbf{(16)}$$

$$r_3 = K_3\ (P_{eb}) \quad \textbf{(17)}$$

$$r_4 = K_4\ ({P_{H_2O}}^{0.5} C_2H_4) \quad \textbf{(18)}$$

$$r_5 = K_5\ (P_{H_2O} P_{cH4}) \quad \textbf{(19)}$$

$$r_6 = K_6(P_T/T^2)\left(P_{H_2O} P_{CO}\right) \quad \textbf{(20)}$$

The reaction rate constants in these equations are obtained as:

$$K_j\,(molkg^{-1}s^{-1}bar^{-n}) = 10^3 \exp\left(A_1 - \frac{E_i}{RT}\right) \quad \textbf{(21)}$$

$$K_{peb} = exp\ (\frac{-\Delta H}{RT}) \quad \textbf{(22)}$$

$$\Delta H = a + bT + cT^2 \quad \textbf{(23)}$$

Since the rate equation in (15-23) is in form of partial pressure, converting it to be in terms of fractional conversion.

recall from the ideal gas equation

$$PV=nRT \quad \textbf{(24)}$$

Divide equation (24) by V

$$\frac{PV}{V} = \frac{nRT}{V} \quad \textbf{(25)}$$

$$P = \frac{n}{v} RT \quad \textbf{(26)}$$

Recall: $C = \frac{n}{v}$

Putting (26) into (24)

P=CRT **(27)**

Putting equation (27) into the rate equation.

$$r_1 = k_1 (P_{eb} - \frac{P_{sr} P_{H2}}{K_{peb}}) \quad \textbf{(28)}$$

$$r_1 = k_1 [RT\, C_{eb} - \frac{RT(C_{st} - C_{H2})}{K_{peb}}] \quad \textbf{(29)}$$

$$r_1 = RTK\, [C_{eb} - \frac{(C_{st} C_{H2})}{K_{peb}}] \quad \textbf{(30)}$$

Total moles of reactant = 2 mole of E_B + 30 moles of Steam = 32 moles **(31)**

$$\delta = -1 + 1 + 1 = 1$$

$$y_{EB} = \frac{1-X}{Total\ moles + X} \quad \textbf{(32)}$$

$$y_{st} = \frac{X}{Total\ moles + X} \quad \textbf{(33)}$$

$$y_{H_2} = \frac{1-X}{Total\ moles + X} \quad \textbf{(34)}$$

$$P_{EB} = y_{EB} \,.\, P_T \quad \textbf{(35)}$$

$$P_{ST} = y_{ST} \,.\, P_T \quad \textbf{(36)}$$

$$P_H = y_H \,.\, P_T \quad \textbf{(37)}$$

Inputting rate equation into design equation

$$V_{RC} = \frac{F_{AO}}{\rho_c} \int_O^{X_A} \frac{dXA}{K1\ (P_T y_{eb} - P_T 2 y_{st} y_{H2})/Keb} \quad \textbf{(38)}$$

The equation will be solved in MATLAB to determine the volume of the reactor and the performance model for an adiabatic packed bed reactor.

2.2.5 Design Equation for Reactor Parameters

Reactor performance is a measure for the direction of the entire reaction process. In steady state reactors like Fixed bed reactor, the performance is measure with space time, space velocity and mean residence time.

Space time (τ)

Space time is the time required to process one reactor volume of feed at specific condition. It is defined mathematically as the ratio of volume of reactor to volumetric flow rate. That is,

$$\tau = \frac{V_R}{V_{AO}} \quad \textbf{(39)}$$

V_R = Volume of reactor

V_0 = Initial volumetric flow rate

Space Velocity (S_V)

Space velocity is the number of reactor volumes of feed at specific condition which can be treated in a unit time. Mathematically, it is the reciprocal of space time (τ).

$$S_V = \frac{V_{AO}}{V_R} = \frac{1}{S_T} = \frac{1}{\tau} \quad \textbf{(40)}$$

Length of Reactor

Fixed bed catalytic reactor is cylindrical in shape; volume of cylinder

$$v = \pi r^2 \, l = \frac{\pi d^2 l}{4} \quad \textbf{(41)}$$

$$L_R = \frac{4V_{RC}}{\pi d^2}$$

Heat Load Q

The total heat generated is expressed as

$$Q = \Delta H_{rA} \, F_{AO} \, X_A \quad \textbf{(42)}$$

Where

Q = Total heat load

ΔH_{rA} = Heat of reaction

F_{A0} = Initial molar flow rate of A

X_A = Fractional conversion

Heat Generated Per Unit Volume of Reactor

$$H_R = \frac{Q}{V_R} \quad \textbf{(43)}$$

Where

H_R = Heat generated per unit volume of reactor

Q = Total heat load

V_R = Volume of reactor

Input Parameters

The following data were obtained from literatures and used to run the MATLAB program for the designed reactor and Heat exchanger for styrene production via the catalytic dehydrogenation of ethylebenzene adopting an adiabatic condition for reactor operations

