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Prophetic Appraisal of Response Surface Methodology and Artificial Neural Network Methods for Carbon Dioxide Reforming of Methane over Ni/MgO Catalyst

Tahani Gendy[1], Radwa El-Salamony[1,*], Seham El-Temtamy[1], Salwa Ghoneim[1], Dalia Abd El-Hafiz[2], Ahmed El Naggar[2] and Mohamed Ebiad[3]

[1]Process Development Department, Egyptian Petroleum Research Institute (EPRI), Cairo, Egypt
[2]Refining Department, Egyptian Petroleum Research Institute (EPRI), Cairo, Egypt
[3]Analysis and Evaluation Department, Egyptian Petroleum Research Institute (EPRI), Cairo, Egypt

***Corresponding Author:** Radwa El-Salamony, Process Development Department, Egyptian Petroleum Research Institute (EPRI), Cairo, Egypt, Tel.: 00201010707023, E-mail: radwa2005@hotmail.com

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Abstract

Radial Basis Function Neural Network (RBFNN) has been accomplished to evaluate the effect of the different operating parameters, namely the hourly space velocity, the reaction temperature, and [$C0_2$: CH_4] mole ratio on the conversion and formation of the different components involved in the dry reforming of methane over Ni/MgO catalyst. A three-layered Feed Forward Neural Network in conjugation with the Radial Basis Function, and an optimized topology of 3:10:1 (input neurons: hidden neurons: output neurons) has been developed, trained, and tested. Moreover, the RBFNN has been employed to elucidate such effects in the three and two dimensions and to display the location of the predicted maxima. The results are compared to our previosuley pblished RSM results. The preeminence of ANN was indicated in the prediction capability demostrating the R^2_{adj} & F Ratio are 0.78 - 0.99 & 17.39- 231.09 for RSM method compared to 1.00 & 9.92E+29 - 1.30E+39 for ANN method beside lower values for error analysis terms. This is due to ANN capability to approximate the non-linearity between the input and output variables.

Keywords: Modeling; RSM; ANN; quadratic models; Dry reforming of methane

Nomenclature: MDR: methane dry reforming; RSM: Response Surface Methodology ANN: Artificial Neural Network; RBFNN: Radial Basis Function Neural Network; CO_2: carbon dioxide; CH_4: methane; CO: carbon monoxide H_2: hydrogen; R^2_{adj}: regression significance; Rt: coded molar ratio of CO_2/ CH_4; SV: coded space velocity; T: coded temperature; Y: the response variable; Xi and Xj are the input-coded values of the variables that affect the response variable; e: represents the random error or uncertainties between predicted and measured values; k : the number of variables; β_0,β_i,β_{ii},β_{ij} are the regression constants of intercept, linear, quadratic, and interaction terms, respectively; ADC_{max}%: *the relative error in the prediction of maximum concentration* max_{error}%

Introduction

The frequent environmental pollution often encountered from the consumption of energy derived from fossil fuels has aroused the quest for the production of alternative and cleaner energy sources. One such alternative means of energy production is catalytic methane dry reforming (MDR) whereby the two principal greenhouse gases, carbon dioxide (CO_2) and methane (CH_4) are utilized for the production of hydrogen and syngas using active catalysts.

The dry reforming of methane has a dual advantage of mitigating the greenhouse effect by utilizing the two principal components of greenhouse gases CH_4 and CO_2 as feedstocks. Hydrogen and syngas produced can be used directly as fuel or as a chemical intermediate for synthesizing value- added chemicals and synthetic fuel. Thermo-catalytic methane decomposition is a prospective route for producing Cox-free hydrogen [1]. Hydrogen, which has been tagged as the energy of the future as being environmentally friendly, finds wide applications in electricity generation when combined with oxygen in fuel cells so it can be employed for powering cars, heating houses, and so on [2]. Hence, obtaining a compromise on the optimum conditions that can maximize the hydrogen and the syngas yield has been a bone of contention to date [3].

