

NONISOTHERMAL MODELLING OF DEHYDROGENATION OF CYCLOHEXANE IN HYBRID MEMBRANE REACTOR

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ABSTRACT

Simple mathematical model is developed for a membrane reactor used for the catalytic dehydrogenation of cyclohexane under nonisothermal condition and plug flow pattern. An FAU- type zeolite membrane reactor for the dehydrogenation of cyclohexane was chosen for the study. The tubular reactor is of hybrid type, which is a combination of fixed bed and membrane reactor with a fixed bed as the first stage and membrane reactor as the second stage. Simulation studies have been done both for the isothermal and the non-isothermal cases. From the results of this study, it has been established that the non-isothermal model is the adequate representation of the dehydrogenation of cyclohexane in a membrane reactor. Besides, a hybrid reactor is a better choice for a comparative study of membrane and conventional fixed bed reactor.

Keyword: Hybrid Membrane Reactor, Knudsen diffusion, Permeance, Perselective, Sweep Gas, Zeolite Membran

I. INTRODUCTION

Benzene (B) and cyclohexane (C) is important starting materials for a variety of petrochemical products. Since the boiling points of these compounds are very close (353.2 and 353.9K, respectively), azeotropic distillation and extraction distillation are used frequently for their separation with the addition of a third component as a separating agent. Therefore, it would be desirable to develop a process in which B and C could be separated directly. In this regard the dehydrogenation of cyclohexane in a catalytic membrane reactor has shown much attention and has been adopted as a promising process to produce H₂ and C₆H₆ [10,20].

Most of these systems are used for dehydrogenation where a thick or composite metallic membrane (palladium or ceramic) [10] is used to removal of hydrogen from the reaction mixture. Metallic membranes are more selective than glass and ceramic membranes. Recently, zeolite materials have great potential for membrane reactor application due to their regular porous structures with pore of molecular size. Zeolites are also able to separate close boiling point organic mixtures with high efficiency than a traditional distillation and also molecules with same molecular weight which cannot be separated by Knudsen diffusion governed by porous inorganic membrane [5]. As far as the literature on dehydrogenation of cyclohexane in membrane reactor concerned, a large number of research studies on performance of catalytic membrane reactor [24] have modelled the reactor to study the optimum ratio of permeation rate to reaction rate corresponding to the maximum conversion of cyclohexane and concluded that a membrane which exhibits a high permselectivity for the products over the reactants should be used to achieve high conversion. [10] has selected Pd membrane to

demonstrate experimentally and theoretically that conversion of cyclohexane enhances by using Pd membrane reactor.[11] have discussed the permeance and separation properties of the FAU type zeolite membrane for the mixture of benzene and cyclohexane. Experimentally it has been investigated that the conversion of cyclohexane in the FAU type zeolite membrane reactor reached 72.1% at 473 K as compared to the calculated equilibrium value of 32.2%. The above mentioned studies reveal that in dehydrogenation reactions, the selective removal of product H_2 through a selective membrane such as Pd alloy membrane increases the conversion. The conversion of cyclohexane can also be increased by simultaneous removal of both the products C_6H_6 and H_2 through the membrane. [14,15] and [12,13] have investigated that FAU type zeolite membrane may be successfully used to separate mixture of hydrocarbons. [12] and [14] reported the separation properties of FAU type zeolite membrane for binary mixture of C_6H_6 and saturated $C_4 - C_7$ hydrocarbons and mixture of C_6H_6 and n-alkanes. [14] has reported the separation properties of FAU type zeolite membrane for ternary mixture of C_6H_6 , cyclohexane and H_2 . This study shows that the selective adsorption of C_6H_6 in the pores is very high which in turn blocks the cyclohexane molecules from permeating. Thus FAU type membrane is considered as benzene selective and so may be successfully used for dehydrogenation of cyclohexane reaction in membrane reactor.

In the present simulation study, FAU type zeolite tubular membrane is used for dehydrogenation of cyclohexane reaction in catalytic membrane reactor under the assumption of nonisothermal. 1.0 wt% Pt / Al_2O_3 type catalyst is used and is packed in shell side. The reaction is carried out in shell side of the membrane reactor and gaseous components are permeated through the membrane to tube side of the reactor. The standard operating conditions and physical parameters are given in Table 1, these conditions have taken from the experimental studies[15].

II. MATHEMATICAL MODEL

Simple mathematical model is developed for a membrane reactor used for the catalytic dehydrogenation of cyclohexane under nonisothermal condition and plug flow pattern. One dimensional non-isothermal model equations are developed to describe the behaviour of hybrid reactor at steady state on the basis of the following assumptions:

1. Non Isothermal conditions,
2. Non Adiabatic operation,
3. Heat resistance offered by the membrane is negligible and so is the external heat resistances between bulk gas and catalyst particle due to high conductivity of catalyst particle, Therefore T_s and T_t are assumed to be identical and equal to T,
4. Plug flow in both the feed and permeate sides, No axial or radial diffusion,
5. Permeation through the membrane is proportional to the difference in partial pressures between the feed and permeate sides,
6. Ideal bulk gas behavior on the both sides of the reactor,
7. Pressure drop along the reactor length are negligible, and
8. There are axial variations in the gas temperature on the both sides (shell and tube); However, radial variations are negligible.

