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Modeling and Simulation of Natural gas dehydration reactor

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Abstract:

Natural gas is an important source of primary energy that, under normal production conditions, is saturated with water vapor. Water vapor in a natural gas stream can result in line plugging due to hydrate formation, reduction of line capacity due to collection of free water in the line, and increased risk of damage to the pipeline due to the corrosive effects of water. Therefore, water vapor must be removed from natural gas to prevent hydrate formation and corrosion from condensed water. Gas dehydration is the process of removing water vapor from a gas stream to lower the temperature at which water will condense from the stream; this temperature is called the ''dew point'' of the gas. There are several methods of dehydrating natural gas. The most common of these are liquid desiccant (glycol) dehydration, solid desiccant dehydration, and refrigeration. Molecular sieves are considered as one of the most important materials that are used as solid desiccant materials in industrial natural gas dehydration. In the present study, a steady state mathematical model was developed to simulate an adsorption process for dehydration of a gas stream in a fixed bed reactor using molecular sieves. Pressure drop inside the bed was calculated by Ergun equation. Heat transfer outside the solid particles was assumed to be convective and inside the particle was assumed to be diffusive. The results obtained from the mathematical model were verified against the ones obtained from a Liquefied Natural Gas Company in Egypt. The model predictions agreed well with the industrial data and the percentage error was very small. The percentage error in case of applying momentum balance equations was -6.7% and -2.9% in case of applying heat balance equations. The error in case of applying heat balance equation was less than that applied by momentum balance equation. Different parameters such as bed voidage, particle diameter, superficial gas velocity, gas density, and gas viscosity were studied to determine their effects on the pressure drop inside the reactor. It was found that pressure drop increases linearly with increasing superficial gas velocity, gas density, and gas viscosity and decreases linearly with increasing bed voidage, and particle diameter. The most effective parameter on the pressure drop is the bed voidage.

Key words: Dehydration, Fixed bed Reactor, heat transfer, Mathematical Modeling, Natural Gas Treatment, pressure drop, Simulation.

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1. Introduction:

Natural gas is one of the most important fuels in our life and one of the principle sources of energy for many of our day to day needs and activities [1]. Natural gas is used primarily as a fuel and as a raw material in manufacturing. It is used in home furnaces, water heaters, and cooking stoves. As an industrial fuel, it is used in manufacturing brick, cement, and ceramic-tile kilns; in glass making; aviation; hydrogen production; for generating steam in water boilers; and as a clean heat source for sterilizing instruments and processing foods. As a raw material in petrochemical manufacturing, natural gas is used in a range of fertilizers and as a secondary feed stock for manufacturing other chemicals, including nitric acid and urea. Ethylene, an important petrochemical, is also produced from natural gas [2]. Natural gas is considered as an environmentally friendly clean fuel, offering important environmental benefits when compared to other fossil fuels. The superior environmental quantities over coal or crude oil are that emissions of sulfur dioxide are negligible or that the levels of nitrous oxide and carbon dioxide emissions are lower. This helps to reduce problems of acid rain, ozone layer, or green house gases. Natural gas is also a very safe source of energy when transported, stored, and used [2]. Natural, associated, or non-associated gas usually contains water, in liquid and/or vapor form, at source and/or as a result of sweetening with an aqueous solution, which condense and form solid gas hydrates to block pipeline flow and especially control systems. Natural gas in transit to market should be dehydrated to a controlled water content to avoid hydrate as well as to minimize the corrosion problems [2].There are several methods of dehydrating natural gas. The most common of these are liquid desiccant (absorption) dehydration, solid desiccant (adsorption) dehydration, and refrigeration (i.e., cooling the gas) [3]. Adsorption (or solid bed) dehydration is the process where a solid desiccant is used for the removal of water vapor from a gas stream. The solid desiccants commonly used for gas dehydration are those that can be regenerated and, consequently, used over several adsorption-desorption cycles [1]. The two types of adsorption are physical adsorption and chemical adsorption (chemisorption). Adsorption process has many advantages such as: ability to provide extremely low dew points, less susceptible to corrosion or foaming, simplicity of operation and design of units, less affected by small changes in gas pressure, temperature, or flow rate, and adaptability to dehydration of very small quantities of gas at low cost [4]. The adsorbents most commonly used for dehydration are: Activated carbon, Activated alumina, Silica gel, and Molecular sieves (Zeolites) [5]. In this study, a mathematical model based on the linear driving force model was developed to simulate an adsorption process for dehydration of natural gas stream. The model evaluates the temperature distribution and pressure drop inside the fixed bed reactor. The effects of different parameters on pressure drop inside the reactor were studied. These parameters are: the density of gas mixture, the superficial gas velocity, bed porosity, particle diameter, and gas mixture viscosity. The results obtained from the mathematical model were verified against the ones obtained from a Liquefied Natural Gas Company in Egypt.