RSM and ANN modeling are suitable approaches to solve problems in a way that fits reality [4] so they have been enormously employed in diverse fields to investigate the various aspects of these processes as they do not need accurate expressions or the physical meaning of the system under exploration [5]. They help determine the level of importance of the process parameters and thus reduce the computational cost involved in simulation and sensitivity analyses [6]. RSM requires the specification of a polynomial function where the number of terms in the polynomial function is limited to the number of experimental design points. Selecting an appropriate polynomial equation can be tedious since each response requires an individual one. The ANN approach is quite flexible, robust technique structured in nature, it has the ability of universal approximation for almost all kinds of nonlinear functions, without the need for complicated equations, and can explore regions that are otherwise omitted when using statistical approaches. It provides sensitivity analysis determining the level of importance of the process parameters besides revealing the interactive effect of two factors on the system fitting function thus allowing the determination of the optimal parameters for designing [7]. Numerous studies have been performed to scrutinize the various aspects of RSM and ANN and to compare the significance of the models concerning different statistical parameters. In most of these works the superiority of ANN, its appropriateness, and adequacy over the RSM has been verified especially when dealing with a high degree of non-linearity systems [8]. The supremacy of ANN supremacy over RSM has been validated in predicting permeable concrete properties and Pavement Condition Index (PCI); its accuracy in optimizing methane yield from palm oil mill effluent and forecasting the mechanical performance of recycled aggregate concrete surpassed that of RSM [9-12]. Further ANN models outperform traditional Multiple Linear Regression (MLR) in predicting the properties of previous concrete blended with Ground Granulated Blast-furnace Slag. Similarly, Nejad et al. (2024) observed that ANNs provide a more effective approach for predicting the fatigue life of riveted joints in AA2024 aluminum alloy plates compared to analytical or numerical methods. Despite the vast number of researches dealing with ANN application to model and analyze different systems including methane steam reforming, only a few articles report ANN application to MDR. The papers published by [13-18] discuss the application of ANN to different catalytic systems not including Ni/MgO catalyst. In our previous publication [19] we studied in detail the application of RSM to methane dry reforming using Ni/MgO catalyst. The present study highlights the evaluation of the predictive competencies of the RSM and ANN methodologies for the formerly reported experimental data. This has been accomplished by comparing the values of the coefficient of determination (R^2), and F-Ratio besides the various error analysis parameters. Furthermore, the ANN method has been utilized to illustrate the effect of input experimental parameters on the response in three and two dimensions and to show the location of the optima.

Experimental

Preparation of Catalyst

Commercial magnesium oxide (MgO) from Fisher, Germany was calcined at 900 °C for five hours to create the magnesium oxide support. Using aqueous $Ni(NO_3)_2.6H_2O$ (Fisher, Germany) with a 10 wt% loading, the Ni/MgO catalyst was prepared using the impregnation method. This was followed by drying at 110 °C and calcining in air at 550 °C for three hours.

Catalytic Activity

A homemade fixed-bed flow system apparatus was adjusted and used to test the catalytic activity of the Ni/MgO catalyst toward dry reforming of methane [20]. Mass flow controllers were used to alter the CO_2/CH_4/Ar reaction mixture at the ratios of 1:1:4, 1:1.5:4, and 1:2:4 to produce flow rates that matched the GHSV values of 2000, 4000, and 6000 $ccg^{-1}h^{-1}$, in that order. Atmospheric pressure, and reaction temperatures of 600, 700, and 800 °C were investigated. An online quantitative gas analysis system (HIDEN Analytical QGA, England) was used to evaluate the gaseous products. Here is the calculation for the reactants' conversion:

$$CO_2\ conversion\% = \left\{\frac{CO_{2,in} - CO_{2,out}}{CO_{2,in}}\right\} X100$$

$$CH_4 conversion\% = \frac{CH_{4,in} - CH_{4,out}}{CH_{4,in}} x100$$

Evaluation of the predictive ability of RSM and ANN Models

A brief description of RSM and ANN in addition to the selection of the suitable ANN network has been presented in Supplementary data. Many approaches have been stated in the literature for evaluation of the goodness of model fitting and prediction accuracy of RSM & ANN besides error analyses as presented through the application of 24 performance and error functions' equations in Tables (1S: a-d) [Supplementary data].

To make the model computationally more tractable codification of both the input and output data variables should be performed to the range of -1 to 1, to eliminate the effect of the variation of natural independent variables units and ranges and to achieve fast convergence to obtain the minimal RMSE values [21], employing the most frequently used equation seen below [22]

$$Coded\ value = \frac{actual\ value - mean}{half\ of\ the\ range} \quad [1]$$

A second-order equation of the following form has been established for the functional relationships between the coded independent and dependent variables using the multiple regression technique:

$$Y = \beta_0 + \sum_{i=1}^{n} \beta_i X_i + \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \beta_{ij} X_i X_j + \sum_{i=1}^{n} \beta_i X_i^2 \quad [2]$$

Details of this method have been dealt with in [19, 23-27].