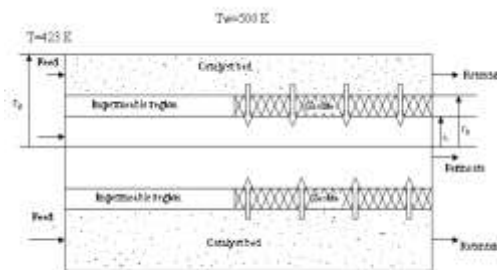


Figure 1. Cross-Sectional Diagram of the Hybrid Reactor

2.1 Shell Side Mole Balance (Reaction Zone)

$$\frac{dN_i F}{dl} = n_i S_R r_c - 2prQ_i p_i \quad (1)$$

2.2 Tube side Mole Balance (Permeate Zone)

$$\frac{dN_i F}{dl} = 2prQ_i p_i \quad (2)$$

where , $p_i = (P_F x_i - P_P y_i)$ (3)

Whereas before i refers to the species cyclohexane, argon, benzene, hydrogen.

The molar flow rate of the parameter Q_i , appearing in Equations (1 & 2) depend upon membrane characteristic and temperature.[28] have fitted the experimental permeation data reported by [15] for cyclohexane, benzene, argon, and hydrogen at different temperatures by polynomials for each of the components using MATLAB 6.1`

$$Q_c = 1.025 \times 10^{-14} T^3 - 2.365 \times 10^{-11} T^2 + 1.643 \times 10^{-8} T - 3.408 \times 10^{-6} \quad (4)$$

$$Q_b = 1.14 \times 10^{-12} T^3 - 1.691 \times 10^{-9} T^2 + 8.317 \times 10^{-7} T - 1.341 \times 10^{-4} \quad (5) \quad \dots(4)$$

$$Q_H = 6.503 \times 10^{-13} T^3 - 9.703 \times 10^{-10} T^2 + 4.823 \times 10^{-7} T - 7.911 \times 10^{-5} \quad (6)$$

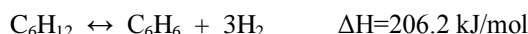
2.3 Energy Balance

The energy balance differential equation is derived by assuming that the membrane offer no resistance to heat transfer, and external heat resistance between bulk gas and catalyst particle are negligible due to high conductivity of catalyst particle. Therefore T_t and T_s are assumed to be identical and equal to T . The energy balance gives the equation for overall temperature gradient as follows:

$$\frac{dT}{dl} = \frac{(R_i (-DH_i) + hA (T_w - T))}{\dot{a} N_i C_{p_i}} \quad (7)$$

2.4 Kinetic Model

The stiochiometry of the dehydrogenation of cyclohexane is represented by



The following kinetic rate expression used by various authors in the past has been (10,15 and 28)

$$r_c = -k \left(\frac{\left(\frac{K_P P_C}{P_H^3} \right) - P_B}{1 + \left(\frac{K_B K_P P_C}{P_H^3} \right)} \right) \quad (8)$$

p_i is the partial pressure of component i .

Where k , K_B , and K_P are the reaction rate constant, the adsorption equilibrium constant for benzene, and the reaction equilibrium constant respectively given by the following expressions.

$$K_p = (4.89 \times 10^{35}) \exp\left(\frac{-26490}{T}\right) \quad (\text{Pa}^3) \quad (9).$$

$$K_b = (2.03 \times 10^{-10}) \exp\left(\frac{6270}{T}\right) (\text{Pa}^{-1}) \quad (10).$$

$$k = 0.44 \exp\left(\frac{-4270}{T}\right) (\text{mol.m}^{-3} \text{Pa}^{-1} \text{s}^{-1}) \quad (11)$$

The conversion of cyclohexane, X_C , is calculated from the ratio of the molar fractions of cyclohexane at the outlets of the feed and the permeate sides to those for cyclohexane at the inlets of both sides as follows:

$$X_C = 1 - \frac{u_{x,1} X_{C,1} + u_{y,1} Y_{C,1}}{u_{x,0} X_{C,0} + u_{y,0} Y_{C,0}} \quad (12)$$

Where, $u_{x,0}$, $u_{x,1}$ - gas flow rates at the inlet and the outlet of the feed side, $u_{y,0}$, $u_{y,1}$ - gas flow rates at the inlet and the outlet of the permeate side. The model operating conditions for the simulation as used in this study are summarized in TABLE 1.

III. RESULTS AND DISCUSSION

The results are presented for both isothermal and non-isothermal cases. In isothermal model, effect of feed temperature, feed rate, sweep flow rate and co-feeding of hydrogen on cyclohexane conversion were examined in detail while in the non-isothermal model, the effect of wall temperature (while keeping feed temperature constant), feed flow rate and temperatures profile in the reactor, and the effect of co-feeding of hydrogen have been investigated in full detail.

In order to simulate the model, two cases were chosen.

1. Isothermal condition with fixed temperature throughout the reactor length.
2. Non isothermal condition with varying temperature across the reactor length.

The variation of temperature was incorporated by fixed wall temperature outside the reactor.

3.1 Isothermal Model

The isothermal model of the hybrid membrane reactor has been simulated using the reactor data given in Table 1.

1. As stated earlier, simulation has been performed for both the conventional (fixed bed) and the hybrid membrane reactor for comparison.

3.1.1 Effect of Feed Temperature on Conversion of Cyclohexane

Conversion of cyclohexane at different feed temperatures for a conventional reactor and hybrid reactor are shown in Figure 2. The figure shows that conversion increases with increasing the feed temperature as reported in the experimental studies by [15]. This may be attributed to the fact that the dehydrogenation reaction is endothermic in nature and on increasing the temperature, the forward reaction rate increases which leads to increase in conversion of cyclohexane. The figure also shows that the increase in conversion at higher temperature is larger as compared to the increase at lower temperatures in both the fixed bed as well as the hybrid reactor. This again is explained by the same reason of endo-thermicity. For instance, at the temperature of 448 K the conversions are 23.49 % and 38.90 % for the fixed bed and hybrid membrane reactor respectively.

