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Modeling and Simulation of Styrene Monomer Reactor: Mathematical and Artificial Neural Network Model

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Abstract— A pseudo-homogeneous model was developed for fixed bed catalytic styrene monomer reactor based on the reaction mechanisms and mass and energy balance equations. With the proposed mathematical model, the profiles of ethyl benzene conversion, styrene yield and selectivity were achieved through the length of catalytic bed reactor. Good agreement was found between model results and industrial data. The effects of some input parameters such as the molar ratio of the steam to ethyl benzene in the feed (S/E) and inlet temprature were investigated on final conversion of ethyl benzene and styrene selectivity using proposed mathematical model. USING THE RESULTS OF mathematical model, a three-layer perceptron neural network was developed for simulation of the effects of feed composition and operation condition on conversion and selectivity. The optimum structure of neural network was determined by a trial-and-error method and different structures were tried.

Index Terms—Artificial Neural Network, Fixed bed catalytic reactor, Mathematical modeling, Styrene monomer

1 INTRODUCTION

Styrene is one of the simplest and most important monomers produced worldwide, and finds major use in the production of polystyrene, acrylonitrile/butadiene/styrene resins (ABS), and various miscellaneous polymers in the petrochemical industry [1]. Styrene produced commercially by catalytic dehydrogenation of ethyl benzene, which firstly presented in 1869 by Berthelst. Recently, optimal design and operation of the styrene reactor needed, as it is the critical equipment in the styrene manufacturing process.

Dehydrogenation reaction of ethyl benzene is equilibrium, endothermic reversible reaction and thermally proceeds with low yield but catalytically with high yield such as iron oxide and supper heated steam [2]. This reaction strongly depends on temperature and pressure conditions and the favorite conditions for it is high temperature and low pressure. In addition to dehydrogenation of ethyl benzene to styrene reaction, a set of parallel endothermic reactions can occur that lead to benzene and toluene production. These competitive endothermic reactions cause decrease of styrene yield. Therefore an optimal operating temperature must be selected to achieve high conversion of ethyl benzene to styrene [3]. Additionally, selectivity of catalyst for conversion of ethyl benzene to styrene must be considered. Generally, yield and selectivity of styrene monomer can be influenced by some parameters such as temperature, pressure, molar ratio of the steam to ethyl benzene in the feed and selectivity of catalysis. Conversion of ethyl benzene and selectivity of the styrene increases with increasing of temperature, pressure and molar ratio of steam to ethyl benzene in the feed [4].

Many studies on kinetics, reactor modeling, simulation and optimization of the styrene reactor have been reported. More than 50 years ago, Wenner and Dybdal [5] obtained rate data from experiments for two types of catalysts. Sheel and Crowe [6] determined rate coefficients and heat of reactions from the industrial data of an adiabatic styrene reactor using a pseudo-homogeneous model. They obtained the best kinetic model by calibrating several models using catalyst manufacturers' data. The kinetic model proposed by Sheel and Crowe has been widely used by most researchers for simulation and optimization of industrial reactors [7-9]. Elnashaie et al. developed a heterogeneous model based on the dusty gas model [9]. They used the model to extract intrinsic kinetic data from industrial data iteratively. In another paper, Abdalla et al. reported intrinsic kinetics for three promoted iron oxide catalysts using pseudo-homogeneous and heterogeneous models, and compared the performance of these catalysts [4].

In the present work, results of mathematical modeling of styrene monomer production process were reported. With this pseudo-homogeneous model, the profile conversion of ethyl benzene and steam, styrene yield and selectivity, temeperature and pressure were achieved through the length of catalytic fixed bed reactor and were compared with an industrial reactor as a case study. The best molar ratio of the steam to ethyl benzene in feed has been investigated for optimal conversion of ethyl benzene and styrene selectivity. Using results of mathematical model, an Artificial Neural Network model has been developed for simulation of the effects of feed composition.