In the present study, the following cases have been considered

Case a: The response concentration has been employed as it is for *Y* in eq. [2], and for training in the case of ANN, the predicted concentrations were compared with the corresponding experimental concentration values [CH_4,CO_2,CO,H_2] The RSM quadratic equations are as follows:

For CH_4 conversion, $CH_4 = 78.07 + 1.476^{*}SV + 19.12^{*}T + 3.34^{*}Rt + 5.408^{*}SV^2 - 11.86^{*}Rt^2$

For CO_2 conversion, $CO_2 = 63.21 + 16.52^{*}T - 7.902^{*}Rt - 2.598^{*}T^{*}Rt$

For CO production, $CO = 35.44 + 7.879^{*}T - 4.649^{*}Rt^2$

For H_2 production, $H_2 = 34.58 + 8.896^{*}T - 6.456^{*}Rt + 3.131^{*}SV^2 - 3.694^{*}Rt^2 - 1.866^{*}T^{*}Rt$

Applying the Box-Cox method to RSM reached the following transformations to represent the response Y in equation [2] for the various components of the reaction system: $(CH_4)^2$, $(CO_2)^3$, $(CO)^3$ $(H_2)^3$. The corresponding equations are given below [19]:

For CH_4 conversion, $(CH_4)^2 = 6388.0 + 233.9^{*}SV + 2726.3^{*}T + 470.5^{*}Rt + 602.3^{*}SV^2 - 1655.5^{*}Rt^2$

For Carbon dioxide conversion, $(CO_2)^3 = 291853.0 + 188499.3^{*}T - 100008.9^{*}Rt - 82693.3^{*}T^{*}Rt$

For Carbon monoxide formation $(CO)^3 = 46804.6 + 23602^{*}T^{*}12571.7^{*}Rt^2$

For Hydrogen formation, $(H_2)^3 = 47007.2 + 31312.9^{*}T - 23750.6^{*}Rt + 7992.2^{*}SV^2 - 6651.9^{*}Rt^2 - 17321.9^{*}T^{*}Rt$

Case b- The $(CH_4)^2$, $(CO_2)^3$, $(CO)^3$ & $(H_2)^3$ have been employed in eq.[2] as Y and for training in the case of ANN, and the predicted results in both cases have been transformed back to the equivalent original responses to be compared with the corresponding experimental ones [CH_4, CO_2, CO & H_2].

Case c- The (CH_4), (CO_2), $(CO)^3$ & $(H_2)^3$ have been employed in eq.[2] as Y and for training in the case of ANN, and the predicted results in both cases have been compared with the corresponding experimental $(CH_4)^2$, $(CO_2)^3$, $(CO)^3$ & $(H_2)^3$.

Results and Discussions

These above-mentioned 24 formulas in Tables (1S: a-d) (Supplementary Data) have been employed in this study for performance evaluation and error analyses and the results are recorded in Tables (1: a-c). The performance estimation results revealed that the ANN was found to be highly efficacious with superior reliability and accuracy of performance prediction as well as fitting the target responses.

Comp_ Case _Method	Average concentration		Maximum concentration		Minimum concentration		R_square	R^2_{adj}	F_ratio	SD	Elapsed time
	Exp.	Pred.	Exp.	Pred.	Exp.	Pred.					
CH4_ case a_NN	74.63	74.63	99.05	99.05	39.05	39.05	1	1	4.60E+30	1.91E-16	8.4454
CH4_ case a_Reg	74.63	74.63	99.05	104.07	39.05	43.76	0.9578	0.9343	40.81	0.0578	0.0649
CH4_ case b_ NN	74.63	74.60	99.05	99.05	39.05	39.05	1	1	9.48E+35	1.77E-16	8.4726
CH4_ case b_Reg	74.63	74.72	99.05	99.75	39.05	39.19	0.9893	0.9834	159.29	0.0341	0.0349

