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Full Length Article

Hydrogen production as a green fuel in silica membrane reactor: Experimental analysis and artificial neural network modeling

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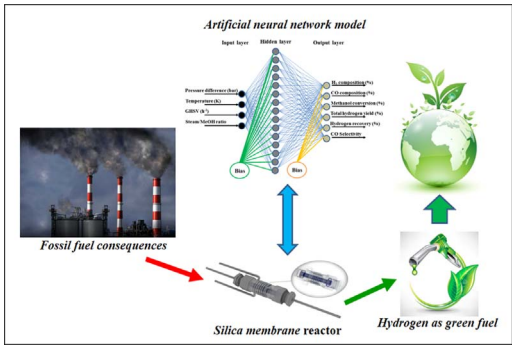
GRAPHICAL ABSTRACT



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ABSTRACT

In this work, artificial neural networks (ANNs) model has been developed for investigation of the silica membrane reactor (MR) performance during methanol steam reforming (MSR) reaction. Particularly, such parameters as the transmembrane pressure (from 0.5 to 1.5 bar), reaction temperature (from 513 to 573 K), gas hourly space velocity (GHSV) between 3300 and 10000 h^{-1} and Steam/MeOH molar ratio (from 1 to 3) have been taken to account from both experimental and modeling viewpoints in order to analyze their influences on the silica MR performance with respect to traditional reactor (TR) in terms of methanol conversion, CO selectivity, total hydrogen yield, hydrogen recovery, hydrogen and carbon monoxide compositions. The ANN model results have been validated by using portion of the experimental data. Moreover, regarding to optimization results of ANNs model, reaction temperature was selected as the most effective operating parameter in the silica membrane reactor and traditional reactor during MSR reaction.

1. Introduction

Nowadays, one of the main worldwide environmental challenges is devoted to the search for clean energy sources. Reducing the content of gas emissions that contributes to the global warming and greenhouse effect is imperative, and fuel cells are one of the most promising attractive options to solve this problem. As only heat and water are released hydrogen fuel cells can be used as a producer of clean electrical power [1–4]. In general, to generate electrical power, polymer electrolyte membrane fuel cells (PEMFC) need hydrogen as fuel. However, direct consumption of hydrogen in the PEMFC presents transport and storage problems make happen by its low density of energy. Therefore,

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Acronyms list

ANN	artificial neural networks
CFD	computational fluid mechanic
DLS	damped least-squares
DMFC	direct methanol fuel cell
GHSV	gas hourly space velocity
LMA	Levenberg–Marquardt algorithm
MAE	mean absolute error
MeOH	methanol
MD	methanol decomposition
MLP	multilayer perceptron
MR	membrane reactor
MSE	mean square error
MSR	methanol steam reforming
PEMFC	polymer electrolyte membrane fuel cells
SR	steam reforming
TR	traditional reactor
WGS	water gas shift

Nomenclature list

B	scalar bias
$E_{a,i}$	transport activation energy of component i (J/mol)
I_j	relative importance
J_i	permeating flux of component i through the membrane ($mol/m^2.s$)
N_i	numbers of input neurons
N_h	numbers of hidden neurons
Pe_i^*	permeance of component i ($mol/m^2.s.Pa$)
$Pe_{0,i}^*$	pre-exponential coefficient of component i
Pe_i	permeability of component i ($mol.m/m^2.s.Pa$)
$p_{i,retentate}$	partial pressure of component i in the retentate side (Pa)
$p_{i,permeate}$	partial pressure of component i in the permeate side(Pa)
R	gas constant (8.314 $Pa.m^3/mol.^\circ K$)
T	temperature ($^\circ K$)
W	scalar weight
$y_{i,pred}$	neural network prediction
$y_{i,exp}$	experimental response

