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Chemical Engineering Journal 115 (2005) 113–120

Chemical Engineering Journal

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Hybrid artificial neural network—First principle model formulation for the unsteady state simulation and analysis of a packed bed reactor for CO_2 hydrogenation to methanol

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Received 18 February 2005; received in revised form 26 August 2005; accepted 26 August 2005

Abstract

Carbon dioxide emission is well recognized as the main source of global warming. The catalytic hydrogenation of carbon dioxide to methanol represents an effective method for preventing this side effect. The objective of this paper is to present a hybrid neural network model (NNM) for the simulation of a differential catalytic hydrogenation reactor of carbon dioxide to methanol. The hybrid model consists of two parts: a mechanistic model and a neural model. The mechanistic model employs heat transfer, mass transfer and pressure drop equations and calculates the effluent temperature of the reactor by taking outlet mole fractions from the output of a neural network model.

The prepared hybrid model was used to simulate and identify an existing industrial methanol reactor. The bed of the reactor was assimilated to a pile of layers, each corresponding to a neural network (NN) model that can predict outlet composition of each layer as a function of time. The model was successfully tested with plant experimental data. The insights of this research indicate a very fast responding model in comparison to traditional models to demonstrate CO_2 reduction as a function of time and reactor length. Variation of temperature and other compositions with time and bed height are also investigated in this article.

Keywords: CO_2 reduction; Methanol synthesis; Neural network; Packed bed reactor

1. Introduction

CO_2 is considered to be the major cause of global warming. The net increase of 13,000 million tonnes of carbon dioxide estimated to be added to the atmosphere annually is alerting [1]. The rising level of CO_2 is already affecting the atmosphere, sea level and ecological systems. The global sea level rose 10–20 cm over the past century and in this century it may rise by as much as 88 cm. The current atmospheric concentration of carbon dioxide at 380 ppm is 30% higher than the pre-industrial level and is expected to increase to somewhere between 800 and 1000 ppm by the year 2010. The chemical reduction of carbon dioxide is regarded as the most effective method to reduce carbon dioxide concentration in the atmosphere [2]. Catalytic hydrogenation of CO_2 is one of the chemical reduction methods that can produce low grade hydrocarbons. Especifically, methanol is considered to be the most valuable product because of its use as feed stock to produce other valuable products [3].

For chemical reactor modeling, the accurate knowledge of kinetics is necessary. However, the kinetic modeling of complex chemical reactions usually suffers from a number of problems:

1. Despite the fact that some reactions have been carried out in practice for many years, reaction mechanisms still remain not understood, e.g., hydrogenation of propionic anhydride [4].
2. Large number of reactions and intermediates play significant roles in reaction systems.
3. In many cases, kinetic modeling depends on hidden state variables, such as adsorbed surface components, gas phase radicals, or radicals (i.e. polymerization chain reactions) whose concentrations cannot be quantified using conventional measurement techniques.

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doi:10.1016/j.cej.2005.08.018

Nomenclature

A	output of network Input layer
A_i	constant of Eq. (10)
A_c	reactor surface area (m^2)
B	output of network hidden layer
B_i	constant of Eq. (10)
C	output of network
C_i	constant of Eq. (10)
C_p	specific heat (J/kg)
d	diameter (m)
D_i	constant of Eq. (10)
E	error
F	neuron activation function
F	total molar flow rate (mol/s)
I	input data of network (mol/(s kg))
MPR	methanol production rate (kg/day)
M_w	molecular weight (g/mol)
M	mass (kg)
N	number of outputs in ANN
N_C	number of components
N_r	number of reactions
P	pressure (Pa)
r	rate of formation in each time (kg)
R_i	rate of reaction for reaction I (mol kg/(cat. s))
Re	Reynolds number
T	temperature (K)
$\overline{T}$	average temperature (K)
U	overall heat transfer coefficient (W/(m^2 K))
u_g	gas velocity (m/s)
V	weight on network Hidden layer
W	mass of catalyst (kg)
W_{ij}	weight on network output layer
y	mole fraction of specified component
z	bed height (m)

Subscripts and superscripts

g	gas
i	component number
in	input
0	zero time condition (fresh catalyst)
out	output
p	particle
r	reaction
R	reference

Greek letters

ΔH	heat of reaction (J/mol)
ε	bed voidage (m^3/m^3)
μ	viscosity (Pa s)
ρ	density (kg/m^3)

4. Even in the presence of elementary reaction networks, the use of unique global reaction rate law can be impossible because the rate determining steps may change with varying operating conditions. For instance for CO oxidation over Pt-alumina catalyst, the rate determining step shifts from surface reaction to adsorption depending on temperature [5].
5. In hydrogenation of CO and CO_2 to produce methanol on $Cu/ZnO/Al_2O_3$ catalyst, preliminary results indicated that it is not possible to use Langmur–Henshelwood reaction rate expression to predict the rate of reaction in low activities [6].