CH4_ case c_ NN	5826.4	5826.4	9810.9	9810.9	1524.9	1524.9	1	1	7.53E+30	3.43E-16	8.9934
CH4_ case c_Reg	5826.4	5826.4	9810.9	9950.5	1524.9	1535.8	0.9917	0.9871	215.73	0.0718	0.0649
CO2_ case a_NN	63.20	63.20	86.09	86.09	28.89	28.89	1	1	2.10E+30	3.48E-16	7.6958
CO2_ case a_Reg	63.20	63.20	86.09	90.22	28.89	41.38	0.8258	0.7783	17.39	0.1573	0.0555
CO2_ case b_ NN	63.20	63.20	86.09	86.09	28.89	28.89	1	1	1.30E+39	3.80E-16	7.9174
CO2_ case b_Reg	63.20	63.91	86.09	87.20	28.89	44.15	0.8456	0.8035	17.47	0.1664	0.0345
CO2_ case c_ NN	291853.0	291853.0	638077.2	638077.2	24100.0	24100.0	1	1	3.00E+30	1.37E-15	7.4684
CO2_ case c_Reg	291853.0	291853.0	638077.2	663054.5	24100.0	86038.2	0.9311	0.9124	49.58	0.7446	0.0425
CO _ case a_NN	32.96	32.96	41.93	41.93	17.93	17.93	1	1	1.45E+30	3.81E-16	8.5165
CO _ case a_Reg	32.96	32.96	41.93	43.32	17.93	22.92	0.8332	0.8054	29.96	0.1091	0.0365
CO _ case b_ NN	32.96	32.96	41.93	41.93	17.93	17.93	1	1	8.97E+37	3.35E-16	8.5575
CO _ case b_Reg	32.96	33.26	41.93	41.29	17.93	21.99	0.9011	0.8846	44.88	0.0860	0.0335
CO _ case c_ NN	40099.7	40099.7	73707.6	73707.6	5767.1	5767.1	1	1	5.26E+30	1.07E-15	8.4855
CO _ case c_Reg	40099.7	40099.7	73707.6	70406.6	5767.1	10630.9	0.8883	0.8697	47.72	0.2907	0.0396
H2_ case a_NN	34.28	34.28	48.32	48.32	15.18	15.18	1	1	9.92E+29	5.25E-16	8.6338
H2_ case a_Reg	34.28	34.28	48.32	48.11	15.18	17.40	0.9638	0.9438	47.98	0.0617	0.0385
H2_ case b_ NN	34.28	34.28	48.32	48.32	15.18	15.18	1	1	5.54E+37	5.82E-16	8.6112

H2_ case b_Reg	34.28	34.25	48.32	48.31	15.18	13.77	0.9908	0.9857	200.83	0.0354	0.0373
H2_case c_ NN	34.28	34.28	48.32	48.32	15.18	15.18	1	1	9.92E+29	5.25E-16	9.9131
H2_ case c_Reg	47722.1	47722.1	112818.6	112740.9	3499.3	2613.7	0.9923	0.9880	231.09	0.1032	0.0355
Min NN =	32.96	32.96	41.93	41.93	15.18	15.18	1.00	1.00	9.92E+29	1.77E-16	7.468
Max NN =	291853	291853	638077.20	638077.20	24100.00	24100.00	1.00	1.00	1.30E+39	1.37E-15	9.913
Min Reg =	32.96	32.96	41.93	41.29	15.18	13.77	0.8258	0.7783	17.39	0.0341	0.0335
Max Reg =	291853	291853	638077.20	663054.50	24100.00	86038.20	0.9923	0.9880	231.09	0.7446	0.0649

Table (1:c): Performance and Error Evaluation of RSM and ANN Methods for Dry Reforming of CH4 Over Ni/MgO Catalyst

Similar annotations were obtained by many research groups studying various engineering problems as mentioned earlier in this manuscript. This is conveyed in the very high values of the R^2 & F ratio and the exceedingly low value of error indicators for the ANN results compared to that of RSM ones. Considering the results of the studied case a, the values of R^2_{adj} are (0.9343, 0.8054, 0.7783, & 0.9438) for RSM compared to the values of 1.00 in the case of ANN, and of F-ratio for RSM case (40.81, 17.39, 29.96, & 47.98) matched to (4.60E+30, 2.10E+30, 1.45E+30, & 9.92E+29) in case of ANN for CH_4, O_2, CO, & H_2 respectively, designating the preeminence of ANN in prediction. Furthermore, the ranges of R^2_{adj} & *F-ratio* in all the studied cases are 0.7783 - 0.9880 & 17.39 - 231.09 for RSM method compared to 1.00 & 9.92E+29 - 1.30E+39 for ANN method. Also, in all cases studied the max_{error}% for the ANN method was less than that for the RSM method. The max_{error}% range is 2.87E-14 - 5.88E-14 for the ANN compared to the range 3.22 - 28.20 for the RSM. The relative error in the prediction of maximum concentration AD_{Cmax}% ranges from 0.0230 to 5.065 for RSM, while that for ANN lies within the range 0-4.41E-14. Furthermore, for the ANN method, there is no remarkable difference in the values of max_{error}% & AD_{Cmax}% in the three studied cases, which reveals the ability of the ANN method to establish the relation of the input variables and the response in any form. On the contrary, there is a marked difference between case (a) and those of (b & c) cases. This indicates the importance of choosing the suitable equation form for representing the data in the case of the RSM.