2. Model Development:

In this study, a mathematical model based on the linear driving force model was developed to simulate an adsorption process for dehydration of natural gas stream. The model evaluates the temperature distribution and pressure drop inside the fixed bed reactor. The effects of different parameters on pressure drop inside the reactor were studied. These parameters are: the density of gas mixture, the superficial gas velocity, bed porosity, particle diameter, and gas mixture viscosity. The results obtained from the mathematical model were verified against the ones obtained from a Liquefied Natural Gas Company in Egypt.

2.1 Assumptions:

In driving the model, the following assumptions were made [6]:

1- The temperature and concentration variation are absent in the redial direction.
2- The temperature and concentration varies in the axial direction (one dimensional flow).
3- Profiles of temperature and concentrations are assumed flat.
4- The flow of gas among the cylinder bed length is assumed to follow the plug flow pattern.
5- The bed wall is fully insulated.
6- The heat capacity of the bed wall is neglected.
7- Heat transfer in the bed is result of the generated heat due to conduction through the solid particles and the heat transferred from the solid surface to the gas phase by convection.
8- Steady state conditions are assumed.
9- Ergun's equation is applied to predict pressure drop across the bed.

2.2 Model Equations for the fixed bed:

2.2.1. Momentum balance equations:

Ergun's equation was applied to predict pressure drop across the bed by means of the following momentum balance equation [7]:

$$\frac{\Delta P}{L} \cdot \frac{g d_p \phi}{2 \rho_f u^2} \cdot \frac{\varepsilon^2}{(1-\varepsilon)} = 75 \frac{(1-\varepsilon)}{\phi (R_e)_p} + 0.875 \qquad (1)$$

2.2.2. Heat balance equations:

Adsorption is an exothermic process, so heat is generated. The generated heat is conducted to the surface of particles and then transferred to the gas phase by convection: the following equations [6] were obtained:

$$\frac{\partial}{\partial z}\left(k_{eff}\frac{\partial T_b}{\partial z}\right)-\frac{\partial\left(\rho_g U C_{p_g} T_b\right)}{\partial z}-\frac{6(1-\varepsilon_b)h_b}{\varepsilon_b d_p}\left(T_p-T_b\right)=\frac{\partial}{\partial t}\rho_g C_{p_g} T_b$$

$$\frac{\partial}{r^2\partial r}\left(k_s r^2\frac{dT_p}{\partial r}\right)+\sum_{i=1}^{n}\Delta H_i^{ads}\frac{\partial q_{ci}}{\partial t}=\frac{\partial}{\partial t}\left(\rho C_{p_s} T_p\right)$$

(2,3)

The above equations were used to find the distribution of temperature both inside the particles and along the bed.