Table 3.1: Input Data for Packed bed Reactor for Styrene Production

Variable	Symbol	Value	Units
Reaction Temperature	T	903	K
Initial Concentration of A	C_A	1000	mol/m^3
Initial Volumetric Flow rate of A	VAO	0.001	m^3/sec
Initial molar flow rate of A	FAO	181.65	mol/sec
Pre-exponential factor	Ko	0.0000351	-
Reactor Diameter	D	0.5	m
Activation Energy of reaction	E	0.851	-
Conversion rate	x	0.90	
Gas constant	R	8.314	J/mol.K
Standard Heat of reaction	dHr	124.9	kJ/mol
Heat transfer coefficient of product	Kh	0.58	W/m.K
Mass flow rate of product	mp	2.42	Kg/sec
Viscosity of reaction mixture	n	5.2	kg/sec.m
Viscosity correction factor	nh	0.932	Kg/sec.m
Linear velocity of reaction mixture	v	0.0224	s^{-1}
Density of ethybenzene (A)	ρ	790	Kg/m3
Specific heat capacity	C_p	4.184	
Viscosity correction factor of product	np	20	kg/sec.m
Reactor thickness	Tr	0.05	m
Dirty overall film transfer coefficient	Ud	0.764	KJ/m^2K

Table 3.2: Data for Heat Exchanger Design

Variable	Symbol	Value	Units
Hot fluid	-	-	-
Inlet temperature	Ti	836.23	K
Outlet temperature	T_2	377.319	K
Mass flowrate	m	500	kmol/hr
Cold fluid			
Inlet temperature	Ti	433	K
Outlet temperature	T_2	793	K
Mass flow rate	m	181.64	kmol/hr

3. RESULTS AND DISCUSSION

3.1 Results

Table 3.1: Results for Reactor functional Parameters

Variable	Symbol	Value	Units
Volume of reactor	V_R	60.1	m^3
Length of reactor	L_R	7.6	m
Space velocity	Sv	9.5	min
Space time	St	6.5	min

Table 3.2: Design Results for Heat exchanger for Styrene Production

Variable	Symbol	Value	Units
Heat duty	Q	17289471.93	kJ/hr
Exchanged Area	A	1.263	m^2
Long men Temperature	LMTD	52.716	K
Shell side pressure drop	Gs	38242.78	atm
Pressure	P	0.01	atm
Tube side pressure drop	P	19284.7	atm
Over all coefficient	U_0	72.11	$W/m^{20}C$
Tube side velocity	v_t	0.0453	m/s

Manual calculations of the heat exchanger design were computed and simulated using MATLAB and the following results tabulated (see Table 4.1). The heat duty is 4802.63W and the area of the exchanged heat is $1.263m^2$. The values indicate that the heat exchanger design is good and reliable for the set function.

Table 3.3: Design Results for Heat exchanger's Parameters

Variable	Symbol	Value	Units
Correction constant	R	1.045	-
Correction constant	S	0.874	-
Tube length	L_t	6.10	m
Area of single tube	A_t	0.4867	m^2
Density	ρ	354	kg/m^3
Heat transfer Coefficient	Uo	72.58	

Shell side velocity	v_s	0.00947	m/s
Volumetric flow rate	v_0	0.0025	m3/s
Shell diameter	D_s	476	mm
Baffle spacing	L_b	0.512	m
Cross flow area	A_c	0.2639	m^2
Shell diameter	D_s	0.025	m
Number of baffles	N_b	11	
Reynolds number	Re	24.5-444.5	-

Table 4.2 indicates also some of the heat exchanger design parameters that were gotten from the manual and simulation calculations. The values must be obtained in other to determine, evaluate and rate the performance of the heat exchanger and the area of the exchanged heat.

