Simultaneous Mass, Heat and Momentum Transfer in an Adiabatic Packed Bed Reactor

Ban A.Ahmed , Sattar J.Hussen ,Saba A.Yosif
Petroleum Research & Development Centre,Iraq

Abstract:

Process modeling or computer simulation is one of the most important studies which gives the engineer a whole description about certain processes including all the mathematical relationships that are relating the process variables.

Transport phenomena on fixed bed reactor was studied because of their importance and their effects on the catalyst performance in all chemical reactions.

Simultaneous mass , heat and pressure drop were studied and all the process variables such as temperature, rate of reaction , pressure along length of the reactor were calculated and the data obtained from the mathematical package showed that with the increase the reaction temperature the process production , rate of reaction and pressure drop will increase.

Key words: mass transfer heat transfer fixed bed reactor pressure drop catalytic reactor .

الخلاصة :

تعتبر دراسة العمليات الصناعية نظريا أو ما يسمى (Process Modeling) أو لمحاكاة بالحاسوب (Computer simulation) من الدراسات الضرورية والتي تعطي المهندس وصفا عما يحدث في عملية معينة ضمن علاقات رياضية متناسقة تربط بين متغيرات العملية.

يتضمن البحث دراسة ظواهر الانتقال في مفاعل الحشوة الثابتة حيث تعتبر ظواهر الانتقال من الظواهر المهمة وذات تأثير كبير على أداء العامل المساعد في مختلف التفاعلات الكيميائية التي يدخل بها.

انطلاقا من هذه الأهمية تم دراسة سرعة التفاعل وتاثير الضغط و دراسة

التغيير في درجات الحرارة خلال المفاعل وتم تحليل البيانات المحسوبة من الموديل الرياضي ومعرفة التغير في إنتاجية التفاعل والحرارة والضغط على طول حشوة العامل المساعد .

حيث بينت النتائج انه بزيادة كمية العامل المساعد يمكن زيادة إنتاجية العملية ضمن معامل انتشار وحرارة محددة بالاضافة الى زيادة هبوط الضغط على طول الحشوة .

كل هذه العوامل تعطي وصف شامل لما هو موجود فعلا في موقع العمل الفعلي وبذلك يمكن تحديد فيما إذا كان أداء الوحدة منسجم مع تغيير العوامل المؤثرة فيها.

Introduction:

One of the most important and critical processes in petroleum refineries is the catalytic process in which we get more valuable products used in industry. The mathematical modeling for such processes will be very important to evaluate and to understand the performance and how to overcome the operating problems that may occurs. Many factors are affecting any processes such as the operating conditions, catalyst types and its properties.

So in our model we first try to study these factors theoretically and how it affect the results we get, and second to compare the actual data obtained from refinery with our model and how does the data deviate in these two cases. This report deals with the first case and in our future work we shall study the second case [1, 2] .

Energy Balance ;

Our attention was focused on heat effects in chemical reactors. The basic design equations rate laws and stoichiometric relationships will be derived for non-isothermal reactor. An energy balance will be carried out on the open system as shown in figure(1) [3] .

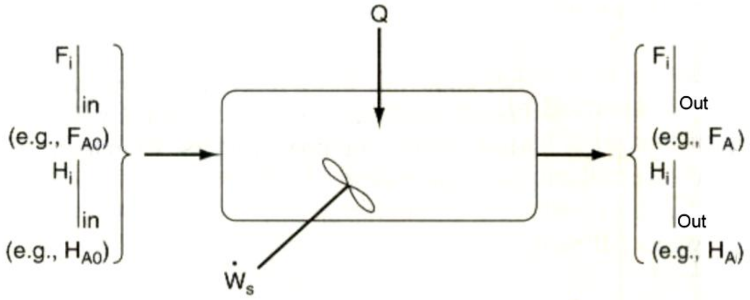

Figure (1) Energy balance on an open system: schematic.

[flow rate of heat to the system from the surrounding] - [rate of work done by the system on the surrounding] + [rate of energy added to the system] - [rate of energy leaving the system] = [rate of accumulation of energy with in the system]

$$Q - w^{\circ} + \sum E_i * F_i |_{in} - \sum E_i * F_i |_{out} = \frac{dE_{sys.}}{dt} \quad ....1$$

Evaluating the Work Term :

The work can be classified into flow work and shaft work. Flow work is the work that is necessary to get the mass into and out of the system and the shaft work could be produced from a stirrer in a CSTR or a turbine in a PFR.

as in eq. below [3]

$$w^{o} = -\sum F_i * p * V_i |_{in} + \sum F_i * p * V_i |_{out} + w_s \quad ....2$$

sub eq. 2 in 1 we get

$$Q - w_s + \sum F_i * \left(E_i + P * V_i\right)|_{in} - \sum F_i * \left(E_i + P * V_i\right)|_{out} = \frac{dE_{sys.}}{dt} \quad ....3$$

The energy E_i is the sum of the internal energy (U_i), kinetic energy ($u_i^2/2$),and the potential energy (gz_i). In almost all chemical reactor the kinetic, potential energy terms are negligible in comparison with in the enthalpy so the energy equal to the internal energy [3, 4]

$$E_i = U_i \qquad \text{……… 4}$$

The enthalpy (Hi) is defined in terms of the internal energy and the product PV .as below :-

$H_i = U_i + P*V_i \longrightarrow U_i = H_i - P*V_i$ ……..5

sub eq. 5 into eq.3

$$Q - w_s + \sum F_i * H_i \mid_{in} - \sum F_i * H_i \mid_{out} = \frac{dE_{sys.}}{dt} \qquad \text{……… 6}$$

Eq. 6 describes the Overall Energy Balance on a flow reactor.