2.2.3. Momentum and heat transport properties correlations:

2.2.3.1. Bed porosity [8]:

$$\varepsilon_b = 0.4 + 0.5\left(\frac{d_p}{D}\right)+0.412\left(\frac{d_p}{D}\right)^2 \qquad \frac{d_p}{D}\le 0.5$$

(4)

2.2.3.2. Density for ideal gas mixture:

$$\rho = \frac{PM_{wt}}{ZRT}$$

(5)

2.2.3.3. Density of gas mixture:

$$\rho_{mix} = \Sigma y_i \rho_i$$

(6)

2.2.3.4. Heat capacity of gas mixture [9]:

$$C_{p_{mix}} = \Sigma y_i C_{p_i} \qquad (7)$$

2.2.3.5. Viscosity of gas mixture [10]:

$$\mu_{mix} = \frac{\Sigma x_i \mu_i (M_i)^{1/2}}{\Sigma x_i (M_i)^{1/2}} \qquad (8)$$

2.2.3.6. Reynolds number:

$$R_e = \frac{\rho_g v d_p}{\mu_g} \qquad (9)$$

2.2.3.7. Thermal conductivity of gas mixture [11]:

$$(k_g)_{mix} = \frac{\Sigma y_i k_i (M_i)^{1/3}}{\Sigma y_i (M_i)^{1/3}} \qquad (10)$$

2.2.3.8. Convective heat transfer coefficient [6]:

$$h_b = \frac{N_u k_f}{d_p}$$

$$Nu_D = 2 + 1.1 \Pr^{1/3} R_e^{0.6} \qquad R_e = \text{up to } 4000 \qquad (11,12)$$

2.2.3.9. Effective thermal conductivity [12]:

$$K_{eff} = (1-\varepsilon)K_S + K_{g_{mix}} \tag{13}$$

2.2.3.10. Superficial velocity:

$$U = \frac{Q}{cross\ sectional\ area} \tag{14}$$

3. Results and discussion:

The model developed for dehydration of natural gas was checked against a liquefied natural gas plant in Egypt. The measured and calculated values of pressure drop and temperature were in good agreement. Different parameters were studied to determine their effects on pressure drop and heat transfer inside the reactor. This analysis was applied using momentum and heat balance equations. MATLAB software which is a tool for solving numerical mathematics both linear equations and differential equations was used for solving the heat balance equation.

3.1 Validation of the model:

3.1.1. Validation of pressure drop inside the reactor:

The calculated values of pressure drop obtained by this model were compared with the actual values and a deviation of -6.71% was obtained as shown in table (1).

3.1.2. Validation of temperature inside the reactor:

The results indicated that a very good agreement between the model predictions and industrial values have been reported for evaluating temperature inside the reactor. A deviation of -2.9% was found to be for temperature values inside the reactor as shown in table (2).

3.2 Effect of particle diameter on pressure drop:

As shown in figure (1), when the particle diameter increases the pressure drop decreases. The particle diameter affects the friction factor which has a direct effect on the pressure drop. Increasing the particle diameter decreases the friction factor and according to that the pressure drop decreases.