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TABLE1
Kinetic Equation And Frequency Factors And Activation Energy Of Ethylbenzene Dehydrogenation

Num	Reaction	Reaction rate	A_i	$E_i \times 10^{-5}$ (j.mol^{-1})
1	$C_6H_5CH_2CH_3 \longrightarrow C_6H_5CHCH_2 + H_2$	$R_1 = k_1\left(p_{EB} - {p_{ST}p_{H_2}}/{K_{EB}}\right)$	8.32×10^3	0.909
2	$C_6H_5CH_2CH_3 \longrightarrow C_6H_6 + C_2H_4$	$R_2 = k_2 p_{EB}$	4.29×10^9	2.80
3	$C_6H_5CH_2CH_3 + H_2 \longrightarrow C_6H_5CH_3 + CH_4$	$R_3 = k_3 p_{EB} p_{H_2}$	6.13×10^2	0.915
4	$2H_2O + C_2H_4 \longrightarrow 2CO + 4H_4$	$R_4 = k_4 p_{H_2O} p_{ETH}^{0.5}$	3.95×10^2	1.040
5	$H_2O + CH_4 \longrightarrow CO + 3H_2$	$R_5 = k_5 p_{H_2O} p_{MTH}$	1.42×10^2	0.675
6	$H_2O + CO \longrightarrow CO_2 + H_2$	$R_6 = k_6\left({P_T}/{T^3}\right) p_{H_2O} p_{CO}$	5.82×10^{12}	0.736
$k_i = A_i\, exp\left[-\left({E_i}/{RT}\right)\right]$ $K_{EB} = exp\left(-{\Delta F^0}/{RT}\right)$, $\Delta F^0 = 122725 - 126.267T - 0.002194T^2$ $\left(\frac{J}{mol}\right)$				

2 EXPERIMETAL

2.1 Proccess Description

In styrene monomer reactor fresh ethyl benzene mixed with recycled ethyl benzene and steam is preheated using the product stream from the reactor, and then mixed with the superheated steam to reactor inlet temperature of over 875 K before injecting into the fixed bed catalytic reactor [10]. Superheated steam provides the necessary heat of reaction and prevents coke formation, reduces partial pressure of styrene and hydrogen to shift the thermodynamic equilibrium in favour of the styrene production [9, 10]. The reactor effluent is cooled to quench all reactions in several heat exchangers, and then directed to the separator to recover styrene.

Six main reactions occur in styrene reactor. Rate equations and frequency factors and activation energy of those reactions are listed in Table 1 [6]. The kinetic constants of the reactions are expressed by Arrhenius equation. Dehydrogenation of ethyl benzene (Eq. (1)) is an endothermic reversible reaction, and proceeds thermally with low yield but catalytically with high yield. As it is an endothermic reaction producing two moles of product with one mole of reactant, low pressure and high temperature favour forward reaction producing styrene. The competing reactions, (Equations (2) and (3)) degrade ethyl benzene to by-products such as benzene and toluene, thus reduce styrene yield [6]. As the rate of formation of by-products increases with temperature, an optimal operating temperature is necessary to compromise between conversion of ethyl benzene to the styrene and by-product formation. Moreover, a selective catalyst is desirable to achieve high styrene yield at the low temperature and to minimize side reactions.

2.2 Development of Models

For modeling of styrene monomer reactor, assuming a plug flow reactor was employed. Heat and mass transfer as well as diffusion in catalyst pellets were lumped in the rate constants. Catalyst activity is considered to be constant because of lack the available data, even though it varies with time and reactor length, also steady state conditions are considered. Thus, the model is a pseudo-homogeneous model and reactor is considered single phase. Since in the multi-phase reactor, molar flow rates of components are preferred rather than molar fractions, mass balance equations are written based on molar flow rate of components.

$$\frac{dF_i}{dl} = \rho_c (r_i) A \quad (1)$$

Where i represent components; The energy balance equation for adiabatic operation is given by equation (2). Relationship of partial pressure and molar flow rate of components with the assumption of ideal gas is given by equation (3).