In addition to the above drawbacks leading to inaccuracies in detailed kinetic models, such models are also not computationally tractable because they often lead to stiff differential equations. The complexity of these models and their associated solution times render them of little practical use for dynamic unsteady state reactor simulations, for optimization studies and for online process control applications. Adopting aNN approach for solving kinetic problems can be an attractive alternative.

Neural networks have been used as a promising technique, when complex reaction systems cannot be well identified, or in the case of lack of basic knowledge of reaction mechanisms. It has been claimed that artificial neural networks (ANN) are 120–5000 times faster than phenomological models [7], and can therefore lead to significant reductions in computation times. Recently, ANN have been used to formulate kinetic models for biological as well as conventional chemical reactors [7–17]. Various aspects of kinetic modeling of chemical reactors with multilayer feed forward networks have been studied by Molga [12]. This work makes no comparison and judgment about other NN architectures and training algorithms. In the work of Jose et al. [13], only a back-propogation algorithm was considered. Both studies of Jose and Molga [12,13] based on simulation data for training the NN. The effect of bed height was not studied in their works.

Most published works on methanol synthesis and kinetics, including our recent work [18], are based on mechanistic models. No attempt has been made to incorporate the use of neural networks in modeling such processes. In this paper, a hybrid neural network model is developed that combines both first principle models and neural network models. The ANN is adopted to estimate the outlet composition only (Fig. 1) and the first principle model is used to calculate the outlet pressure and temperature from the reactor. The outlet temperature of each layer was calculated by simultaneous solution of governing equations (heat, mass and pressure drop). The pressure drop across the bed was calculated based on Ergun correlation [19]. Different experimental reaction conditions (feed composition, pressure and temperature) are applied to the hybrid model.

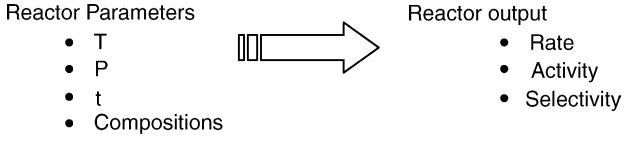

Fig. 1. Scheme of application of ANN in kinetic modeling, as a black box model.

The second part of this paper uses the developed hybrid model to study an existing industrial reactor. Because the hybrid model is based on experimental kinetic data from a lab scale reactor, the bed of industrial methanol reactor was divided into differential layers, each corresponding to the hybrid model conditions. The output of each layer is fed as input to the succeeding layer. The procedure is continued until the outlet of industrial reactor can be estimated.

2. Hybrid simulation of reactor

Hybrid models may be developed in many different combinations. Knowledge of the process can guide how to build them. A usual approach is having the first principle model as the basis, while the NN calculates unknown parameters. Another way is using the NN to learn deviation between mathematical model output and the aimed output. Another alternative is to use the deterministic model as reinforcement for the relation between inputs and outputs [8,20].

In this study, a NN model is used to learn the relationship between certain input and output data. The input data are time, pressure, temperature and feed compositions and effluent compositions are output data. The scheme is described in Fig. 2. The NN model receives information from input variables and estimates output compositions. The results are then fed to a first principle model to compute the reactor outlet temperature and pressure.

2.1. Mathematical modeling of Kuechen–Hoffmann differential reactor (first principle model)

The following three reactions can be assumed to occur in methanol synthesis:

$$CO + 2H_2 \Leftrightarrow CH_3OH \quad (1)$$

$$CO_2 + 3H_2 \Leftrightarrow CH_3OH + H_2O \quad (2)$$

$$CO_2 + H_2 \Leftrightarrow CO + H_2O \quad (3)$$

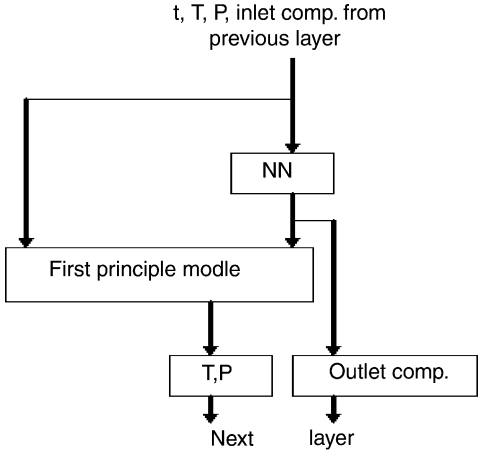

Fig. 2. Hybrid model scheme.