Assumptions:-

- Steady state conditions, $\frac{dE_{sys.}}{dt} = 0$
- Reaction is carried out is first order in a packed bed reactor.
- Adiabatic condition. $Q = o$
- Neglected the work done. $W_s = 0$

So eq.6 become:-

$$\sum F_i * H_i \mid_{in} - \sum F_i * H_i \mid_{out} = 0 \qquad \text{………7}$$

The express the molar flow rate in terms of conversion:-

For reaction $A \longrightarrow B$

$$F_i = F_{Ao} * (\theta_i + \upsilon_1 * \chi) \qquad \text{.........} 8$$

So the flow rate for A and B

$$F_A = F_{Ao} * (1 - \chi)$$

$$F_B = F_{Ao} * (\theta_B + \chi) \qquad \text{........} 9$$

sub. Eq. 9 into eq. 7

In $$\sum H_{i^o} * F_{i^o} = H_{A^o} * F_{A^o} + H_{B^o} * F_{B^o}$$

Out $$\sum H_i * F_i = H_A * F_A + H_B * F_B$$

Subtraction

$$H_{A^o} * F_{A^o} + H_{B^o} * F_{B^o} - H_A \times [F_{A^o} * (1 - \chi)] - H_B \times [F_{A^o} * (\theta_B + \chi)]$$

$$F_{A^o} * (H_{A^o} - H_A) + F_{A^o} * \theta_B * (H_{B^o} - H_B) - \underbrace{[H_B - H_A]}_{\Delta H_R} * F_{A^o} * \chi \qquad \text{.......}10$$

Express the enthalpy term:-

$$H_{i^o} - H_i = \int_{T_o}^{T} cp_i * dT \qquad \text{.........}11$$

sub. eq. 11 and eq. 10 into eq. 7

$$\left(\int_{T_o}^{T}\sum \theta_i * cp_i * dT\right) * F_{A^o} - \Delta H_R * F_{A^o} * \chi = 0 \quad \ldots\ldots\ 12$$

Express the heat of reaction term:-

$$\Delta H_R = \Delta H_{R^o(TR)} + \int_{T_R}^{T} cp_i * dT \quad \ldots\ldots 13$$

sub. eq.13 into eq. 12

$$\chi * \left[\left(\Delta \mathrm{H}_{R^o(TR)}\right) + \int_{T_R}^{T}\Delta cp * d\mathrm{T}\right] = \int_{T_o}^{T}\sum \theta_i * cp_i * d\mathrm{T} \quad \ldots\ldots\ldots\ 14$$

This is the Energy Balance eq. for Adiabatic Packed Bed Reactor (PBR).

Open the brackets on eq. 14

$$\Delta \mathrm{H}_{R^o(TR)} * \chi + \int_{T_R}^{\mathrm{T}}\Delta cp * d\mathrm{T} * \chi = -\int_{\mathrm{T}_o}^{\mathrm{T}}\sum \theta_i * cp_i * d\mathrm{T} \quad \ldots\ldots\ldots 15$$

Differentiate eq. 15 with respect to V

$$\Delta \mathrm{H}_{R^o(TR)} * \frac{d\chi}{dV} + \int_{T_R}^{\mathrm{T}}\Delta cp * d\mathrm{T} * \frac{d\chi}{dV} + \chi * \Delta cp_i * \frac{d\mathrm{T}}{dV} = -\theta_i * cp_i * \frac{d\mathrm{T}}{dV}$$

$\ldots\ldots\ldots 16$

Rearrange eq. 16

$$-\left(\Delta \mathrm{H}_{R^o(TR)} + \int_{T_R}^{\mathrm{T}}\Delta cp * d\mathrm{T}\right) * \frac{d\chi}{dV} = \left(\sum \theta_i * cp_i + \Delta cp_i * \chi\right) * \frac{d\mathrm{T}}{dV} \quad \ldots\ldots\ldots 17$$

Eq. 17describes the change of temperature and conversion across the volume of a PBR.

Mole Balance:

We will now perform the general mole balance equation for PBR reactor as shown in figure 2. [3, 4]

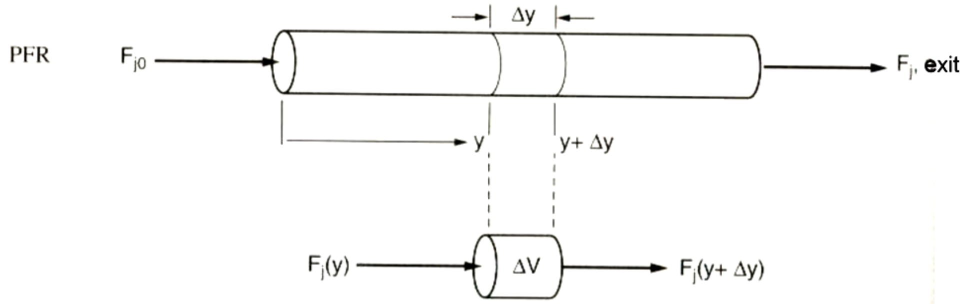

Figure (2) Tubular reactor.

$$F_{i(x)} + F_{i(x+\Delta x)} + r_i * \Delta V = \frac{dN_i}{dt}$$

………18

Assumptions:

- ❖ Steady state conditions, $\frac{dN_i}{dt} = 0$
- ❖ Reaction that is carried out is a first order in a packed bed reactor.