$$dT/_{dl} = {\sum_i^6(-\Delta H_i) \times \rho_c \times A \times R_i}/{\sum_j F_j \times C_{P_j}} \quad (2)$$

$$p_j = P\frac{F_j}{F_t} \quad , \quad F_t = \sum_j F_j \quad (3)$$

The Ergun equation (4) is used to compute pressure profiles along the reactor.

$$\frac{dP}{dl} = -10^{-5}\left[\frac{(1-\varepsilon)G_0}{D_c \varepsilon^3 \rho_G}\right]\left[\frac{150(1-\varepsilon)\mu_G}{D_c} + 1.75G_0\right] \quad (4)$$

$$\rho_G = \sum \rho_i = \sum {p_i M_i}/{RT} \quad (5)$$

Density of gases with the assumption of ideal gas is given in equation (5). Viscosity of the mixture of gas in catalyst bed is calculated by Chapman-Enskog theory (equation (6)).

$$\mu_G = (-10.035 + 0.25191T - 0.000037932 \times T^2) \times (3.6 \times 10^{-4}) \quad (6)$$

The characteristics of the industrial reactor at Polymer Corporation, Ontario, Canada are given in Table 2 [4].

3 RESULTS AND DISCUSSION

The differential Equations of reactor model (1-6) were numerically solved using MATLAB. The set of differential equation is solved with Runge-Kutta-Verner fourth and fifth order method with variable step size. Fig. 1 shows ethyl benzene conversion, styrene yield and selectivity profiles through the length of the reactor.

TABLE 2
Industrial Reactor Specifications, Catalyst Properties And Feed Conditions

	Value	Dimension
Reactor diameter	1.95	m
Catalyst bed depth	1.70	m
Catalyst density	2146.27	kg/m^3
Catalyst diameter	4.7	mm
Catalyst pore radius	2400	Å
Catalyst porosity	0.35	
Inlet pressure	2.0	Bar
Inlet temperature	922.59	K
Inlet Ethylbenzene molar flow rate	36.87	Kmol/h
Inlet Styrene molar flow rate	0.67	Kmol/h
Inlet Benzene molar flow rate	0.11	Kmol/h
Inlet Toluens molar flow rate	0.88	Kmol/h
Inlet Steam molar flow rate	453.10	Kmol/h
Total molar feed	491.63	Kmol/h
Total mass flow	12238.79	Kg/h

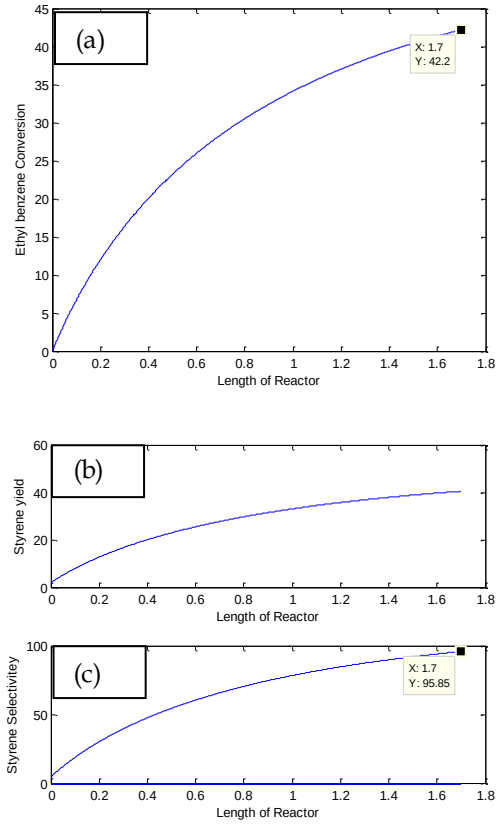


Fig. 1: a) Ethyl benzene conversion, b) styrene yield and c) selectivity profile through the length of the reactor

The results of pseudohomogeneous model and industrial reactor are compared in Table 3. The simulation results of the reactor give ethyl benzene conversion and styrene yield of 42.11% and 40.41% respectively. This indicates that the selectivity for styrene production from ethyl benzene is 95.85%. According to this table it is concluded that except in the case of benzene, results are close to the values of the industrial reactor, and the error is negligible.