Skrzypek et al. [21] indicated that only two of these equations are stoichimetrically independent and can define an equilibrium composition of gas mixtures. Approximating an internally recycled reactor with a differential mixed flow reactor, the governing equations in terms of component mass balance can be expressed as:

$$Fy_i - F^0 y_i^0 = WR_i \quad (4)$$

where y_i is the mole fraction of component i, W the catalyst weight in the reactor, R_i the rate of formation of component i, F^0 the total molar flow rate at the reactor inlet and F is the total molar flow rate at the reactor outlet. The relationship between F and F^0 in an isobaric non-isothermal CSTR reactor can be written as:

$$F = F^0 + W\sum_{i=1}^{N_C} R_i \quad (5)$$

where N_C is the number of reaction components. The reaction components in methanol synthesis are H_2, CO, CO_2, CH_3OH and H_2O. CH_4 and N_2 are inert components. Combining Eqs. (4) and (5) and rearranging gives:

$$\left[\frac{y_i - y_i^0}{\left(\frac{W}{F^0}\right)}\right] + y_i\sum_{i=1}^{N_C} R_i = R_i \quad (6)$$

from which the mole fraction of component i can be calculated at each time.

The exit pressure is calculated using Ergun's equation [19]:

$$\frac{dP}{dz} = -10^{-5}\left(1.75 + 150\frac{1-\varepsilon}{Re}\right)\left(\frac{1-\varepsilon}{\varepsilon^3}\right)\left(u_g^2\frac{\rho_g}{d_p}\right) \quad (7)$$

where dP is pressure drop in increment dz, ε the bed voidage and u_g, ρ_g and d_p denote gas velocity, density and packing diameter, respectively. Outgoing temperature is obtained by numerical solution of the energy balance equation:

$$\sum_{i=1}^{N_C} M_{in}(i)\frac{C_p}{M_w}(T_{in} - T_R) - \sum_{i=1}^{N_C} M_{out}(i)\frac{C_p}{M_w}(T_{out} - T_R) + \sum_{i=1}^{N_r}\left(\frac{-\Delta H_r(i)}{M_w}\right) r_i - UA_c(\bar{T} - T^{shell}) = 0 \quad (8)$$

where

$$\bar{T} = \frac{T_{in} + T_{out}}{2} \quad (9)$$

N_r is the number of reactions and T_R is a reference temperature. According to Vanden Bussche and Froment [22], there are two equilibrium reactions and their rates r_1 and r_2 could be obtained from Eq. (6). Physical properties of methanol are obtained from [23] as:

$$\begin{aligned} \mu &= 67.2 \times 10^{-7} + 0.21875 \times 10^{-7}\bar{T}, \\ C_p &= 1000(A_i + B_i\bar{T} + C_i\bar{T}^2 + D_i\bar{T}^3), \\ -\Delta H_r(1) &= 57980 + 35(T - 498.15), \\ -\Delta H_r(2) &= -39892 + 8(T - 498.15) \end{aligned} \quad (10)$$

where A_i, B_i, C_i and D_i are constants.

Table 1
Comparison of mean square errors of various training algorithms

Training method	M.S.E.
Back-propagation	3.0051×10^{2}
Adaptive variable learning rate	0.7321
RP (resilient propagation)	2.2×10^{-10}
RBE	6.9×10^{-11}
RB	1.2×10^{-10}

2.2. Kinetic modeling with neural networks (NN model)

ANN inputs should be selected carefully if the best results are to be achieved. The inputs should reflect the underlying physics of the process to be analyzed. In the methanol reactor, inlet mole fractions play a prominent role in affecting the system behavior. Additionally, pressure, temperature and reactor operation time have strong effect on the rate of methanol production. Experimental data in terms of mole fractions of components reported by Kuechen and Hoffmann [24] have been used in this study. Two sets of experiments are used at two different space velocities. At a space velocity of 2.9 kg cat. s/mol, 118 data points for a period of 1034 h of operation are obtained. At a space velocity of 3.1 kg cat. s/mol, 48 data points for a period of 426 h of operation are used.

