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SIMULTANEOUS MASS, HEAT AND MOMENTUM TRANSFER IN AN ADIABATIC PACKED BED REACTOR

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ABSTRACT

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

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

Simultaneous mass , heat and pressure drop have been 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 shows that with increasing the reaction temperature the process production , rate of reaction and pressure drop will increase.

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 its affects on the results we get, and second we want to compare between the actual data obtained from refinery with our model and how does the data deviate between these two cases. This report deals with the first case and in our further work we shall study the second case.[1],[2]

ENERGY BALANCE

We are now focus our attention on heat effects in chemical reactors. The basic design equations rate laws and stoichiometric relationships will derive for non-isothermal reactor. We shall carry out an energy balance on the open system as shown in figure 1.

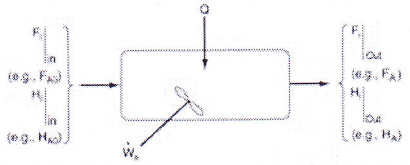

Figure (1) Energy balance on an open system schematic.

[rate of flow 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][2]

$$Q - w^{o} + \sum E_i * F_h \mid_{in} - \sum E_i * F_i \mid_{out} = \frac{dE_{sys.}}{dt} \qquad (1)$$

Evaluating the Work Term

The work is separate into flow work and shaft work.
Flow work is work that is necessary to get the mass into and out the system and the shaft work could be produced from such things as a stirrer in a CSTR or a turbine in a PFR.
As in eq. below[3]

$$w^{o} = -\sum F_i * p * V_i \mid_{in} + \sum F_i * p * V_i \mid_{out} + w_s \qquad (2)$$

Sub. Eq.1 into eq.2

$$Q - w_s + \sum F_i * (E_i + P * V_i) \mid_{in} - \sum F_i * (E_i + P * V_i) \mid_{out} = \frac{dE_{sys.}}{dt} \qquad (3)$$

The energy E_i is the sum of the internal energy (u_i), the kinetic energy ($u_{i2}/2$),the potential energy (gz_i),and 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.[2],[3]

$$E_i = U_i \qquad (4)$$

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

$$H_i = U_i + P * V_i$$

$$\downarrow$$

$$U_i = H_i - P * V_i \qquad (5)$$

Sub eq. 5 into eq.3

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