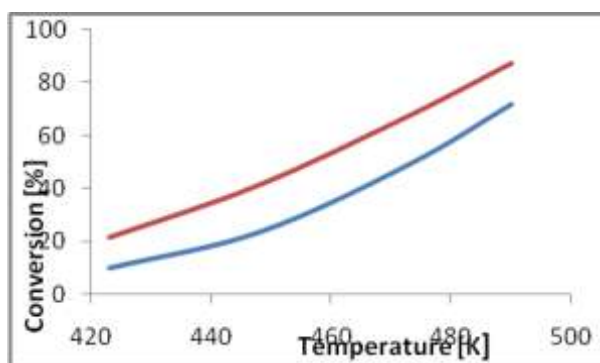


Fig.2 Exit Conversions vs Feed Temp. of Hybrid Membrane Reactor and Fixed Bed Reactor
(--Hybrid Membrane Reactor,---Fixed Bed Reactor)

3.1.2 Conversion Profile

The conversion of cyclohexane was evaluated along the length of the reactor for both cases viz. hybrid membrane reactor and fixed bed reactor setups. Figures 3 to 5 show the variation in conversion along the length of reactor for the feed temperature of 423 K, 448 K and 473 K respectively. The percent conversion in the hybrid reactor is found to be higher than that of fixed bed at all temperatures. This is due to the fact that in the hybrid membrane reactor, one of the reaction products is permeated through the membrane thereby shifting the equilibrium forward to the right. The conversion, in case of fixed bed is limited by the thermodynamic equilibrium, when forward and backward reaction rate are balanced giving a maximum of 48.96 % conversion at 473 K whereas 67.70 % is achieved in case of hybrid membrane reactor. The increase in reaction rate is not only enough to produce high conversion but also increases permeance rate of the components. Thus, increase of temperature has significant effect on the enhancement of the conversion. Figure 5, clearly indicates the advantage and necessity of the removal of one of the products from the reaction zone in order to shift the equilibrium forward. It is clear from this figure that the conversion is same up to 0.0335 m, the length of the impermeable region (common in both the fixed bed and the hybrid reactor). However, beyond that length, the membrane dominates the equilibrium effect and yields higher conversion. Almost 72% of the conversion increased beyond the impermeable region. In other words, this much of the conversion advantage is possible with the membrane reactor to the fixed bed reactor. Thus, it may be concluded that hybrid membrane reactors yields higher conversion than of fixed bed reactors of the same specifications and at the same operating conditions.

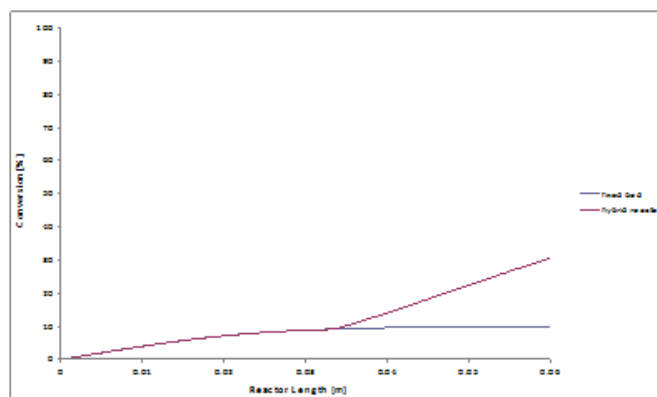


Fig. 3. Conversion of Cyclohexane Along the Length of Hybrid Membrane Reactor and Fixed Bed Reactor ($T_f = 423$ K, $N_f = 9.6E-6$ mol/s)

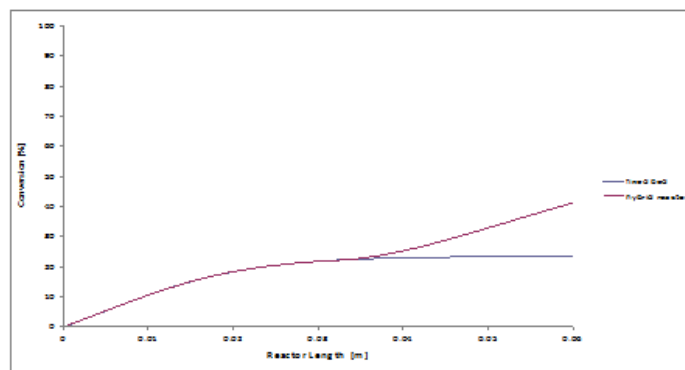


Fig. 4. Conversion of Cyclohexane Along the Length of Hybrid Membrane Reactor and Fixed Bed Reactor ($T_f = 448\text{ K}$, $N_f = 9.6\text{E-}6\text{ mol/s}$)

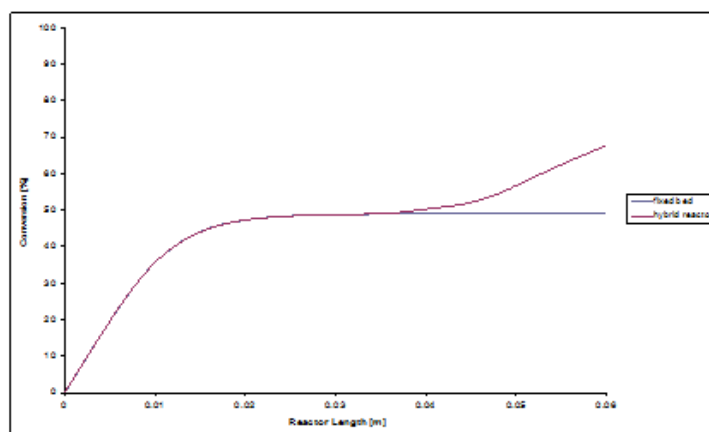


Fig. 5. Conversion of Cyclohexane Along the Length of Hybrid Membrane Reactor and Fixed Bed Reactor ($T_f = 473\text{ K}$, $N_f = 9.6\text{E-}6\text{ mol/s}$)