Various architectures of multi layer perceptron (MLP) and radial basis function network (RBFN) are used to predict experimental reactor outlet compositions. Among these architectures, radial basis (RB) and exact RBFN (RBE) methods were found to be able to generalize well. Each ANN was trained with 2/3 of the data set and the remaining 1/3 was used for validation of the trained NN and few data were used for validation of the hybrid model as will be explained later.

As shown in Table 1, RBFN method is more accurate than the other ANN structures. Table 1 compares the mean square error (M.S.E.) of various networks. Among the RBFN trained networks, RBE algorithm had a good performance and was used for the generation of the kinetic data with the hybrid model (Section 3). Table 2 provides the percent error between simulation and experimental results.

Fig. 3 compares the predictions of the NN with experimental data for two different inlet conditions, condition A, of $T = 513$ K, $P = 5$ MPa, $x_{H_2} = 0.7022$, $x_{CO} = 0.2780$, $x_{CO_2} = 0.0198$ and $x_{CH_4} = 0.000077$ and also for condition B, $T = 513$ K, $P = 5$ MPa, $x_{H_2} = 0.7020$, $x_{CO} = 0.1490$, $x_{CO_2} = 0.1490$ and $x_{CH_4} = 0.000085$. It is obvious that the network cannot estimate well beyond the training range, but for the training range the network prediction of hydrogen outlet mole fraction matches the experimental data very well.

Table 2
Comparison of predicted data with experimental data of Kuechen and Hoffmann at condition A

Time (h)	Experimental x_{H_2}	Predicted x_{H_2}	Error (%)
228	0.6904	0.6951	0.68
428	0.6997	0.7006	0.12
506	0.7010	0.7032	0.31

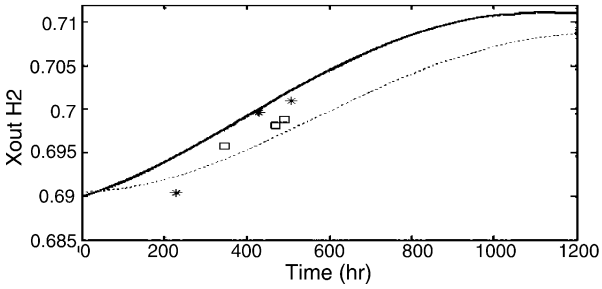

Fig. 3. Estimation of H_2 mole fraction in reactor effluent. Dotted line and square experimental data correspond to condition A in the feed. Solid line and star experimental data stand for condition B.

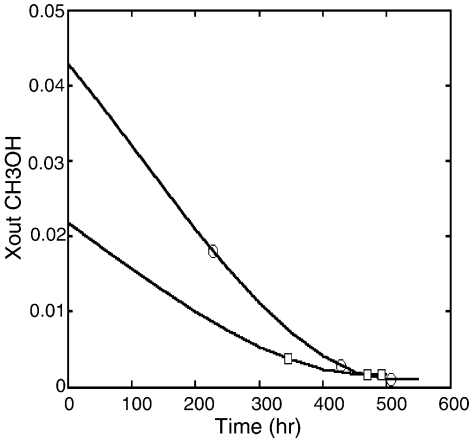

Fig. 4. Methanol mole fraction estimation NN predictions as a function of time for two different conditions. Circles represent experimental data for condition A, while squares represent condition B.

Fig. 4 represents the network estimation as a function of time. This figure clearly shows the catalyst deactivation by the passage of time. Fig. 5 gives NN simulations at different temperatures.

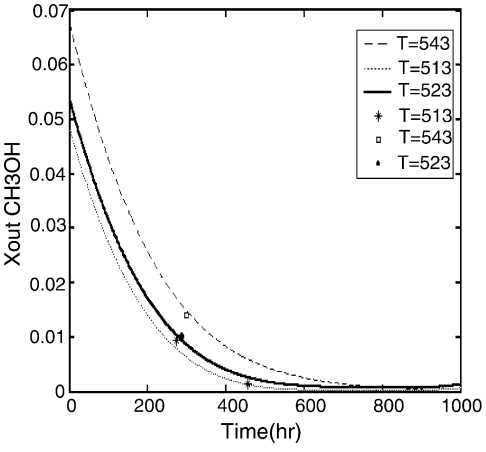

Fig. 5. NN simulations of deactivation data at different temperatures. Feed conditions are: $P = 5$ MPa, $x_{H_2} = 0.7011$, $x_{CO} = 0.2390$, $x_{CO_2} = 0.0599$ and $x_{CH_4} = 0$.