After applying the assumptions

$$F_{i(x)} + F_{i(x+\Delta x)} + r_i * \Delta V = 0 \quad ....19$$

The volume ΔV is the product of the cross sectional area A of the reactor length Δx.

$$\Delta V = A * \Delta x \quad ....20$$

Sub eq. 20 into eq. 19 and divide by Δx and then taking the limit as Δx approaches zero

$$\frac{dF_i}{dV} = -r_i \quad ....21$$

Recall eq. 9 $F_A = F_{Ao} * (1 - \chi)$

After differentiate eq. 9 and sub it in eq. 21

$$\frac{d\chi}{dV} = \frac{1}{F_{\mathrm{A}^o}} * (-r_A) \quad ....22$$

Eq. 22 is the Mole Balance eq. on the steady state PBR.

Sub. eq. 22into eq. 17

$$-\left(\Delta \mathrm{H}_{R^o(TR)} + \int_{T_R}^{T} \Delta cp_i * d\mathrm{T}\right) \times (-r_{\mathrm{A}}) = F_{\mathrm{A}^o} * \left(\sum \theta_i * cp_i + \Delta cp_i * \chi\right) * \frac{d\mathrm{T}}{dV}$$

.........23

Arrangement of eq.23

$$\frac{d\mathrm{T}}{dV} = \frac{-\left(\Delta \mathrm{H}_{R^o} + \int_{\mathrm{T}_R}^{\mathrm{T}} \Delta cp_i * d\mathrm{T}\right) \times (-r_{\mathrm{A}})}{F_{\mathrm{A}^o} * \left(\sum \theta_i * cp_i + \Delta cp_i * \chi\right)} \quad ....24$$

Eq.14 describes the change on temperature a long the volume of PBR.

Heat Capacity Calculations:

The form of energy balance in the case where heat capacities are strong functions of temperature over a wide temperature range. Combining equation (24)with the quadratic form of the heat capacity [5] .

$$cp_i = \alpha_i + \beta_i * T + \gamma_i * T^2 \quad \text{.........25}$$

$$\Delta cp_i = \Delta\alpha_i + \Delta\beta_i * \mathrm{T} + \Delta\gamma_i * \mathrm{T}^2 \quad \text{.........26}$$

Sub. Eq. 25,and eq,.26 into eq.24, and integrating :

$$\frac{d\mathrm{T}}{dV} = \frac{-\left[\Delta \mathrm{H}_{R^o} + \Delta\alpha_i * (\mathrm{T} - \mathrm{T}_R) + \frac{\Delta\beta_i}{2} * (\mathrm{T}^2 - \mathrm{T}^2{}_R) + \frac{\Delta\gamma_i}{3} * (\mathrm{T}^3 - \mathrm{T}_R{}^3)\right] \times (-r_A)}{F_{\mathrm{A}^o} * \left[(\theta_i * \alpha_i + \theta_i * \beta_i * T + \theta_i * \gamma_i * T^2) + \chi * (\Delta\alpha_i + \Delta\beta_i * T + \Delta\gamma_i T^2)\right]} \quad \text{.........27}$$

Eq. 27 describes the Energy Balance for the case of highly Temperature sensitive heat capacities for PBR.

Pressure Drop:

It is important to predict the drop in pressure for the flow of the fluid through a packed column. In reactor design there is a pressure drop through a packed of catalyst bed, when there is a liquid – phase reactions, the concentration of reactant is insignificantly affected by even relatively large change in the total pressure. Consequently, we can totally ignore the effect of pressure drop on the rate of reaction when sizing liquid – phase chemical reactors.

However, in gas – phase reactions, the concentration of reacting species is proportional to the total pressure and consequently, proper accounting for the effect of pressure drop on the reaction system can, in many instances, be a key factoring the success or failure of the reactor operation [6, 7].

Pressure drop & the Rate Law:

Our attention is focused on the accounting for the pressure drop on the rate law, for gas - phase reactions pressure drop may be very important. [8]

For an ideal gas, the concentration of reacting species (I)

$$C_i = \frac{F_i}{v_i} \qquad = \frac{F_{A^o} * (\Theta_i + \nu_1 * \chi)}{v_o * (1+\varepsilon * \chi) * \left({}^{P_1}\!/_{P} \right) * \left({}^{T}\!/_{T_o} \right)}$$

$$C_i = \frac{C_{A^o} * (\Theta_i + \nu_i * \chi)}{(1+\varepsilon * \chi)} * \left({}^{P}\!/_{P_1} \right) * \left({}^{T_o}\!/_{T} \right) \quad \text{……..28}$$

Now determine the ratio (P/P∘) as a function of volume of the reactor to account for pressure drop then combine the concentration , rate law , temperature and design equations in differential form and then solved simultaneously to understand the behavior of reactor

First order isomerization of n-hexane reaction is being carried out in a packed – bed – reactor [8] ,

$$A \longrightarrow B$$

The differential form of material balance in term of volume of reactor

$$F_{A^o} * \frac{d\chi}{dV} = -r_A \quad \text{………29}$$

$$-r_A = k * C_A \quad \text{………30}$$

sub. Eq. 28 into eq. 30,

$$-r_A = k * \frac{C_{A^o} * (\Theta_i + \nu_1 * \chi)}{(1 + \varepsilon * \chi)} * \left({}^{P}\!/_{P_1} \right) * \left({}^{T_o}\!/_{T} \right) \quad \text{……….31}$$

sub. Eq. 31 into eq. 29,

$$\frac{d\chi}{dV} = \frac{k}{F_{A^o}} * \frac{C_{A^o} * (\Theta_i + \nu_1 * \chi)}{(1 + \varepsilon * \chi)} * \left({}^{P}\!/_{P_1} \right) * \left({}^{T_o}\!/_{T} \right) \quad \text{……….32}$$