3.2 Result of the Reactor Design and Simulation

The computer program written with MATLAB 2011 compiler for the design of a Packed bed Reactor for the production of ethybenzene via the Catalytic dehydrogenation of ethylbenzene produced the following results at T = 630 K are C_A= 1187mol/m^3 and V_{AO} = 0.001 m^3/sec. The effect of conversion on Volume, Length, Space time and Space velocity of the reactor were studied and the results are presented as profiles shown below:

3.3 Discussion of Heat Exchanger Results

The differential models were simulated using MATLAB 2011 Compiler to obtained Temperature profiles over the length of the heat exchanger at steady state time as shown below:

3.3.1 Steady State Temperature Profile of Shell and Tube Heat Exchanger Length at time of 90 sec

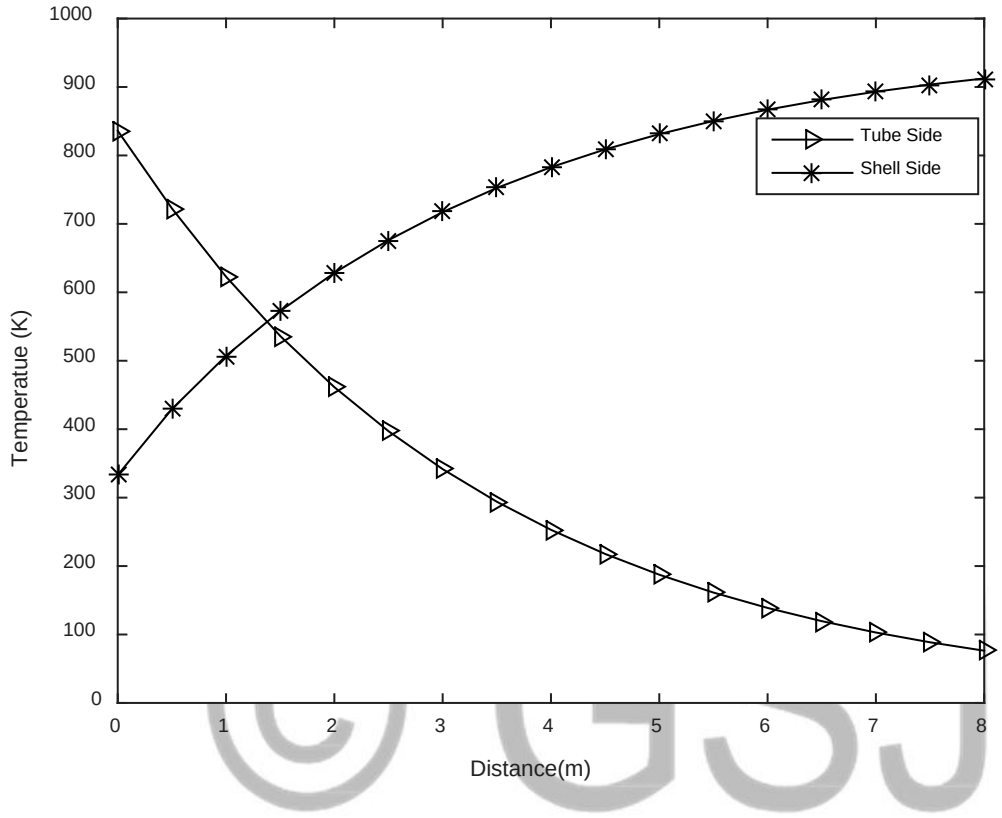


Figure: 4.1 Plots of Temperature Profiles for Heat Exchanger

The temperature profile of heat exchanger design at steady state along the length of the exchanger is shown in Figure 4.1. The profile is obtained at 90secs. The rating of the exchanger is at 333K and 836K initially for the heat exchanger and increases and decreases respectively exponentially to 912Kand 76K when the length increases from 0m to 8m and then remains constant throughout the remaining length.

4 Conclusion

The research on design of Adiabatic Packed bed reactor for styrene production has been carried out, the performance model for adiabatic Packed bed Reactor was used for simulation over a

fractional conversion of 92% for the feed $x_A = 0.92$ was obtained , From the results obtained it shows clearly that the results gave a reliable data for the functional parameters of the reactor. These parameters includes reactor volume, reactor length, space time, space velocity, and rate of heat generation per reactor volume, the analysis of the energy balance equation of a packed bed reactor was essential in predicting the conversion of reactant along the reactor length with other process parameters. The relationship between the model obtained and the performance of the packed bed reactor depends on the process parameters such as the concentration of the feed (reactant), its speed of rapidness and the temperature of the reaction, hence an exponential increase in reactor temperature will give rise to the formation of side reaction an optimization of the operating condition will be necessary in other to ensure economic operate ability of the reactor.

The analysis of the heat exchanger yields a favorable steady state for reactor operations for styrene production the heat transfer coefficient was obtained as $U_0 = 72.58 W/m^2.^oC$ with shell side pressure $P_t = 38242.78 atm$

Area of the exchanger, $A = 1.263 m^2$, tube length 6.10m, LMTD = 52.716K heat duty Q= 17289471.93kJ/hr and the steady state time was obtained to be 90 sec, the results obtained shows the design models are correct, predicting the amount of heat transferred for the heat exchanger and the steady state time for the designed reactor compares favorably with the output of an industrial reactor.

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