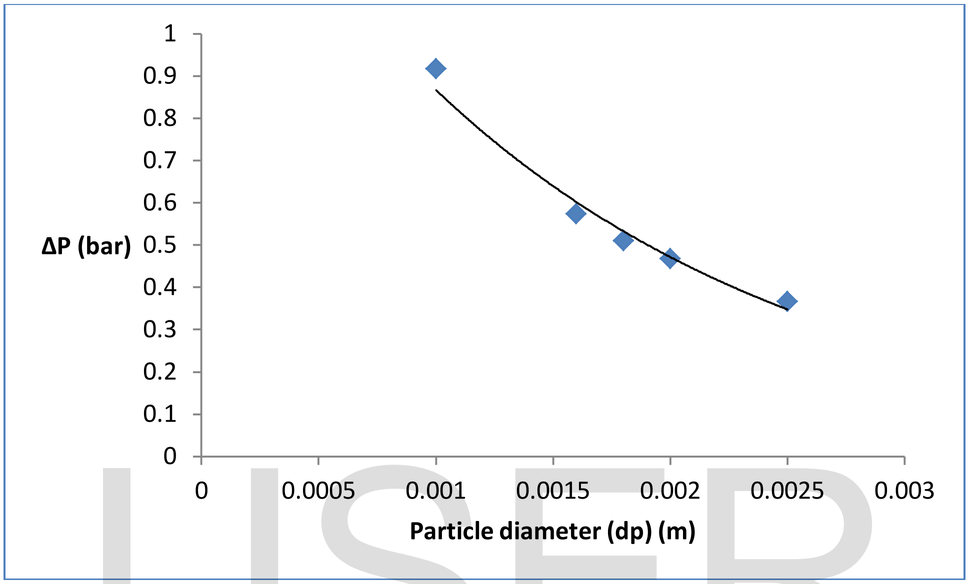

Fig 1. Effect of particle diameter on pressure drop

3.3 Effect of gas density on pressure drop:

Increasing gas density increases the pressure drop as shown in figure (2). High densities are responsible for high frictional shear stress forces which increases the pressure drop inside the bed.

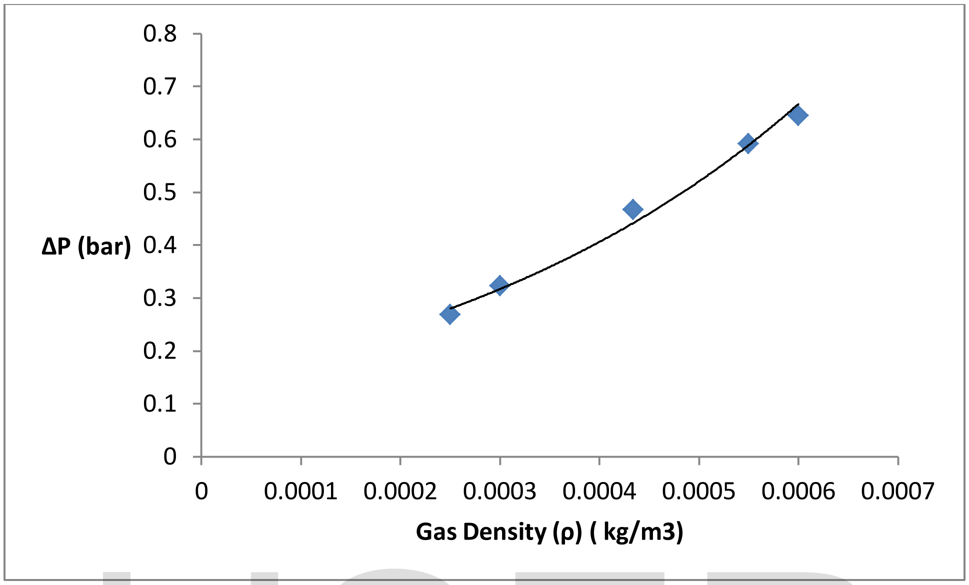

Fig 2. Effect of gas density on pressure drop

3.4 Effect of superficial velocity:

As shown in figure (3), increasing superficial velocity increases the pressure drop. Superficial velocity is directly proportional to friction factor and according to that when it increases, the pressure drop increases.