Pressure Drop Equation:

The most equation used to calculate the pressure drop in a packed of porous bed is the Ergun equation:

$$\frac{\partial P}{\partial L} = -\frac{G}{\rho * g * D_p} * \left\langle \frac{1-\varphi}{\varphi^3} \right\rangle * \left[\frac{150(1-\varphi) * \mu}{D_p} + 1.75 * G \right] \quad \text{……..33}$$

The only parameter that varies in eq. 33 is the gas density (ρ) , and because the reactor is operated at steady state , the mass flow rate at any point down the reactor (mo) is equal to the entering mass flow rate(m) (equation of continuity) [7].

$$m_o = m \longrightarrow \rho_o * v_o = \rho * v \qquad \text{........34}$$

Where ,

$$v = v_o * \frac{P_1}{P} * \frac{T}{T_o} * \frac{F_T}{F_{To}} \qquad \text{........35}$$

So ,

$$\rho = \rho_o \frac{v_o}{v} = \rho_o * \frac{P}{P_1} * \frac{T_o}{T} * \frac{F_{To}}{F_T} \qquad \text{.........36}$$

Combine eq.36 with eq.33

$$\frac{dP}{dL} = -\frac{G}{\rho_o * g * D_p} * \left\langle \frac{1-\varphi}{\varphi^3} \right\rangle * \left[\frac{150(1-\varphi) * \mu}{D_p} + 1.75 * G \right] * \frac{P_1}{p} * \frac{T}{T_o} * \frac{F_T}{F_{To}}$$

……..37

Finally substitute for F_T / F_{TO}

$$F_T = F_{To} + F_{Ao} * \delta * \chi$$

$$\frac{F_T}{F_{To}} = \left[1 + \left(\frac{F_{Ao}}{F_{To}} \right) * \delta * \chi \right] \qquad \text{……..38}$$

$$\frac{F_T}{F_{To}} = [1 + y_{Ao} * \delta * \chi] \longrightarrow \frac{F_T}{F_{To}} = [1 + \varepsilon\chi]$$

.

……….39

Sub. Eq.39 into eq. 37

$$\frac{dP}{dL} = -\frac{G}{\rho_o * g * D_p} * \left\langle \frac{1-\varphi}{\varphi^3} \right\rangle * \left[\frac{150(1-\varphi) * \mu}{D_p} + 1.75 * G \right] * \frac{P_1}{p} * \frac{T}{T_o} * (1 + \varepsilon\chi)$$

…..….40

let

$$\beta = -\frac{G}{\rho_o * g * D_p} * \left\langle \frac{1-\varphi}{\varphi^3} \right\rangle * \left[\frac{150(1-\varphi) * \mu}{D_p} + 1.75 * G \right]$$

$$\frac{dP}{dL} = -\beta * \frac{P_1}{p} * \frac{T}{T_o} * (1 + \varepsilon\chi)$$ ………41

Eq. 41 describes the pressure drop down the PFR.

Results and Discussions:

After we described the material, heat and momentum transfer through the adiabatic fixed bed reactor we get 3 differential ordinary equations that we need to solve them simultaneously in order to get how the conversion, temperature and pressure drop varies down the length of the reactor [3].

The equations are shown below

$$\frac{d\chi}{dV} = \frac{1}{F_{A^o}} * (-r_A)$$

$$\frac{dT}{dV} = \frac{-\left(\Delta H_{R^o} + \int_{T_R}^{T} \Delta cp_i * dT\right) \times (-r_A)}{F_{A^o} * \left(\sum \theta_i * cp_i + \Delta cp_i * \chi\right)}$$

$$\frac{dP}{dL} = -\beta * \frac{P_1}{p} * \frac{T}{T_o} * (1 + \varepsilon\chi)$$

To solve these equations a mathematical package is used named ***"Polymath 5.1"*** so the equations with initial and final limits with the definition of the explicit equations, constants and the initial operating condition are entered.

After the run of the program, the final report for data that describe the change in conversion, temperature and pressure drop and rate of reaction down the length of reactor. (Appendix A shows the interface of program) [3]

The case is studied in this research is from reference No. 8

A plot of a conversion& temperature along the length of reactor is shown in figures (3) ,(4).