The Effect of feed rate on cyclohexane conversion at temperature of 423 K, 448 K, 473 K and 490 K is shown in Figure 6. The feed flow rate has been increased from $6.6 \times 10^{-6}\text{ mol/s}$ to $9.6 \times 10^{-6}\text{ mol/s}$. It is observed from the Figure that cyclohexane conversion decreases with increase in the feed rate, residence time decreases with the increase of feed flow rate. Operation at a low feed rate would result in a high conversion at the expense of a very low product flow rate. On the other hand, increasing the feed flow rate would reduce the conversion. This would require use of an extensive product separation system in order to recover the unreacted feed

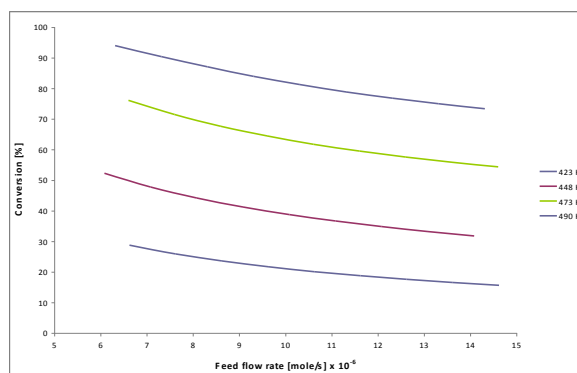


Fig. 6: Conversion vs Feed Rate at Different Feed Temperatures

3.1.4 Effect of Sweep Flow Rate on Cyclohexane Conversion

Exit conversion from the reactor with variation in sweep gas flow rate was evaluated for feed temperatures of 423 K, 448 K, 473 K and 490 K. Argon is used as sweep gas which helps to drift the product towards separation

side. The flow rate was varied from 3.15×10^{-5} to 10.15×10^{-5} . The permeation flux of a component through membrane depends on the partial pressure difference between reaction side and permeate side. The higher flow rate of the sweep gas decreases the partial pressure of the component at permeate side leading to higher driving force for permeation. As a result, the permeation rate increases which in turn increases the conversion of cyclohexane. This is shown in Figure 7 for common sweep gas and feed temperature. At high sweep gas flow rate, the partial pressure of benzene, hydrogen and cyclohexane become very small whereas their partial pressure on the surface of membrane in the reaction side becomes significantly high. This enhances the permeation of product benzene and hydrogen as well as reactant cyclohexane. The permeation of products increases conversion whereas permeation of the reactant decreases conversion.

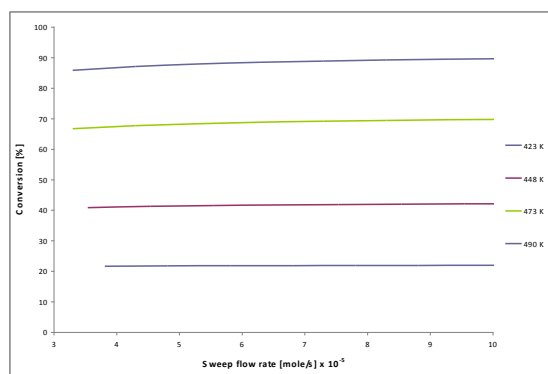


Fig. 7. Conversion vs Sweep Flow Rate at Different Feed Temperatures

3.1.5 Effect of Co-feeding of Hydrogen on Conversion

When the dehydrogenation is carried in the membrane reactor with hydrogen selective membrane, coking on the catalyst due to lack of hydrogen gradually decreases conversion. Figure .8 shows the influence of variation of hydrogen content in feed maintained in the range of 0 - 0.09 (mole fraction). The conversion decreases with increasing mole fraction of hydrogen at inlet. The co-feeding of hydrogen with cyclohexane into the zeolite membrane reactor permits maintaining a certain level of hydrogen concentration on the reaction side, thus inhibiting coking [16] However, the presence of hydrogen in the mixture favors the backward reaction and hence results in decrease of conversion as can be seen in Figure 8. For instance, at 490 K, the conversion is 87.10 % without hydrogen whereas it comes down to 78.81 % with hydrogen.

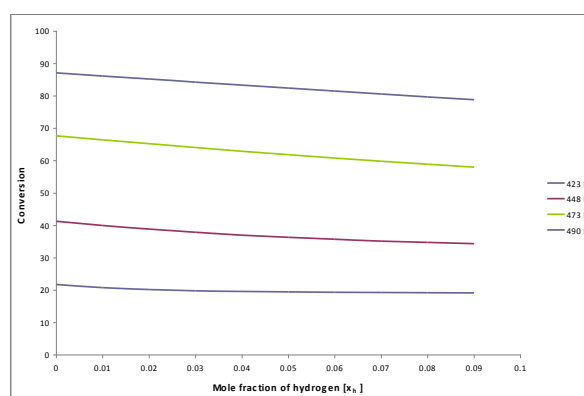


Fig. 8: Effect of Hydrogen Co-Feeding on Conversion (T_f as Parameter)

3.2 Non-Isothermal Model

The non isothermal model has similarly been simulated using the same reactor data as those for isothermal model given in TABLE 1. The temperature of the reactor is affected by the endothermic nature of the reaction.