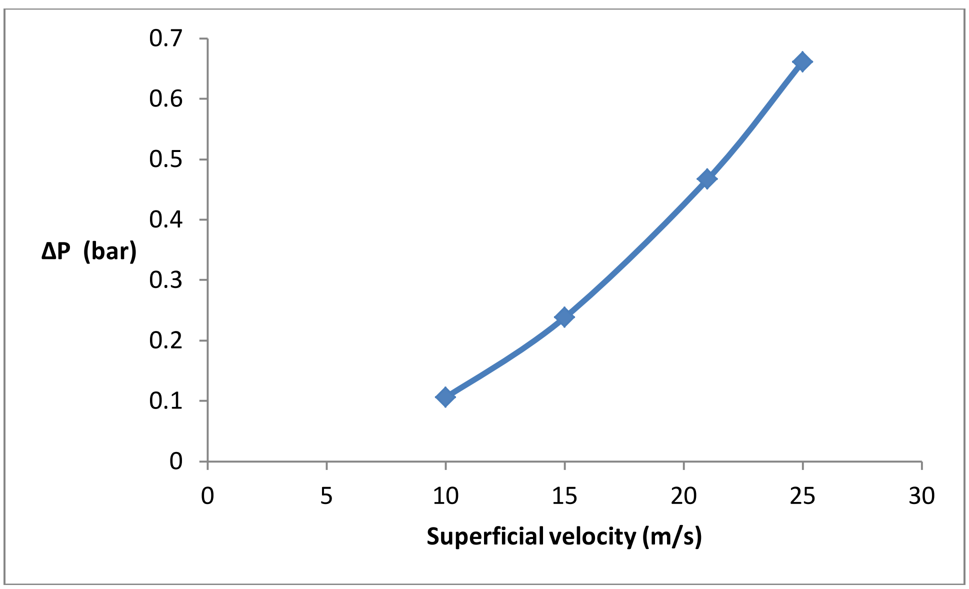

Fig 3. Effect of gas superficial velocity on pressure drop

3.5 Effect of bed voidage on pressure drop:

Increasing the bed voidge decreases the pressure drop inside the reactor very highly compared to the other parameters as shown in figure (4). Because of the large dependence of pressure drop on the bed voidge (as shown in Ergun's equation), it is considered to be the most effective parameter on pressure drop.

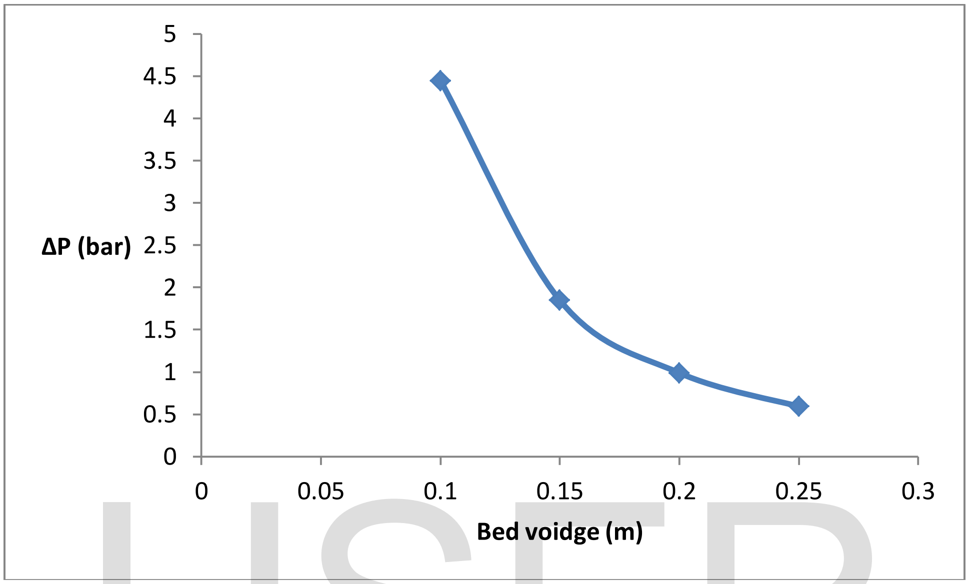

Fig 4. Effect of bed voidge on pressure drop

3.6 Effect of viscosity on pressure drop:

The viscosity inside the fixed bed is affected by increasing the pressure drop. The viscosity is directly proportional to friction factor and according to that when increases the pressure drop also increases as shown in figure (5).