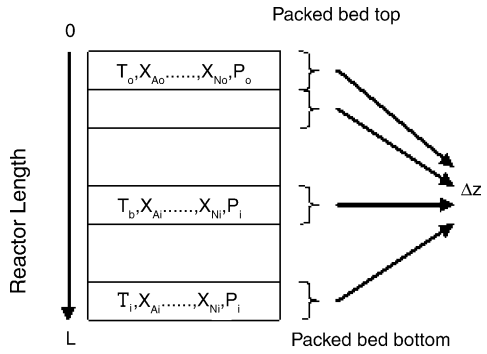

Fig. 6. Configuration of hybrid industrial reactor identification based on discretization of reactor scale.

3. Application of hybrid model to an industrial reactor

As a third modeling effort, a hybrid neural network first principle model is considered in this section. This model was described briefly in Section 2 (Fig. 2) and more details will be given here. To identify the behavior of a real reactor, the bed of reactor is first sliced into increments (Fig. 6). At each time, inlet temperature, feed composition and pressure are fed to the top of the reactor. A NN is used to estimate the outlet mole fraction of the first layer. Pressure drop is calculated from Eq. (7), and outlet temperature is obtained by trial and error as demonstrated in Fig. 7. The outlet composition, temperature and pressure of first layer are fed to the second layer and this process goes on until the end of reactor is reached (Fig. 7). By repeating this procedure, temperature and composition profiles can be estimated. The main reason for slicing the reactor is to have inlet conditions within the range of those of the NN simulation training conditions. Temperature and pressure of NN are close to the plant, Shiraz petrochemical complex (SPC) methanol reactor. In order to have smaller composition increments, the plant reactor has been sliced into sections.

To validate the model, few experimental data of Kuechen and Hoffmann [24], which were not used in training and generalization of the NN are considered. This validation may seem obvious because our NN has been trained by Kuechen and Hoffmann reactor experimental data. But the hybrid simulation is also able to predict concentration and temperature profiles inside the bed. This offers an additional flexibility that the stand alone NN model of the previous section cannot provide. Fig. 8 gives the hybrid NN simulation results for methanol, CO, H_2O and temperatures at the following conditions: $T = 513$ K, $P = 5$ MPa, $x_{H_2} = 0.7022$, $x_{CO} = 0.2780$, $x_{CO_2} = 0.0198$, $x_{CH_4} = 0$, $x_{H_2O} = 0$ and $t = 506$ h. The simulations show the correct behavior as those of other researches [6,19]. In order to check our results further, we compared the concentration of Kuechen and Hoffmann [24], reactor output to those obtained by the hybrid model. The actual concentration of methanol, H_2O and CO were measured at simulation conditions to be 0.018, 0.0008 and 0.2700 while the hybrid model predicts these concentrations to be 0.016, 0.0009 and 0.2703, respectively.

The hybrid NN model is validated further by using collected industrial data from SPC methanol reactor [25]. Tables 3 and 4

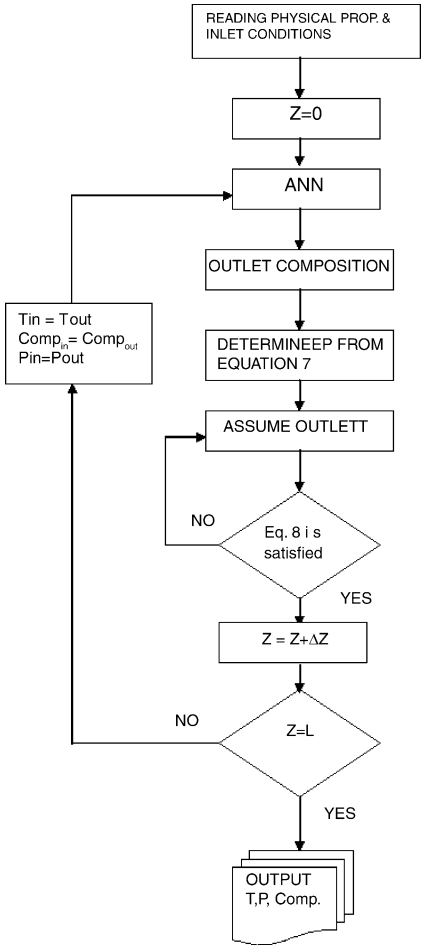

Fig. 7. Hybrid ANN algorithm for packed bed reactor simulation.