There have been many attempts to improve the productivity of the dehydrogenation reactor system. Early researchers were interested in the reaction mechanisms of ethyl benzene dehydrogenation and mathematical modeling of industrial dehydrogenation [10-13]. Prediction of reactor dynamics and variation of some output against variation of some inlet parameters in industrial sites is very difficult because observation of reactor variables is limited, so trial and error tests require a lot of time and cost. Mathematical models using plant data are inadequate for describing reactor dynamics [15]. To predict some of the outputs against variation of some input parameters such as the molar ratio of the steam to ethyl benzene in the feed (S/E) and inlet temperature we proposed an alternative hybrid model. This model is composed of proposed pseudo-homogeneous mathematical model and a neural network model.

TABLE 3
Comparsion of the Results of Model And Industrial Reactor

E%	model		Industrial reactor		
	Conv.	**M.F.R**	**Conv.**	**M.F.R**	
10.87	42.11	21.31	47.25	19.45	**Ethyle benzene**
----	0.707	449.9	Not availeble	Not availeble	**steam**
	yield	**M.F.R**	**Yield**	**M.F.R**	
0.098	40.45	14.91	40.41	15.57	**Styrene**
13.52	3.26	2.15	3.77	1.50	**Benzene**
4.48	2.98	1.75	3.12	2.03	**Tholuene**
0.20	851.77		850		**Temprature**
4.87	2.207		2.32		**Pressure**
M. F. R. : Molar Flow Rate Conv. : Conversion					

Fig. 2 shows the results of proposed mathematical model for effect of the variation of S/E in fixed inlet temperature (900 °C) on conversion of ethyl benzene and styrene selectivity. According to Fig. 2, it can be seen by increasing of S/E in fixed inlet temperature; conversion of ethyl benzene increases firstly with a sharp slope finally becomes almost constant in the ratio of 100. The effect of the increasing of S/E on operation of fixed bed catalytic reactor can be expressed in three ways. Firstly, steam as a diluting agent reduces partial pressure of styrene and hydrogen to shift the thermodynamic equilibrium in favor of styrene production. Secondly, superheated steam provides the necessary heat of endothermic reactions. Thirdly, superheated steam prevents coke formation and catalyst deactivation [11].

Fig. 2 shows that the selectivity of styrene with the variation of S/E has an optimal value as in the molar ratio 14.2 maximum value of styrene selectivity can be achieved. Fig. 3 shows the profile of effect of the inlet temperature in fixed S/E (14) on conversion of ethyl benzene and selectivity of styrene.

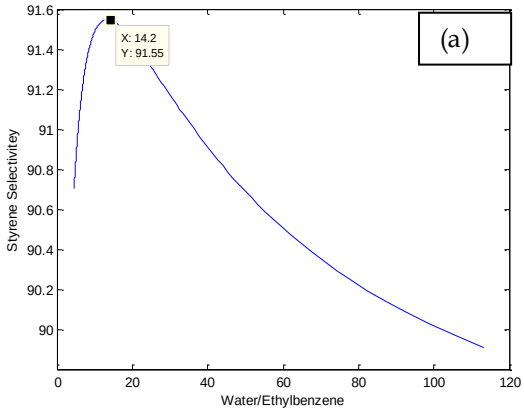
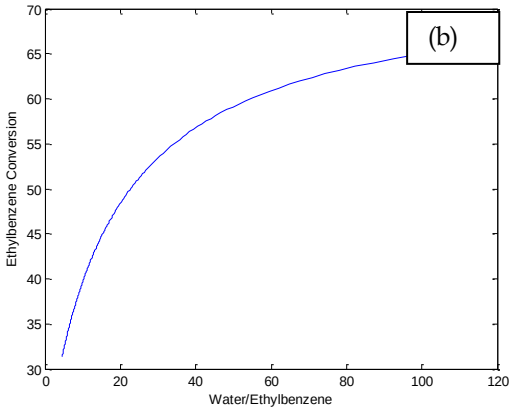