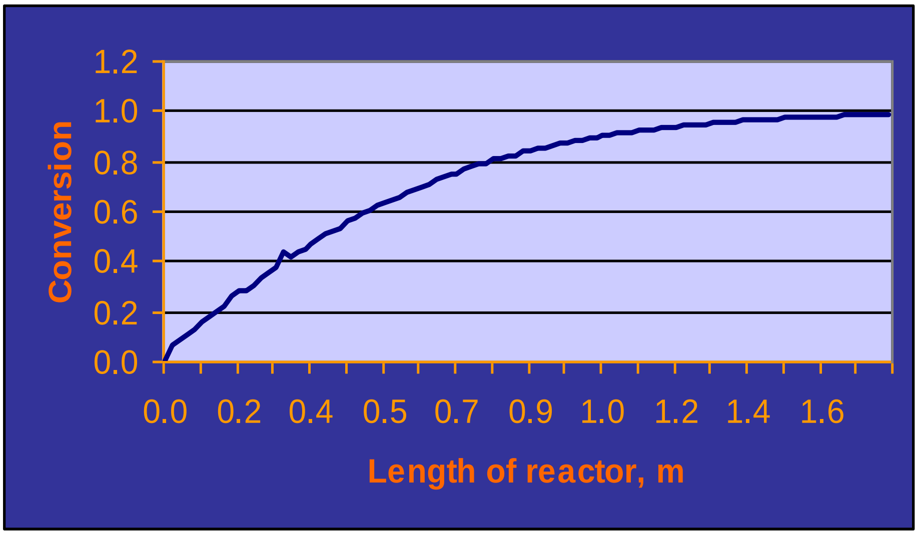

Fig. (3) Conversion down the length of fixed bed adiabatic reactor, T_o =573 K & no pressure drop

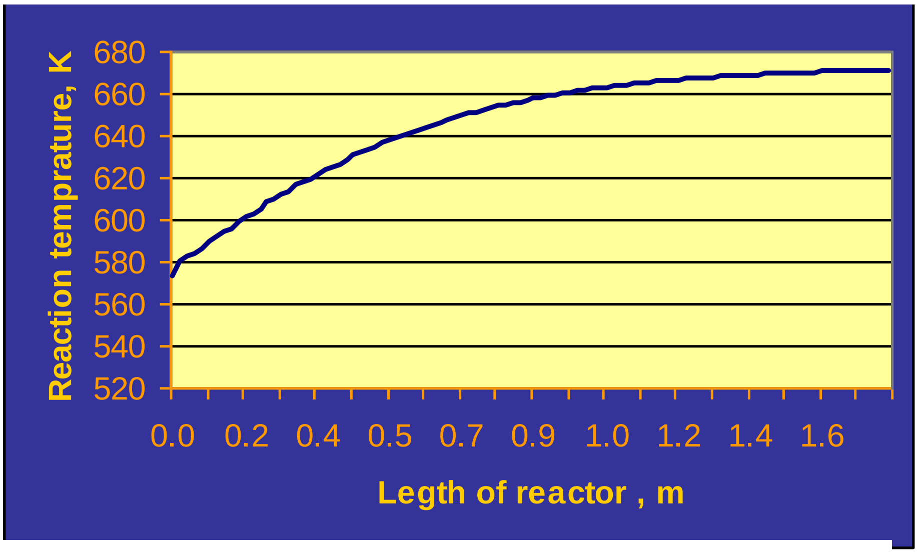

Fig. (4) Change in reaction temperature down the length of fixed bed adiabatic reactor, T_o = 573 K & no pressure drop.

In figure 3 & 4 it is noticed that the conversion increases down the length of the reactor and because of the reaction is exothermic the temperature will also be increased at the same inlet reactor temperature.

Also the reaction rate grows up to maximum value near the entrance of the reactor and then begins to stabilized after 1 m of the reactor length as shown in figure(5).[8]

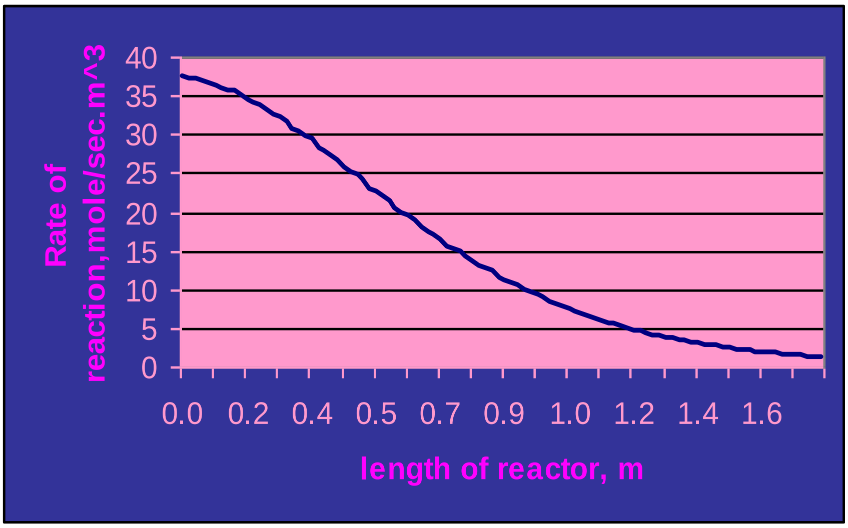

Fig. (5) Rate of reaction down the length of fixed bed adiabatic reactor, T_o =573 K & no pressure drop.

One way may be needed to decrease the accumulated heat or temperature due to the exothermic reaction by adding a coolant to maintain a certain high conversion and reaction rate for the process [9] .

We can see from figures (6) & (7) that increasing bed pressure will results in compressing the bed then reducing the voids between the molecules (dense packing).

Moreover fluid resistance to flow will be high; consequently the substance amount that moves forward the active sites of the catalyst will be slight. Accordingly less conversion and low reaction speed will be obtained [6].