Table 3
Shiraz petrochemical methanol reactor specifications

Quantity	Value
Number of tubes	2962
Length of reactor (m)	7.022
Bulk density of bed (kg/m^3)	1132
Void fraction of bed (m^3/m^3)	0.39

Table 4
Shiraz petrochemical methanol reactor feed inlet conditions

Quantity	Value
CH_3OH (mole%)	0.50
CO_2 (mole%)	9.40
CO (mole%)	4.60
H_2O (mole%)	0.04
H_2 (mole%)	65.90
N_2 (mole%)	9.30
CH_4 (mole%)	10.26
Temperature (K)	503
Pressure (bar)	76.97
Total molar rate per tube (mol/s)	0.64

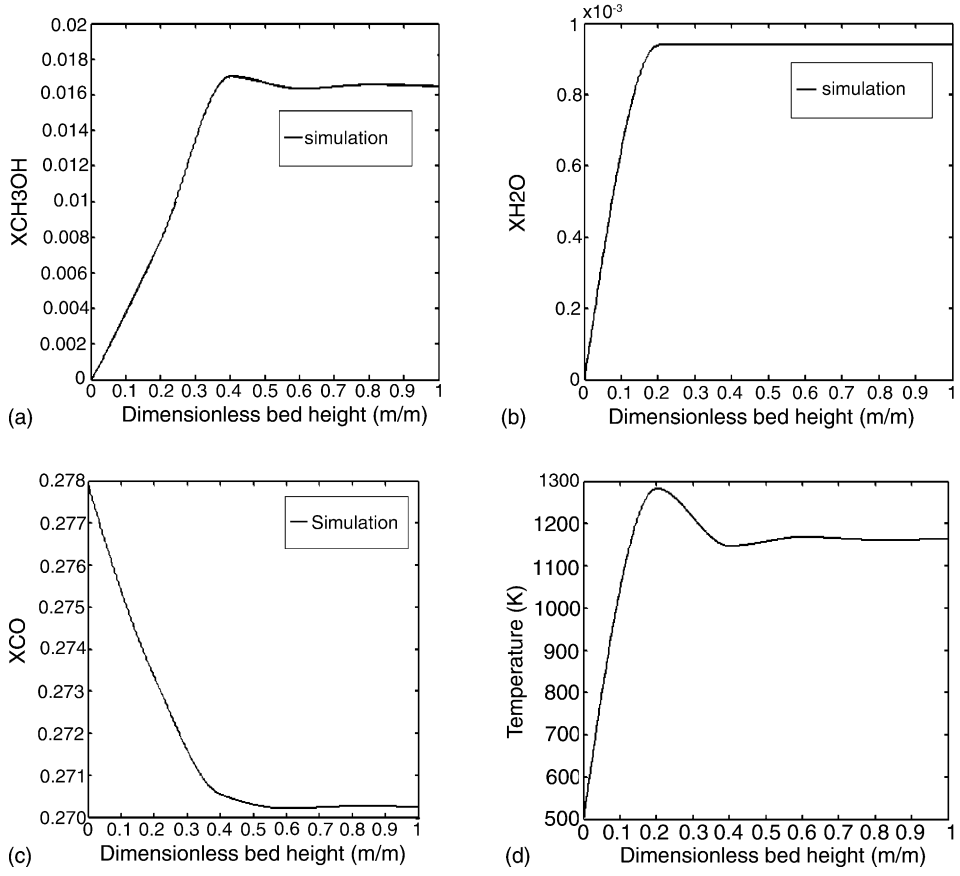

Fig. 8. Methanol, CO, H_2O and temperature profiles from hybrid neural network simulations carried out at conditions: $T = 513$ K, $P = 5$ MPa, $x_{H_2} = 0.7022$, $x_{CO} = 0.2780$, $x_{CO_2} = 0.0198$, $x_{CH_4} = 0$, $x_{H_2O} = 0$ and $t = 506$ h.