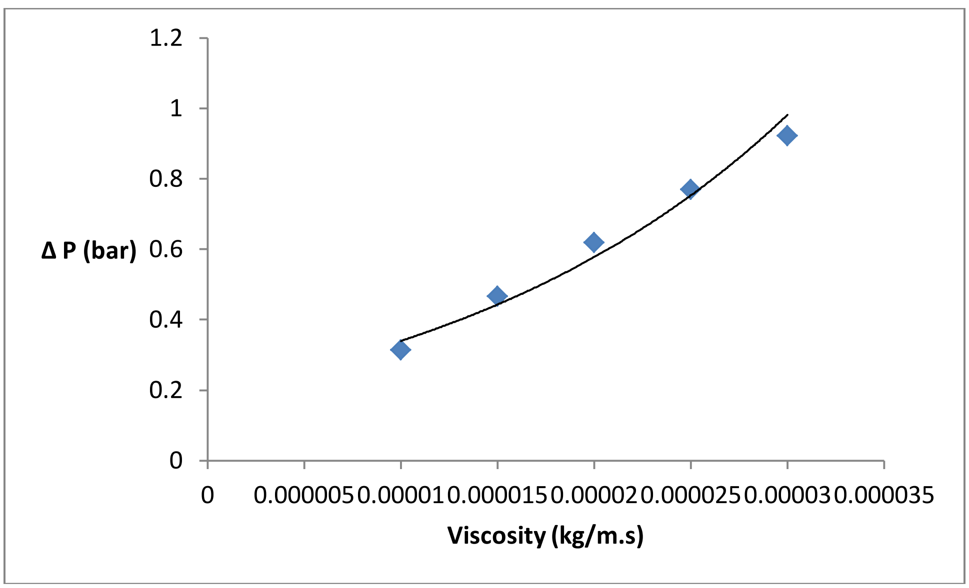

Fig 5. Effect of gas viscosity on pressure drop

4. Conclusions:

From the present work the following conclusions have been arrived at:

- The model predictions agree very well with the actual data from a liquefied natural gas company in Egypt. The model deviation in case of applying momentum balance equations is only -6.7% and -2.9% in case of applying heat balance equations.
- The deviation in case of applying heat balance equation is less than that obtained by applying the momentum balance equation.
- The calculated pressure drop across the bed is close to that obtained from the industrial data. As discussed previously the pressure drop calculated from Eurgn‘s equation is 0.4664 bar which is nearly equal to the actual data that is 0.5 bar.
- The calculated temperature inside the bed is relatively the same that taken from the petrochemical company. The temperature calculated from the model by heat balance equations is 17 °C which is very close to the actual data that is 17.5 °C.
- The particle diameter increases, as a result of this the pressure drop decreases.
- When the gas density increases, this follows an increase in pressure drop.
- Increasing in superficial velocity causes an increase in pressure drop.
- The increase in bed voidage causes a very high decrease in pressure drop.
- When the viscosity increases, the pressure drop increases also.
- The most effective parameter on the fixed bed reactor is the bed voidage in case of applying momentum balance equation.

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NOMENCLATURE

Symbol	Description	Unit
A	Cross sectional area of fixed bed	m^2
C_{pg}	Molar heat capacity of gas	J/mol .°C
C_{pi}	Molar heat capacity of component *i*	J/mol .°C
$C_{p\ gmix}$	Molar heat capacity of gas mixture	J/mol .°C
d_p	Particle diameter	m
D	Bed diameter	m
g	Acceleration gravity	m^2/s
h_b	Gas particle heat transfer coefficient	W/m^2 °C
ΔH_i	Heat of reaction of component i	k J/mol
k	Thermal conductivity of gas	W/m. °C
k_{eff}	Effective thermal conductivity	W/m. °C
k_r	Chemical reaction rate constant	s^{-1}
$k_{g\ mix}$	Thermal conductivity of gas mixture	W/m. °C
k_i	Thermal conductivity of gas *i*	W/m. °C
k_s	Particle thermal conductivity	W/m. °C
L	Total bed Height	m
M	Molecular Weight	kg/kmol
M_i	Molecular Weight of component i	kg/kmol
N_u	Nusselt Number	-