Fig. 2: a) Ethyl benzene conversion, b) Styrene selectivity profile against



According to Fig. 3 with the increase of inlet temperature, the rate of the endothermic reaction such as dehydrogenation of ethyl benzene will be increased. Consequently the conversion of ethyl benzene will be increased with increasing of inlet temperature. According to Fig. 3 it can be seen that the selectivity of styrene in temperature range of 500 – 750 °C is fixed at the maximum amount. However the selectivity of styrene will be reduced in the higher inlet temperature. Consequently, an optimum value of the inlet temperature should be selected to obtain the highest conversion of ethyl benzene and styrene selectivity. According to the results of mathematical model, inlet temperature between 850 °C to 950 °C is the best temperature to get the highest conversion and selectivity.

In recent years, the concept of neural networks has gained wide popularity in many fields of chemical engineering such as dynamic modeling of chemical processes [15, 16], design of catalysts [17], modeling of chemical reactors [18, 19, 20] and modeling of the complex chemical process [21, 22, 23]. In this research, in order to simulate the styrene monomer production reactor and predict the response of the reactor against changes of operation condition such as S/E and inlet temperature, the arrays of appropriate three-layer neural networks have been designed with different number of in hidden layer neurons and network training algorithm. The network includes one input layer which provides input data to the network, a hidden layer and an output layer that represents network response.

The number of input and output nodes is governed by functional requirements of ANN. The number of input neurons corresponds to the number of operational condition that contains the S/E and inlet temperature. The number of output neurons corresponds to the number of response that contains conversion of ethyl benzene and selectivity of styrene. A sigmoid transfer function used for the hidden layer and output transfer function was a linear function.

Training of designed ANN was performed using results of proposed mathematical model in changes of S/E and inlet temperature. Since used transfer function of hidden layers is sigmoid, we scaled all input vectors in the interval [0, 1]. The data were split in three subsets: training, validation and test set. Splitting of samples plays an important role in evaluation of an ANN performance. The training set is used to estimate the model parameters and the test set is used to check the generalization ability of the model. In this work, 480 data were prepared with changing of S/E and inlet temperature using mathematical mode. The training, validation and test sets include 288 data (60% of total data), 96 data (20% of total data) and 96 data (20% of total data), respectively.

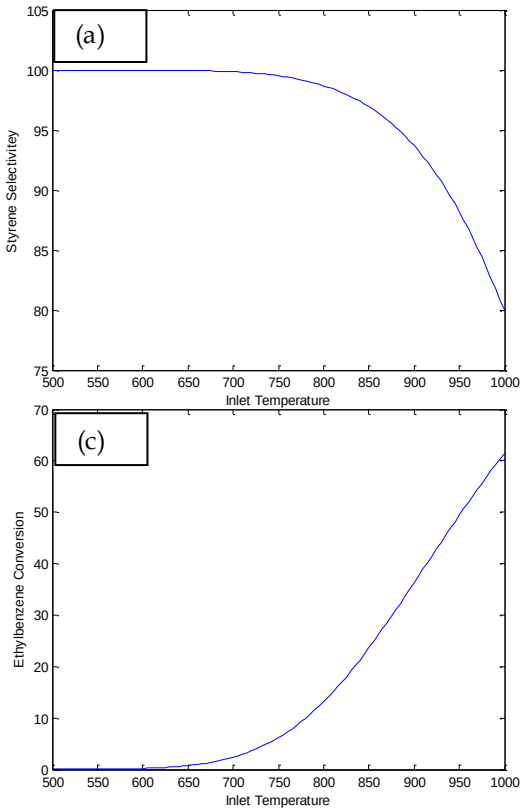


Fig. 3: a) Ethyl benzene conversion, b) Styrene selectivity profile against inlet temprature

It is recognized that the selection of neurons in the hidden layer and training algorithm can have a significant effect on network performance. In this paper, we tried two steps to ob-

tain the optimum model of ANN. In first step, we test different number of neurons in the hidden layer and then, the best design of layers of ANN was considered for the variation of training algorithms such as gradient descent backpropagation (gd), gradient descent with adaptive learning rule backpropagation (gda), gradient descent with momentum backpropagation (gdm) and Levenberg-Marquardt backpropagation (lm). The mean squared error (MSE) for test set was used as the error function.