give reactor specification, and inlet and operating conditions of this reactor, respectively. Introducing initial conditions and specifications of SPC methanol reactor, hybrid NN simulations were carried out to establish the performance of the proposed model. Fig. 9 shows methanol mole fraction as a function of time and bed height. To check the accuracy of results, methanol production rate (MPR) is calculated from the equation:

$$\text{MPR} = FM_{\text{w,methanol}} \int_0^t y_{\text{methanol}}|_{x=1}\, \mathrm{d}t \tag{11}$$

and is compared with plant actual output. After 100 days of operation, the actual production was 296.5 tonnes/day while the hybrid model predicts a production of 276.63 tonnes/day. This represents a very good approximation. Simulation results for other components are shown in Figs. 10–13. These figures show mole fraction of components and temperature as a function of bed height and for different times. The Z direction is denoted by the number of grid points used to assimilate the bed. Sharp variation of temperature is observed in the 0–0.2 region of bed

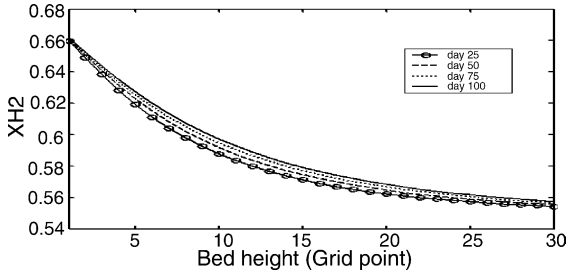

Fig. 10. Hydrogen mole fraction vs. time and bed height.

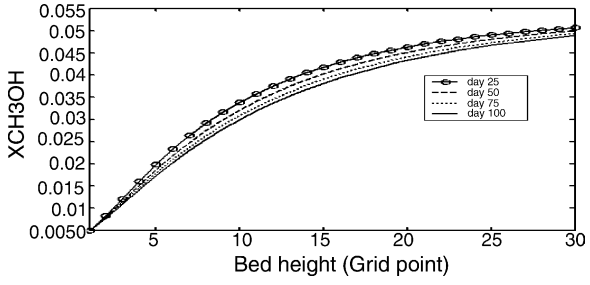

Fig. 9. Methanol mole fraction as a function of time and bed height.

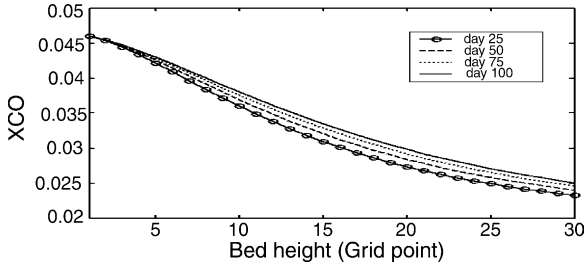

Fig. 11. Mole fraction of CO as a function of time and bed height.

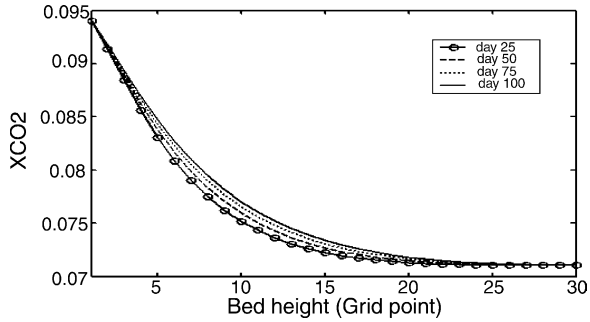

Fig. 12. Dynamic CO_2 mole fraction profiles for industrial reactor.

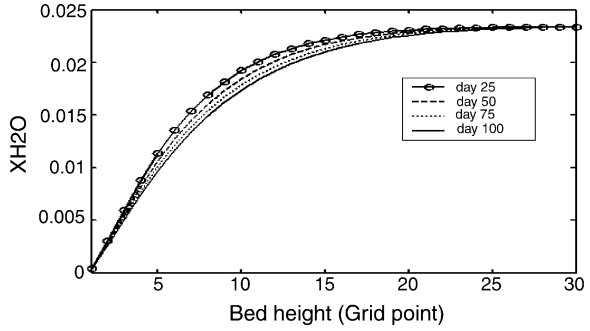

Fig. 13. Estimation of water production inside the industrial reactor vs. operation time.

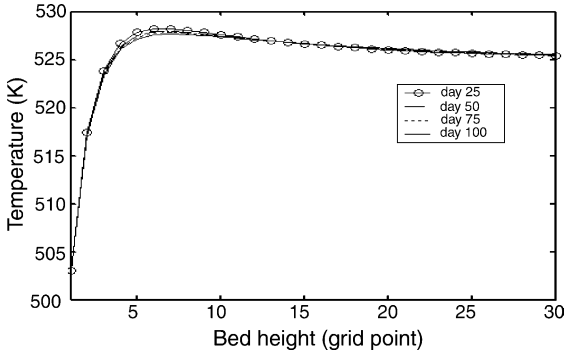

Fig. 14. Variation of temperature inside the industrial rector by the passage of time and length of reactor.

height as demonstrated in Fig. 14. At bed heights beyond 0.2, the temperature drops slowly with time.