However, the outer wall of the reactor is maintained at a constant temperature. Simulation has been performed for both the conventional and the membrane reactor for comparison.

3.2.1 Effect of Wall Temperature on Conversion

An increase in the wall temperature causes heating up of the reaction mixture and thus a rise in reaction temperature, leading to higher conversion. The results are shown in Figure 9. It may be observed from this figure, that 17% (about 28% of total) conversion in the fixed bed section is followed by membrane section, where an exit conversion of 59% cyclohexane occurs at wall temperature of 500 K. When the wall temperature is raised to 550 K, 26% (about 32% of total) conversion in the fixed bed segment is followed by 79% conversion in the membrane section. Likewise, 33% (about 36% of total) conversion in the fixed bed and 91% conversion in membrane section at 550 K. Further, at a wall temperature of 570 K, the conversion increased to 40% and the highest conversion of 99% at the exit of the reactor. This suggests that the membrane section is more effective at elevated temperatures

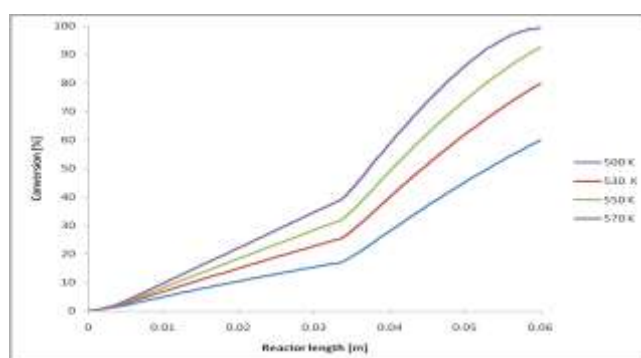


Fig. 9 Conversion Profile in the Hybrid Membrane Reactor, Wall Temperature as Parameter
($T_f = 423 \text{ K}$, $N_f = 9.6\text{E-}6 \text{ mol/s}$)

3.2.2 Temperature Profile in the Hybrid Membrane Reactor

How the temperature of the feed / product stream changes while passing through the reactor was evaluated for the non adiabatic hybrid reactor. The outer wall temperature of the reactor is maintained constant. Figure 10, presents the same results in graphical form. It is observed that temperature rise at the inlet of the packed bed section is faster, because at the entrance of the inlet, conversion is low; therefore sensible heat is used to raise the temperature of the stream. As conversion increases along the reactor length, the rate of temperature rise becomes slow but steady. The rate of change of temperature does not change appreciably from fixed bed to membrane section.

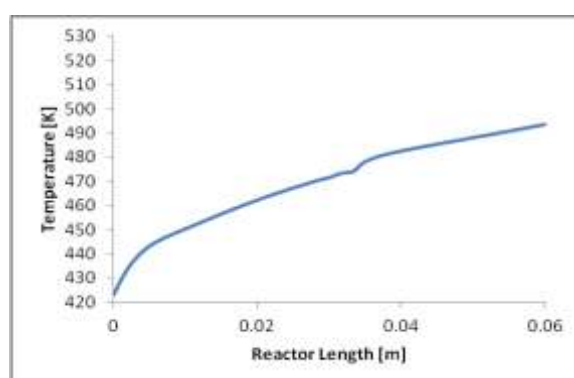


Fig. 10. Temperature Profile in Non-Isothermal Reactor ($T_f=423 \text{ K}$, $T_w = 530 \text{ K}$, $N_f = 9.6\text{E-}6 \text{ Mol/S}$)

However, when the feed was maintained at higher temperature ($T_f = 473\text{K}$), while maintaining the wall temperature still at the same value ($T_w = 530\text{K}$), a different profile results, Figure 11. There is a sharp decline in the temperature of the reaction mixture close to the reactor inlet, reaching a minimum value. This is then followed by almost a steady rise in temperature along the length to the exit of the reactor. This observation is similar to the one reported by [10]. They have simulated the performance of a nonisothermal fixed bed membrane reactor which takes into account the various heat exchanges that takes place inside the reactor. One of the results, in which temperature profile of the reactor has been discussed, closely matches with the trend observed in Figure 10. This behaviour may be explained by the fact that two heat effects take place simultaneously: first the temperature decreases due to consumption of heat by the endothermic reaction while the heat transfer from the wall is not sufficient to maintain the reaction temperature. Next, heat transfer from the wall of the reactor is more than the rate at which heat is absorbed during the reaction. Hence the temperature starts increasing after reaching at minimum value and will continue to increase till the reactor exit.

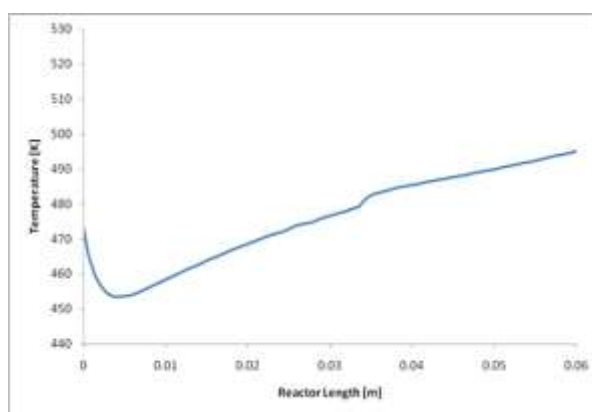


Fig. 11 Temperature Profile in the Nonisothermal Reactor ($T_f=473\text{K}$, $T_w = 530\text{K}$, $N_f = 9.6\text{E}-6\text{Mol/S}$)