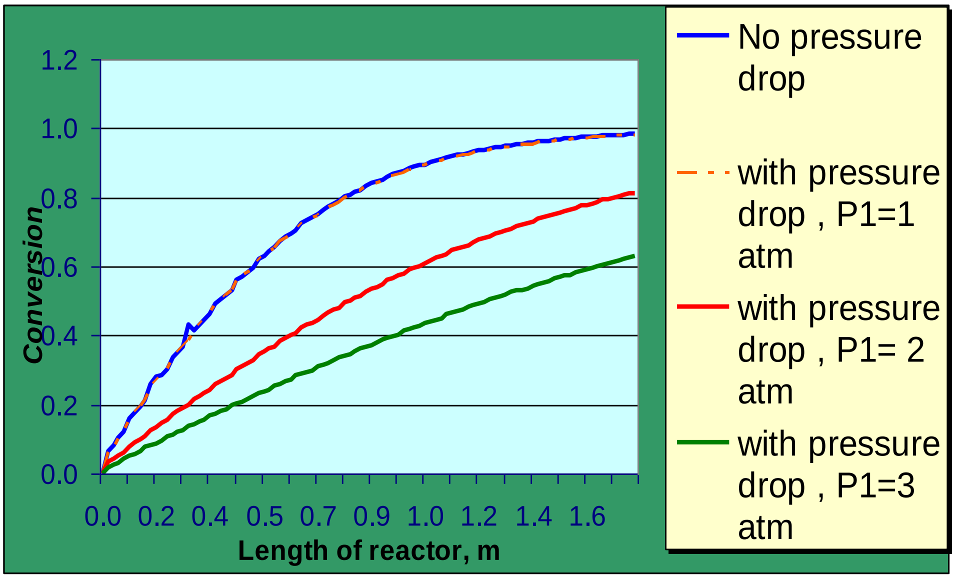

Fig. (6) Change in Conversion down the length of Fixed bed adiabatic reactor ,T_o=573 K.

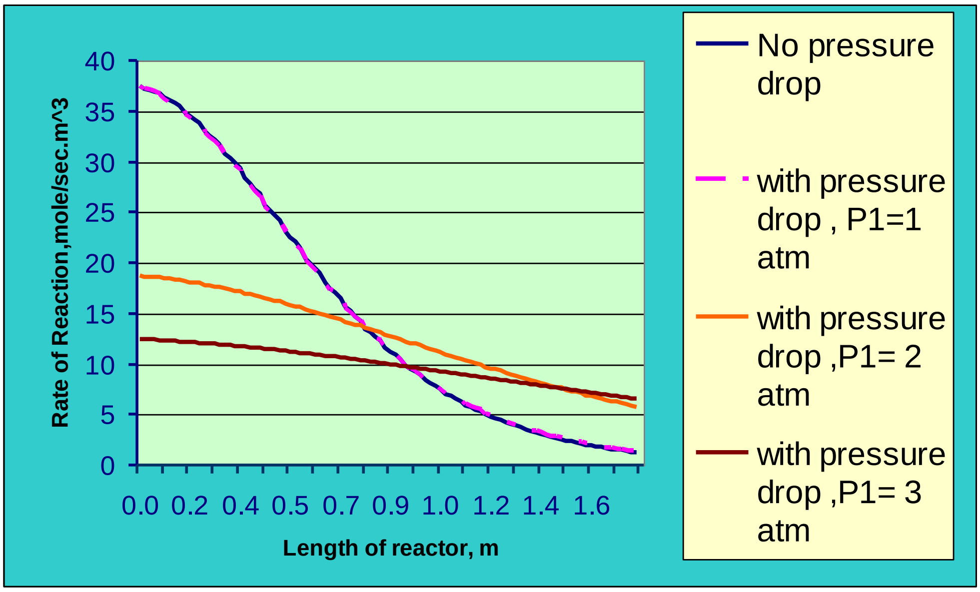

Fig. (7) Change in rate of reaction down the length of Fixed bed adiabatic reactor ,T_o=573 K.

Also we can see that when changing the initial reaction temperature the conversion also increases at a certain operating pressure as shown in figure (8) [10].

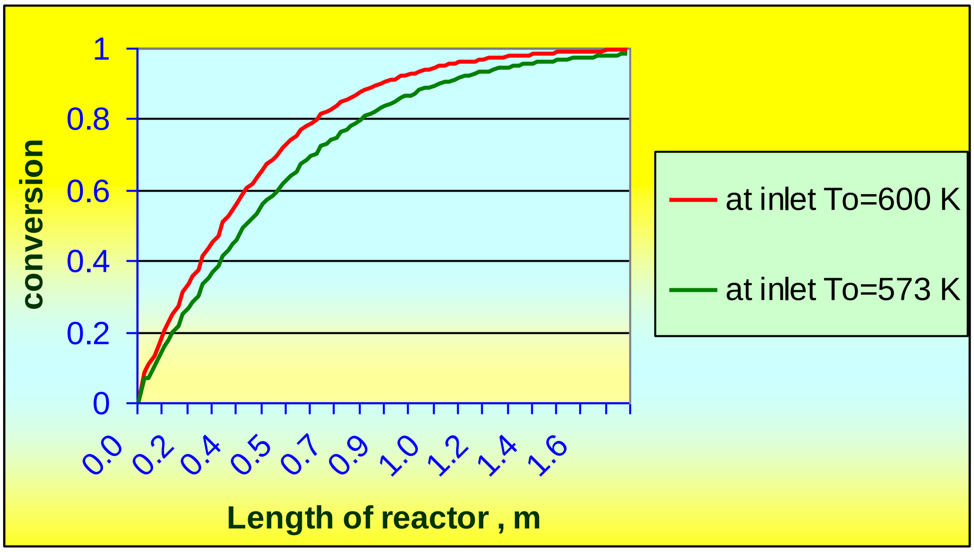

Fig. (8) Change in Conversion down the length of fixed bed adiabatic reactor P1 = 1 atm.

figure (9) shows the change in the pressure drop down the length of the reactor, and it's obviously that pressure increases through the bed of the catalyst and many factors are affecting this pressure such as the fluid mass velocity, porosity of the bed, properties of the reacting fluid and the operating conditions.