In the first step, many networks with different neurons in hidden layer were trained with the Levenberg-Marquardt backpropagation algorithm. Table 4 shows the performance (MSE for training and test sets) of designed network with different neurons in hidden layer. It was found that the network with three neurons in hidden layer has the MSE less than other trained networks. The MSE was 3.48e-10 for training set and 4.63e-8 for test set.

TABLE 4
Comparison of the Performance of Different Designed Network

num	topology	Number of epoch	Training algorithm	MSE for training set	MSE for test set	R^2
1	2-1-2	1000	lm	2.4×10^{-5}	1.8×10^{-4}	0.9801
2	2-2-2	1000	lm	1.2×10^{-6}	2.5×10^{-6}	0.9745
3	2-3-2	1000	lm	3.48×10^{-10}	4.63×10^{-8}	0.9908
4	2-4-2	1000	lm	2.1×10^{-8}	4.1×10^{-6}	0.9815
5	2-5-2	1000	lm	4.7×10^{-5}	1.3×10^{-5}	0.9600
6	2-6-2	1000	lm	3.4×10^{-3}	5.87×10^{-3}	0.9026
7	2-3-2	1000	gd	1.56×10^{-6}	4.16×10^{-5}	0.8794
8	2-3-2	1000	gda	1.4×10^{-5}	2.8×10^{-4}	0.9178
9	2-3-2	1000	gdm	1.89×10^{-5}	1.63×10^{-5}	0.8165

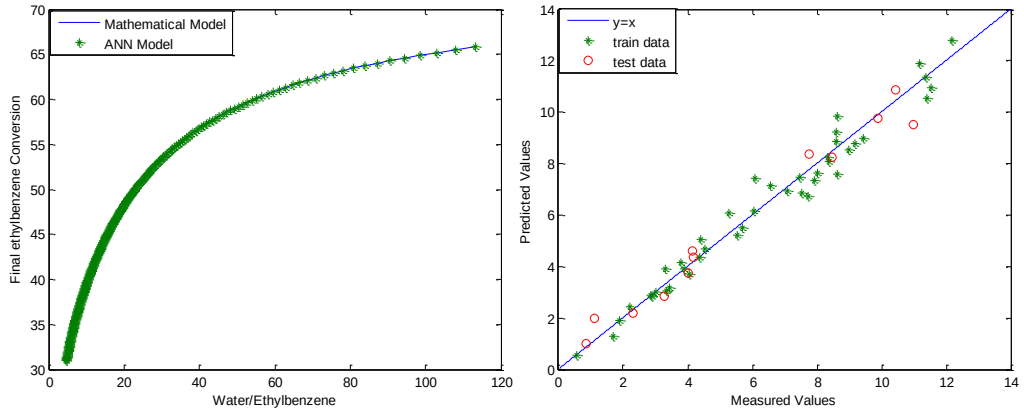


Fig. 4: Comparsion betw ean results of mathematical model and ANN prediction of Ethyl benzene conversion