3.3 Adequacy of Nonisothermal Model

In modeling the reactor, as one operating under isothermal condition, the temperature is assumed at a constant value. That, the temperature does not change along the length of the reactor is not true because the temperature would drop as a result of the endothermic reaction. Therefore, it would be necessary to maintain the temperature by supplying heat (using heating coils etc.). Isothermal operation may be achieved at the expense of a controlled flux of heat from an external source. This has not been considered in the modeling part. However, in the non isothermal modeling, temperature enters the model as a variable and it varies along the length of the reactor. Heat flux is provided by maintaining a constant wall temperature. Temperature drops at the beginning due to the fact that major part of the heat supplied to the reactor is used by the endothermic reaction. When the supplied and the heat required balance each other, the temperature is same; thereafter the temperature starts increasing along the length of the reactor and the achieved conversion increases beyond the equilibrium value at the end of the hybrid reactor. As can be seen from Figure 12, higher conversion is achieved in the isothermal model than nonisothermal model up to specified reactor length because the temperature up to that length in nonisothermal model is less than that in isothermal, hence a low conversion. After that specified length, the reactor temperature exceeds compared to that in the isothermal model. This leads to a higher computed conversion in the nonisothermal model.

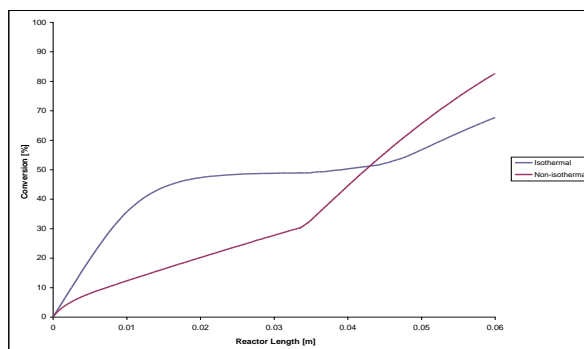


Fig.12 Comparison Between Isothermal and Nonisothermal Model for the Same Inlet Feed Temperature ($T_f = 473 \text{ K}$, $T_w = 530 \text{ K}$, $N_f = 9.6\text{E-}6 \text{ Mol/S}$)

IV. CONCLUSIONS

The catalytic dehydrogenation of cyclohexane in an FAU-type zeolite membrane reactor was simulated by using a simple mathematical model developed under the assumptions of non-isothermal operation and a plug flow pattern. The model equations were solved using “ode solver” of MATLAB at the specified operating conditions. The catalytic membrane reactor provides an efficient means for increasing the conversion through selective permeation of a part of the reaction product. This in turn shifts the reaction equilibrium to higher conversion. Conventionally, low conversion reactions are associated with large size fixed bed reactors together with extensive down- stream separation units that recover and recycle the un-reacted feed. The main attractive feature of the membrane reactor is the possibilities of replacing many of the conventional separation units and recycling devices with a shell and tube membrane reactor or conventional fixed bed reactor together with membrane separation units.

Simulation studies have been done both for the isothermal and the non-isothermal cases. For the isothermal case it was found that Cyclohexane conversion in the hybrid membrane reactor was much higher than the conventional reactor at different feed temperatures: conversion increases with increasing the feed temperature due to endothermic nature of the reaction. Conversion decreases with increase in the feed rate due to lowering of residence time as a result of increase in feed rate. Increase in sweep flow rate also cause increase in conversion. The co-feeding of hydrogen into reaction side causes some decrease in conversion as observed by experimenters in the past and may be attributed to the increase in the concentration of hydrogen on the reaction side. However, use of co-feeding is reported to be effective in preventing coking of the catalyst.

In the case of non-isothermal model it was observed that the conversion of cyclohexane increases with the increase in wall temperature and consequently the reaction temperature; the dehydrogenation reaction being endothermic. The conversion in the hybrid reactor is 35 % higher than the fixed bed reactor at the same operating condition ($T_w = 550 \text{ K}$). The conversion with co-feeding of hydrogen was again observed to be lower than the one without hydrogen. However, as explained earlier, the co-feeding of hydrogen with cyclohexane restrains coke formation on the catalyst and membrane and thus maintaining the stability of both the catalyst and membrane. Conversion decreased with increase in feed rate while maintaining the composition of cyclohexane and argon in the reaction mixture constant. From the results of this study, it has also been established that the non-isothermal model is the adequate representation of the dehydrogenation of cyclohexane in a membrane reactor. Besides, a hybrid reactor is a better choice for a comparative study of membrane and conventional fixed bed reactor.

Table 1 Operating Conditions and Physical Parameters of Reactor

Parameters	Specification/Value
Membrane Type	FAU- type Zeolite
Membrane Reactor	membrane
Length of the reactor (m)	Hybrid Reactor
Length of membrane (m)	6×10^{-2}
Inner radius of shell (m)	2.65×10^{-2}
Inner radius of tube (m)	5×10^{-3}
Outer radius of tube (m)	0.85×10^{-3}
Catalyst bed	1.05×10^{-3}
Diameter of catalyst particle (μm)	1.0 wt.% Pt/Al ₂ O ₃ 140-210
Void fraction of catalyst particle.	0.38
Cross sectional area, S _R (m ²)	
Total flow rate in feed side, V _F (m ³ s ⁻¹)	7.50×10^{-5} 3.34×10^{-7}
Total pressure in feed side, PF (Pa)	1.013×10^5
Mole fraction of C in feed side (x _{C,0})	0.10
Mole fraction of A in feed side (x _{A,0})	0.90
Total flow rate in permeate side, V _P (m ³ s ⁻¹)	1.67×10^{-6}
Total pressure in permeate side, P _P (Pa)	1.013×10^5
Mole fraction of C in permeate side (x _{c,1})	0.00
Mole fraction of A in permeate side (x _{A,1})	1.0
Permeance of argon, Q _A (mol m ⁻² s ⁻¹ Pa ⁻¹)	1×10^{-10}