All these factor are included in the pressure drop equation (41).

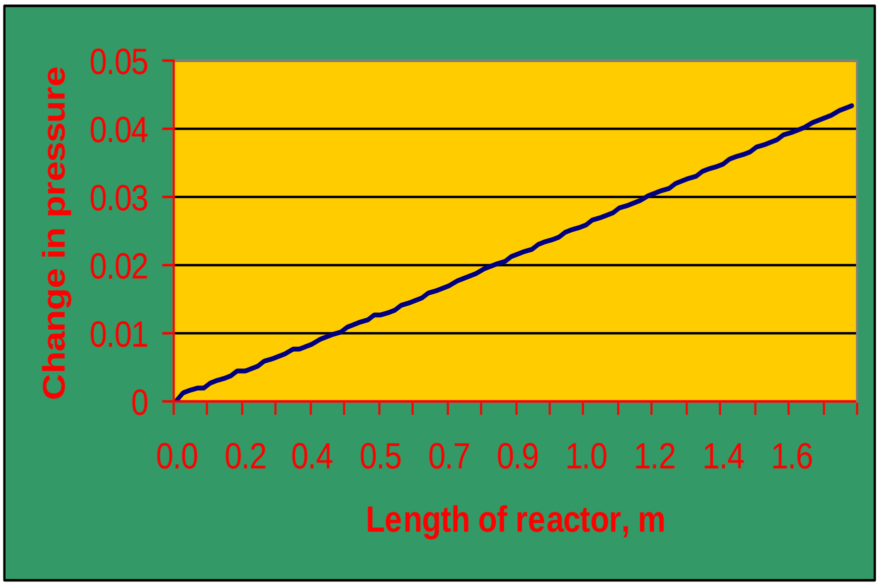

Fig. (9) Change in pressure down the length of Fixed bed adiabatic reactor, T_o=573 K.

Conclusions:

- The pressure drop affects the reaction rate, so by increasing the inlet pressure the rate of reaction will be decreased from 38 to 13 mole / sec.m^{3}when the pressure drop is changed from 0 to 3 atm.
- The conversion will be increased from 80 -90 % by increasing the reaction temperature from 573 –600 K at 1 m length of the reactor.
- The effect of time on operation must be considered on the future work by studying the effect on unsteady state condition on the reactor such as (rate of reaction, temperature and on the pressure drop)

References:

1. Diffusion in Porous Media, Modern Methods in Heterogeneous Catalysis; 2001 lectures at Fritz –Harber Institute.

2. James W.Fulton, Journal of Chemical Engineering, 1988, "Building the Mathematical Model of the Catalyst and Reactor"

3. H .Scott Fogler, 1999,"Elements of Chemical Reaction Engineering", Third Edition.

4. Octave Levenspiel, 1999, "Chemical Reaction Engineering", Third edition.

5. Robert h. Perry, Don w. Green, 1997, "Perry's Chemical Hand Book".

6. Marwa N.Abass, 2008, "Prediction of Pressure Drop in Packed Bed for Water & Air Systems". MS_C.Thesis, Nahreen University.

7. James R.welty, Charles E.wicks, Rober E.wilson and Gregory Romer, 2001, "Fundamentals of Momentum, Heat, and Mass transfer" Fourth Edition.

8. Ban Abdul-Rahman Ahmed, 2000,"Isomerization of n-hexane over Platinum Supported Catalyst by Using Some Monitoring Agents", MS_C.Thesis, Nahreen University.

9. Reactor Design within Excel Enabled by Rigorous Physical Properties and an Advanced Numirical Computation Package. M. Shacham, M.B. Cutlip, Dept. of Chem. Eng., University of Connectcut, USA.

10. Jens Hagen, 2006, "Industrial Catalysis", Second Edition.

Nomenclature

Symbols ***Notations***

A = Cross sectional area of reactor (m^2).

C_{Ao} = Initial concentration (mole / m^3).

C_{Pi} = Heat capacity of species i at temperature T (J/mole.K).

D_p = Diameter of particles in bed (m).

E_i = Energy of species i (J/s).

E_{system} = Total energy of the system (J/s).

F_A = Molar flow rate of species A (mole/s).

F_B = Molar flow rate of species B (mole/s).

F_{A0} = Initial molar flow of species A (mole/s).

F_{B0} = Initial molar flow of species i (mole/s).

F_i = Molar flow rate of species i (mole/s).

F_{io} = Initial molar flow of species i (mole/s).

F_T = Total molar flow (mole/s).

F_{T0} = Initial total molar flow (mole/s).

G = Superficial mass velocity (Kg/m^2.s).

g = Conversion constant.

H_A = Enthalpy of species A at temperature T (J/mole).

H_B = Enthalpy of species B at temperature T (J/mole).

H_i = Enthalpy of species i at temperature T (J/mole).

H_{io} = Enthalpy of species i at temperature T_0 (J/mole)

H_i^o = Enthalpy of formation of species i at temperature T_R (J/mole)

κ = Reaction rate constant (s^{-1}).