4. Comparison of hybrid model with first principle model

In this section, the performance of the hybrid NN model is compared with the first principle model. The first principle model consists of solving the governing heat, mass and pressure drop equations. Fifteen coupled non-linear partial differential equations were solved numerically to obtain the results [18]. SPC methanol reactor conditions are used in this comparison task and the methanol mole fraction profile is selected as a comparison criterion. The bed height has been divided into 30 grid points and profiles of methanol concentrations at three different times are presented versus grid points in Figs. 15–17. The figures

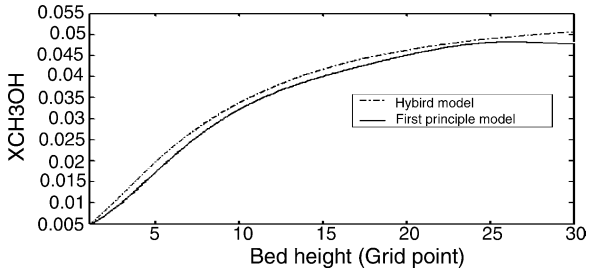

Fig. 15. Comparison of hybrid and first principle models vs. bed grid points after 25 days of operation.

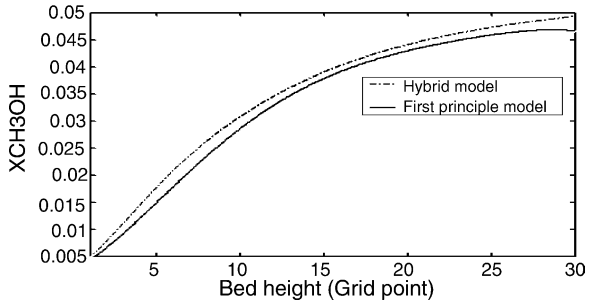

Fig. 16. Comparison of hybrid and first principle models vs. bed grid points after 50 days of operation.

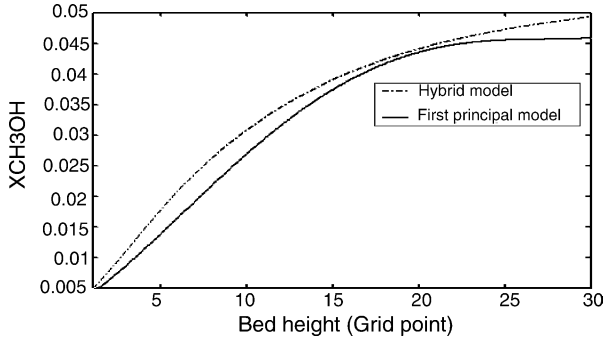

Fig. 17. Comparison of hybrid and first principle models vs. bed grid points after 75 days of operation.

confirm the accurate trend of the hybrid NN model predictions. The hybrid model simulations were performed, however, on an average of 240 times faster than the first principle simulations. The ease of hybrid model simulation represents a major advantage, especially when carrying out optimization studies.

5. Conclusion and remarks

In this work, the catalytic hydrogenation of carbon dioxide to methanol has been considered. Three modeling approaches were investigated: a first principle model, a NN model and a hybrid model. The hybrid model employs both NN model and first principle mechanistic model. The reactor outlet compositions are estimated in this hybrid model based on a neural network approach, while temperature and pressure are calculated based on application of material and energy balances and a correlation to estimate pressure drop. It was found that the hybrid model outperforms the other two modeling approaches

when compared to available experimental data. The performance of the hybrid model was measured based on both model accuracies and computational effort. The hybrid model was also employed in this work to simulate an existing industrial reactor. In order to have inputs to the NN part of the model in the same range as those the network was trained for, the industrial reactor was sliced into increments and the application of the model was carried out for each increment. The predictions of the hybrid model were also acceptable for this industrial reactor.

Acknowledgements

The authors would like to acknowledge Iranian National Petrochemical Company-R&D for its financial support. The financial support of the Natural Sciences and Engineering Research Council (NSERC) of Canada is also gratefully acknowledged.

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