V. NOMENCLATURE

Symbol	Description
C_p	Specific heat of mixture (J/mol.K)
k	Apparent reaction rate constant (mol m ⁻³ Pa ⁻¹ s ⁻¹)
K_B	Adsorption equilibrium constant of benzene (Pa ⁻¹)
K_p	Equilibrium constant (Pa ³)
L	Length of reactor (m)

$N_{i,F}$	Molar flow rate of component i in the feed side (mol s^{-1})
$N_{i,P}$	Molar flow rate of component i in the permeate side (mol s^{-1})
p_i	Partial pressure of component i in the feed side (Pa)
P_F	Total feed pressure (Pa)
P_P	Total permeate pressure (Pa)
Q_i	Permeance of component i ($\text{mol m}^{-2} \text{s}^{-1} \text{Pa}^{-1}$)
R	Outer radius of the porous support tube (m)
r_C	Dehydrogenation rate of cyclohexane ($\text{mol m}^{-3} \text{s}^{-1}$)
R	Gas constant ($\text{m}^3 \text{Pa mol}^{-1} \text{K}^{-1}$)
S_R	Cross-sectional area of catalyst bed (m^2)
$u_{x,0}$	Gas flow rate at the inlet of the feed side ($\text{m}^3 \text{s}^{-1}$)
$u_{x,1}$	Gas flow rate at the outlet of the feed side ($\text{m}^3 \text{s}^{-1}$)
$u_{y,0}$	Gas flow rate at the inlet of the permeate side ($\text{m}^3 \text{s}^{-1}$)
$u_{y,1}$	Gas flow rate at the outlet of the permeate side ($\text{m}^3 \text{s}^{-1}$)
V_F	Total feed flow rate ($\text{m}^3 \text{s}^{-1}$)
V_P	Total permeate flow rate ($\text{m}^3 \text{s}^{-1}$)
x_i	Mole fraction of component i in the feed side
$x_{i,0}$	Mole fraction of component i at the inlet of the feed
$x_{i,1}$	Mole fraction of component i at the outlet of the feed side
X_C	Conversion of cyclohexane
y_i	Mole fraction of component i in the permeate side
$y_{i,0}$	Mole fraction of component i at the inlet of the permeate side
$y_{i,1}$	Mole fraction of component i at the outlet of the permeate side

Greek letters

η_m	Viscosity of gas mixture (kg/m.s)
λ_m	Thermal conductivity of gas mixture (W/m.K)
$\alpha(i/j)$	Separation factor of component i to component j
ν_i	Stoichiometric coefficient of component i

Subscripts

A	Argon
B	Benzene
C	Cyclohexane
H	Hydrogen
i	Component i
j	Component j

REFERENCES

- [1]. Armor, J. N., "Applications of Catalytic Inorganic Membrane Reactors to Refinery Products", *Journal of Membrane Science*, **147**, 217-233 (1998).
- [2]. Caro, J., M. Noack, P. Kolsch and R. Schafer, "Zeolite Membranes- State of their Development and Perspective", *Microporous and Mesoporous Materials*, **38**, 3-24 (2000).