L = Length of reactor (m).

m = Mass flow rate (Kg/s).

m_0 = Entering molar flow rate (Kg/s).

N_i = Number of mole of species i (mole).

P = Partial pressure (atm).

P_1 = Initial pressure (atm).

Q = Heat flow from the surrounding to the stream (J/s).

r_A = Rate of generation of species A (mole/s. m^3).

r_i = Rate of generation of species i (mole/s. m^3).

T = Temperature (K).

T_o = Initial temperature (K).

T_R = Standard temperature 298 K.

U_i = Internal energy of species i (J/mole).

V = Volume of reactor (m^3).

ν = Volumetric flow rate (m^3/s).

ν_1 = Stoichiometric coefficient.

$v_\circ$ = Initial volumetric flow rate (m^3/s).

w^o = Flow work (J/s).

w_s = Shaft work (J/s).

$\mathcal{X}$ = Conversion.

x = Distance (m).

y_A = Ratio of F_{A0}/F_{T0}

Θ_i = Ratio of the number of mole of species i initially (entering) to the number of moles of A initially (entering).

Θ_B = Ratio of the number of mole of species B initially (entering) to the number of moles of A initially (entering).

ΔH_R = Heat of reaction at any T (J/mole).

ΔH_R^0 = Slandered heat of reaction at 298 ^{0}K (J/mole).

Greek Symbols

φ = Porosity of the bed.

μ = Fluid viscosity (kg/m.s).

ρ = Density of the fluid (kg/m^3).

γ = Parameter in heat capacity.

β_i = Parameter in heat capacity.

β = Constant on pressure drop equation.

α_i = Parameter in heat capacity.

APPENDIX (A)

Polymath Report

No Title 2009-23-3 ,Rev5.1.233

Calculated values of the DEQ variables

Variable	initial value	minimal value	maximal value	final value
L	0	0	1.7	1.7
T	600	600	686.12897	686.12897
X	0	0	0.8864842	0.8864842
p	1	0.9142779	1	0.9142779
k	9.6141882	9.6141882	19.257226	19.257226
Fao	1.2	1.2	1.2	1.2
Cp1	91.688	91.688	98.397328	98.397328
Cp2	2.668	2.668	2.7597932	2.759095
Cao	6.08	6.08	6.08	6.08
T0	600	600	600	600
TR	298.15	298.15	298.15	298.15
HR	-9501.7539	-9501.7539	-9214.9245	-9214.9245
p1	2	2	2	2
Ac	0.045	0.045	0.045	0.045
ra	24.355943	4.4275751	24.355943	4.4275751
B	0.0221	0.0221	0.0221	0.0221

ODE Report (RKF45)

Differential equations as entered by the user

[1] $$d(T)/d(L) = (A*r_A)*((-1)*HR)/(F_A{}^o*(Cp_1+X*Cp_2))$$

[2] $$d(X)/d(L) = (A*r_A)/F_A{}^o$$

[3] $$d(p)/d(L) = -1.0*B*(p_1/p)*(T/T_0)$$

Explicit equations as entered by the user

```
[1] k = 2433.291*exp(-3320.256/T)
[2] FAo = 1.2
[3] Cp1 = 17.84+0.17*T-0.000089*(T^2)+0.000000018*(T^3)
[4] Cp2 = -9.02+0.043*T-0.00005*(T^2)+0.000000018*(T^3)
[5] CAo = 6.08
[6] T0 = 600
[7] TR = 298.15
[8] HR = -10125.3+(-9.02385*(T-TR)+0.022*((T^2)-(TR^2))-1.67e-5*((T^3)-
(TR^3))+0.0000000045*((T^4)-(TR^4)))
[9] p1 = 2
[10] A = 0.045
[11] ra = (k*CAo/FAo)*(1-X)*(T0/T)*(p/p1)
[12] B = 0.0221
```

Comments

```
[1] d(T)/d(L) =  (A*rA)*((-1)*HR)/(FAo*(Cp1+X*Cp2))
    energy balance eq .
[2] d(X)/d(L) =          (A*rA)/FAo
    rate eq.[mole balance
[3] d(p)/d(L) =     -1.0*B*(p1/p)*(T/T0)
    pressure drop eq .
[4] k =             2433.291*exp(-3320.256/T)
    rate constant eq .
[5] FAo =      1.2
    molar flow rate mole /sec
[6] Cp1 =      17.84+0.17*T-0.000089*(T^2)+0.000000018*(T^3)
    summation of heat capacity
[7] Cp2 =      -9.02+0.043*T-0.00005*(T^2)+0.000000018*(T^3)
    delta specific heat capacity of reactant and product

[8] CAo =          6.08
    intial concentration of reactant, mole /m^3
[9] T0 =  600
    inlet tepmrature of reactant
[10] TR =                    298.15
     referance temprature
[11] HR =      -10125.3+(-9.02385*(T-TR)+0.022*((T^2)-(TR^2))-1.67e-5*((T^3)-
(TR^3))+0.0000000045*((T^4)-(TR^4)))
     heat of reaction
[12] ra =      (k*Cao/Fao)*(1-X)*(T0/T)*(p/p1)
```

rate equation

[13] Ac = 0.045

cross sectional area of the reactor

[14] p1 = 2

intial pressure

Independent variable

variable name : L

initial value : 0

final value : 1.7

Precision

Step size guess. h = 0.000001

Truncation error tolerance. eps = 0.000001

General

number of differential equations: 3

number of explicit equations: 12