$N_{u\,D}$	Nusselt Number for solid particles	-
P	Total pressure in reactor	N/m^2
P_r	Prandtl Number	-
ΔP	Pressure drop in reactor	N/m^2
q_{ci}	Concentration of component *i* in particle crystal	mol/s
Q	Total volumetric flow rate of gas in feed	m^3/s
r	Particle Radius	m
R	Gas constant	kJ/kmol.K
R_e	Reynolds Number	-
t	Time	s
T	Temperature in Reactor	K
T_b	Temperature of the bed reactor	K
T_p	Particle temperature	K
u	Gas velocity	m/s
U	Superficial gas velocity	**m/s**
$\mathbf{x_i}$	Mole fraction of component *i*	
$\mathbf{y_i}$	Mole fraction of component *i*	
z	Bed Height	m
Z	Compressibility factor	

Greek symbols

	Description	Unit
ε	Void fraction of packed bed	-
ε_b	Bed porosity	
ρ	gas density	kg/m^3
ρ_{mix}	gas mixture density	kg/m^3
ρ_i	Density of component i	kg/m^3
μ	Viscosity	kg/m.s
μ_g	Gas Viscosity	kg/m.s
μ_i	Viscosity of component i	kg/m.s

TABLE 1
VALIDATION OF PRESSURE DROP

Parameter	Value from the model	Actual value	%error
ΔP (bar)	**0.4664**	**0.5**	**-6.71%**

TABLE 2

VALIDATION OF TEMPERATURE INSIDE THE REACTOR

Parameter	Value from the model	Actual value	%error
T_b (°C)	**17**	**17.5**	**-2.9%**

TABLE 3

CHARACTERISTIC OF CATALYST

Pore diameter	***Particle size range***
4ºA	***10 mesh~2mm***

TABLE 4

BED VOIDGE

$$\varepsilon_b = 0.4 + 0.5 \left(\frac{dP}{D}\right) + 0.412 \left(\frac{dP}{D}\right)^2 \qquad \frac{dP}{D} \leq 0.5$$

$$\varepsilon_b = 0.4 + 0.5\,(5.263*10^{-4}) + 0.412\,(5.263*10^{-4})^2$$

$$= 0.4002$$

TABLE 5

PROPERTIES OF NATURAL GAS

Substance	M_{wt}	T_c	T_r	P_c	P_r	μ_a (centipoises)	μ/μ_a	μ (centipoises)
CH_4	16.04	190.6	1.527	45.99	1.087	0.0104	1.1	0.01144
C_2H_6	30.07	305.3	0.953	48.72	1.026	0.0088	1.7	0.01496
C_3H_8	44.09	369.8	0.785	42.48	1.177	0.00775	1.7	0.013175
C_4H_{10}	58.12	425.1	0.685	37.96	1.317	0.007	1.7	0.0119
C_5H_{12}	72.15	469.7	0.619	33.7	1.483	0.006	1.7	0.0102
C_6H_{14}	86.17	507.6	0.573	30.25	1.6528	0.0056	1.7	0.00925
CO_2	44.01	304.2	0.956	73.83	0.677	0.00775	1.7	0.013175
H_2S	34.08	373.5	0.779	89.63	0.557	0.0085	1.7	0.01445

TABLE 6

EFFICTIVE THERMAL CONDUCTIVITY

$$K_{eff} = (1-\varepsilon) K_S + \varepsilon K_g$$

Molecular sieves (K_S) =1.758 W/m. °c

$$K_{eff} = (1-0.4)*1.758+0.4*0.0309$$

$$= 1.06716 \text{ W/m. °c}$$

TABLE 7

CONVECTIVE HEAT TRANSFER COEFFICIENT

a- Calculation of Nusselt number (Nu)

$$Nu_D = 2 + 1.1Pr^{1/3} R_e^{0.6}$$

$$=2+1.1*(1.0313*10^{-3})^{1/3}*(1.2152)^{0.6}$$

$$= 2.1249$$

b- Calculation of convective heat transfer coefficient (h_b)

$$Nu_D = \frac{hd_P}{K_{g_{mix}}}$$

$$2.1249 = \frac{h*2*10^{-3}}{0.0309}$$

h_b=32.829 W/m^2. °c