- [3]. Ciavarella, P., D. Casanave, H. Moveddeb, S. Miachon, K. Fiaty and J.A. Dalmon, "Isobutane Dehydrogenation in a Membrane Reactor: Influence of the Operating Conditions on the performance", *Catalysis Today*, **67**, 177-184 (2001).
- [4]. Coronas, J., R.D. Noble and J.L. Falconer "Separation of C4 and C6 Isomers in ZSM-5 Tubular Membranes", *Ind. Engg. Chem. Res.*, **37** (1), 166–176 (1998).
- [5]. Coronas, J., and J. Santamaria, "Catalytic Reactors Based on Porous Ceramic Membranes" *Catalysis Today*, **51**, 377-389 (1999).
- [6]. Dittmeyer, R., V. Hollein and K. Daub, "Membrane Reactors for Hydrogenation and Dehydrogenation Processes Based on Supported Palladium", *Journal of Molecular Catalysis A: Chemical*, **173**, 135-184 (2001).
- [7]. Dixon, A.G., "Recent Research in Catalytic Inorganic Membrane Reactors", *International Journal of Chemical Reactor Engineering*, **1**, R6, 1-37 (2003).
- [8]. Gokhale, Y.V, R.D. Noble and J.L. Falconer, "Effects of Reactant Loss and Membrane Selectivity on a Dehydrogenation Reaction in a Membrane enclosed Catalytic Reactor", *Journal of Membrane Science*, **105**, 63-70 (1995).
- [9]. Gunn D.J and M. Khalid, "Thermal Dispersion and Wall Heat Transfer in Packed Beds", *Chemical Engineering Science*, **30**, 261-267 (1975)
- [10]. Itoh, N., "A Membrane Reactor Using Palladium", *AIChE Journal*, **33** (9), 1576-1578 (1987)
- [11]. Itoh, N and K. Haraya, "A Carbon Membrane Reactor", *Catalysis Today*, **56**, 103-111 (2000).
- [12]. Jeong, B. H., Y. Hasegawa, K.I. Sotowa, K. Kusakabe and S. Morooka, "Separation of Mixture of Benzene and n-alkanes using an FAU-type Zeolite Membrane", *Journal of Chem. Engg.*, **35**, 167-172 (2002).
- [13]. Jeong, B. H, Y. Hasegawa, K.I. Sotowa, K. Kusakabe and S. Morooka, "Vapor Permeation Properties of a NaY-type Zeolite Membrane for Normal and Branched Hexanes", *Ind. Engg. Chem. Res.*, **41**, 1768-1773 (2002).
- [14]. Jeong, B. H, Y. Hasegawa, K.I. Sotowa, K. Kusakabe and S. Morooka, "Permeation of Binary Mixtures of Benzene and Saturated C4-C7 Hydrocarbons through an FAU-type Zeolite Membrane", *Journal of Membrane Science*, **213**, 115-124 (2003).
- [15]. Jeong, B.H, K.I. Sotowa and K. Kusakabe, "Catalytic Dehydrogenation of Cyclohexane in an FAU-type Zeolite Membrane Reactor", *Journal of Membrane Science*, **224**, 151-158 (2003).
- [16]. Jeong, B.H, K.I. Sotowa and K. Kusakabe, "Modelling of an FAU-type Zeolite Membrane Reactor for the Catalytic Dehydrogenation of Cyclohexane", *Chem. Engg. Journal*, **103**, 69-75 (2004).
- [17]. Julbe, A, D. Farrusseng and C. Guizard, "Porous Ceramic Membranes for Catalytic Reactors- Overview and New Ideas", *Journal of Membrane Science*, **181**, 3-20 (2001).
- [18]. Kariya, N, A. Fukuoka and M. Ichikawa, "Efficient Evolution of Hydrogen from Liquid Cycloalkanes over Pt-containing Catalysts Supported on Active Carbons under "Wet-dry Multiphase Conditions", *Applied Catalysis A: General*, **233**, 91-102 (2002).
- [19]. Kariya, N, A. Fukuoka, T. Utagawa, M. Sakuramoto, Y. Goto and M. Ichikawa, "Efficient Hydrogen Production using Cyclohexane and Decalin by Pulse–Spray Mode Reactor with Pt Catalysts, *Applied Catalysis A: General*, **247**, 247-259 (2003).

- [20]. Koukou, M.K, G. Chaloulou, N. Papayannakos and N.C. Markatos, "Mathematical Modelling of the Performance of Non-isothermal Membrane Reactors", *Int. J. Heat & Mass Transfer*, **40** (10), 2407-2417 (1997).
- [21]. Kumar, S, S. Shankar, P.R. Shah and S. Kumar, "A Comprehensive Model for Catalytic Membrane Reactor", *International Journal of Chemical Reactor Engineering*, **4**, A.5, 1-29 (2006).
- [22]. Lassinantti, M., "Synthesis, Characterization and Properties of Zeolite Films and Membranes", Licentiate Thesis, Lulea University of Technology, May 2001.
- [23]. McLeary, E.E, J.C. Jansen and F. Kapteijn, "Zeolite Based Films, Membranes and Membrane Reactors: Progress and Prospects", *Microporous and Mesoporous Materials*, **90**, 198-220 (2006).
- [24]. Mohan, K and R. Govind, "Analysis of a Cocurrent Membrane Reactor", *AIChE Journal*, **32**, (12), 2083-2086 (1986).
- [25]. Mohamed, Al-Sahali, M. Hisham, Ettouney, Bader, Albusairi, Haitham Lababidi, and Heba A. Al-Hulaila, Non-Isothermal Non-Adiabatic Dehydrogenation of Cyclohexane in Catalytic Membrane Reactors, *Separation Science and Technology*, **42**, 2081–2097, 2007
- [26]. Okubo, T, K. Haruta, K. Kusakabe, S. Morooka, H. Anzai and S. Akiyama, "Equilibrium Shift of Dehydrogenation at Short Space-Time with Hollow Fibre Ceramic Membrane", *Ind. Engg. Chem. Res.* **30**, 614-616 (1991).
- [27]. Reid, Robert C., J. M. Prausnitz, and B. E. Poling, "The Properties of Gases and Liquids, 4e" McGraw Hill International Edition (1988)
- [28]. Sashi Kumar, Tanvi Gaba, S Kumar, "Simulation of Catalytic Dehydrogenation of Cyclohexane in Zeolite Membrane Reactor", *International journal of chemical reactor Engineering*, Volume 7, 2009 Article A13
- [29]. Seader, J. D and E.J. Henley, "Separation Process Principles", John Wiley and Sons, Inc. New York, USA (1998).
- [30]. Sirkar, K. K, V.P. Shanbhag and A.S. Kovvali, " Membrane in a Reactor: A Functional Perspective", *Ind. Eng. Chem. Res.*, **38**, 3715-3737 (1999).
- [31]. Sousa, J.M and A. Mendes, "Simulation Study of a Dense Polymeric Catalytic Membrane Reactor with Plug-flow Pattern", *Chem. Eng. Journal*, **95**, 67–81. (2003)
- [32]. Sun, Y-M and S.J. Khang, "Catalytic Membrane for Simultaneous Chemical Reaction and Separation Applied to a Dehydrogenation Reaction", *Ind. Eng. Chem. Res.*, **27**, 1136-1142 (1988).
- [33]. Yagi, S and Wakao, N., *AIChE Journal*, **5**, 79, 1959
- [34]. Zaman, J and A. Chakma, "Inorganic Membrane Reactors-Reviews", *Journal of Membrane Science*, **92**, 1-28 (1994).