Greek letter list

δ	membrane thickness (m)

hydrogen production in situ from hydrocarbon or alcohol feedstocks can be considered as a reasonable procedure to overcome this problem [5–7]. On the other hand, in this case, methanol indicates several benefits compared to other hydrocarbon fuels (liquid fuels at atmospheric conditions), its reforming temperature is relatively low (473–573 K) and has high hydrogen/carbon ratio [8–10]. Moreover, regarding to the methanol production, it can be obtained from a various source types such as coal, natural gas, and biomass. By the way, to steam reforming (SR) process, methanol can be fed directly to a fuel cell to produce electrical power. However, these systems propose lower power density, lower efficiency and higher catalyst usage over to the PEMFC, which present higher costs [11]. By taking all into account, MSR process is indicated as an acceptable source of hydrogen for PEMFC applications. As stated by literature [12,13], three chemical reactions can be considered in the MSR reaction: one main reaction; namely, the steam reforming itself (SR, Eq. (1)), and two side reactions methanol decomposition (MD, Eq. (2)) and water gas shift (WGS, Eq. (3)):

$$CH_3OH + H_2O \leftrightarrow 3H_2 + CO_2 \quad \Delta H^\circ = 49.4\ kJ.\ mol^{-1} \tag{1}$$

$$CH_3OH \leftrightarrow 2H_2 + CO \quad \Delta H^\circ = 90.5\ kJ.\ mol^{-1} \tag{2}$$

$$CO + H_2O \leftrightarrow H_2 + CO_2 \quad \Delta H^\circ = -41.1\ kJ.\ mol^{-1} \tag{3}$$

It should be noted that besides of the reaction products, namely hydrogen (desired product), carbon dioxide and carbon monoxide (undesired products), the non-reacted methanol and water can be observed. Whereas to feed a PEMFC, the high purity of hydrogen stream is needed, mostly because carbon monoxide poisons the platinum catalyst of the PEMFC and its concentration should be lower than 15 ppm [14]. This low content of carbon monoxide could be carried out by several strategies, namely using a permselective membrane. Combining in the same system both operations, separation and reaction, MRs present several advantages over TRs. Besides decreasing the number of chemical process units, at the same operating conditions, a MR could also attains higher performance than the ones obtained in a TR [15]. However, regarding the membrane kind to be housed in a MR, both MR cost and performance need to be taken into account. In general, several research works have presented on the Pd-based MRs application [16–28,10,29–33]. These membranes are highly selective to hydrogen permeation and allow reaching a high purity hydrogen stream. However, cracking problem during thermal cycling process and readily evidence surface pollution by carbon monoxide can reduce performance of the Pd-based membranes [32]. Moreover, Pd-based membranes are actual expensive and their applications are restricted due to low hydrogen permeance [34,35]. Therefore, a cheaper and usable alternative is strongly needed. On this route, as author's best knowledge, ceramic membranes such as microporous silica membranes are cheaper and indicate higher hydrogen flux, but, in contrast, they show lower hydrogen selectivity with respect to the Pd-based membranes. However, silica membranes, used for carrying out MSR reaction, have not been comprehensively studied [36–44]. Their promising results have justified the need of a detailed analysis of the potential advantages achievable by using silica MR. On the other hand, theoretical modeling indicates an effective possibility to design and optimization chemical/separation processes and, especially, silica MR aimed at performing MSR reaction. Various methods can be applied to develop valid models aimed for evaluation MRs can change under the effect of operating conditions.

Some modeling studies about MSR reaction in the silica MR are currently presented in the particular literatures [42–45]. In fact, all of them 1D models based on mass balance rule or CFD models have been suggested to evaluate the performance of MSR reaction in the silica MRs. Regarding to the complex structure of silica MRs, describing their performances by transport equations is difficult. According to other modeling approaches, a model based on ANNs strategy does not apply any transport equation, which could help to indicate, based on the fundamental principles, the reciprocal relationships existing between the outputs and the inputs. This aspect makes ANNs method as useful tool to model phenomena difficult to be presented by an equation-based approach, since no an initial information about the system under evaluation is essentially required [46].

According to the author's knowledge, the ANNs analysis has been not yet used for modeling MR performance, especially in the silica MRs, during MSR reaction. Therefore, the main purpose of this research work is the development of an ANN model able to forecast the behavior of MSR reaction carried out in a silica MR by varying the operating conditions, subsequently by validation with experimental data.

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