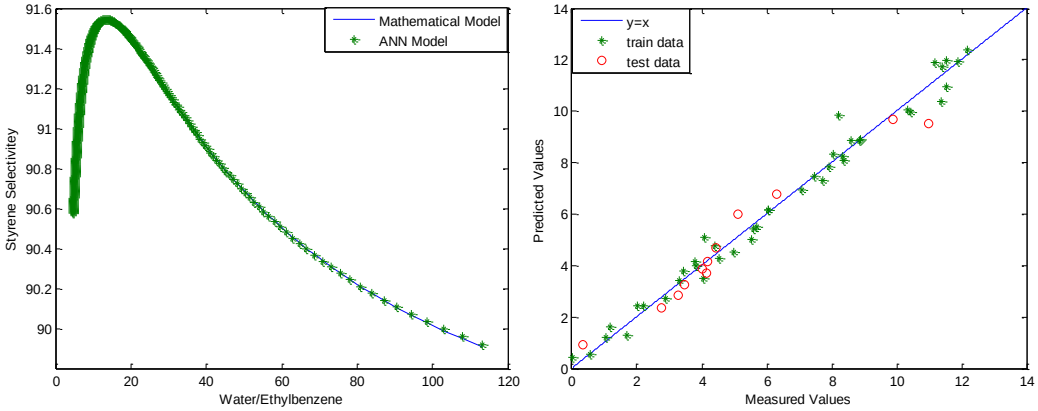


Fig. 5: Comparsion betw ean results of mathematical model and ANN prediction of Styrene selectivity

In second step, an ANN with three neurons in hidden layer was considered for the variation of the training algorithm. In Table 5, the performances (MSE for training and test sets) of designed network with the different training algorithm are listed. It was found that a network with the Levenberg-Marquardt backpropagation algorithm has the MSE less than other trained networks. To test the accuracy of ANN model, a comparison is made between mathematical model and ANN results. Figs. 4-5 show a comparison between mathematical model results and predicted values of the results, using the optimum neural network model with three neurons in the hidden layer and Levenberg-Marquardt backpropagation algorithms. These results confirm that the neural network model can predict adequately the conversion of ethyl benzene and selectivity of the styrene in the styrene reactor under different feed conditions.

4 CONCLUSION

The pseudo-homogeneous model of styrene monomer production reactor was formulated and numerically was integrated with Runge-Kutta-Verner fourth and fifth order method using MATLAB. The profile of effects of some important parameters in the reactor was found by pseudo-homogeneous mathematical model. The results of the proposed model compared to an industrial reactor that was very similar. The proposed mathematical model was used for calculation of the output of the reactor against variation in S/E and inlet temperature. According to the results of the proposed model, with increasing of S/E, the conversion of ethyl benzene increases but the selectivity of styrene decreases. The selectivity of styrene has an optimal value in S/E =13.5-14.5 and inlet temperature between 850 °C to 950 °C is the best temperature to get the highest conversion and selectivity. THEN a three-layer perceptron neural network, with two input nodes, three neurons in hidden layer and two neurons in output layer and Levenberg–Marquardt training algorithm, was developed for simulation of the effect of feed composition and operation condition on conversion and selectivity. These results confirm that the designed neural network model is able to predict the conversion of ethyl benzene and selectivity of styrene in the styrene reactor under different conditions.

4 SYMBOLS

Sym.	definition	dimension
R_i	reaction rates for *i*th component	kg mole/s kg $_{catal}$
k	kinetic constants for *i*th component	kmol.kg $_{catal}^{-1}$ h^{-1} bar^n
K_{EB}	equilibrium constant for styrene formation	Without dimension
p_i	partial pressure for *i*th	bar
P	total pressure	bar
T	temperature	K
F_i	flow rate of component *i*th	$kmol.h^{-1}$
F_t	total flow rate	$kmol.h^{-1}$
ρ_c	density of catalyst	$kg.m^{-3}$
ρ_g	density of gas mixture	$kg.m^{-3}$
μ_g	viscosity of gas mixture	$kg.m^{-1}\ s^{-1}$
Cp_i	Molar heat capacity of component *i*th	kJ $kmol^{-1}$ K^{-1}
M_i	Molecular mass of component *i*th	kg/kmol
A	cross-sectional area of reactor	m^2
l	length of reactor	m
ΔH_i	heat of reaction *i*th	$kJ.kmol^{-1}$
ε	porosity of catalyst	Without dimension
d_c	diameter of catalyst particle	m

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