The range of RMSE cited in Table (1b) varies between 9.06E-15 - 2.16E-10 for ANN while that for RSM is 1.067- 51313.00. These results designate that the ANN method shows a significantly better generalization prediction capacity than that of the RSM. The superior modeling capability of ANN can be accredited to its universal approximation facility for nonlinearity, whereas RSM is only limited to a second-order polynomial regression [7].

Comp_ Case _Method	Er_{av}%	$Er_{a,av}$%	$Er_{a,min}$	$Er_{a,max}$%	*RMSE*	*SEP*	*CC*	*CE1*	*CE2*	Max_{error}%	AD_{cmax}%
CH4_ case a_NN	1.92E-15	1.24E-14	0	4.30E-14	1.85E-14	2.48E-14	1.0	1.0	1.0	4.26E-14	4.30E-14
CH4_ case a_Reg	-0.5759	4.2910	0.9082	13.45	4.257	5.705	0.9787	0.9578	0.9559	6.0344	5.0652

CH4_ case b_ NN	1.16E-14	1.16E-14	0	4.41E-14	1.46E-14	2.51E-16	1.0	1.0	1.0	2.87E-14	0
CH4_ case b_Reg	-0.4356	1.8130	0.3560	11.97	2.138	2.864699	0.9947	0.9893	0.9887	5.32	0.7091
CH4_ case c_ NN	1.98E-14	2.54E-14	0	8.75E-14	2.01E-12	3.44E-14	1.0	1.0	1.0	3.71E-14	0
CH4_ case c_Reg	-0.9795	3.72E+00	0.7132	25.37	261.5	2.727	0.9959	0.9917	0.9917	5.1088	1.4233
CO2_ case a_NN	1.43E-14	2.71E-14	0.00E+00	6.15E-14	2.28E-14	3.61E-14	1	1	1	3.30E-14	1.65E-14
CO2_ case a_Reg	-2.044	1.03E+01	0.5731	43.265	7.206	8.86E-02	0.9088	0.8258	0.7891	14.516	4.7923
CO2_ case b_ NN	2.78E-15	2.54E-14	0.00E+00	1.11E-13	1.81E-14	6.20E-18	1	1	1	3.71E-14	1.65E-14
CO2_ case b_Reg	-3.468	9.2170	0.3564	52.836	6.792	0.0732	0.9194	0.8453	0.7894	17.7273	1.2882
CO2_ case c_ NN	7.99E-14	8.49E-14	0.00E+00	3.77E-13	2.16E-10	7.40E-14	1	1	1	5.47E-14	0
CO2_ case c_Reg	-19.1813	34.7266	1.0654	257.00	51313.0	0.0613	0.9650	0.9311	0.9260	11.0685	3.9145
CO _ case a_NN	3.32E-14	3.32E-14	1.81E-14	6.38E-14	1.21E-14	3.67E-14	1	1	1	4.24E-14	3.39E-14
CO _ case a_Reg	-1.2948	6.9830	0.7767	27.78	3.104	9.416	0.9128	0.8332	0.7998	17.2641	3.3267
CO _ case b_ NN	-1.27E-15	2.27E-14	0	9.91E-14	9.06E-15	2.26E-17	1	1	1	4.24E-14	1.69E-14
CO _ case b_Reg	-2.106	5.4700	0.8879	22.61	2.392	7.256	0.9492	0.9009	0.8660	13.2682	1.5157
CO _ case c_ NN	4.43E-14	6.19E-14	0	3.31E-13	1.82E-11	4.53E-14	1	1	1	3.95E-14	0
CO _ case c_Reg	-8.462	17.5500	2.688	84.34	7271.9	18.13	0.9425	0.8883	0.8743	28.1954	4.4786

H2_ case a_NN	4.28E-14	4.28E-14	0	8.44E-14	2.14E-14	6.24E-14	1	1	1	5.88E-14	1.47E-14
H2_ case a_Reg	-0.6236	4.45E+00	0.1472	14.6373	2.116	6.172	0.9818	0.9638	0.9625	5.8226	0.4388
H2_ case b_ NN	8.07E-15	3.68E-14	0	1.87E-13	1.58E-14	3.32E-17	1	1	1	5.88E-14	4.41E-14
H2_ case b_Reg	0.3071	2.32E+00	0.0230	9.2685	1.067	3.113	0.9954	0.9908	0.9910	3.2226	0.023
H2_case c_ NN	4.28E-14	4.28E-14	0	8.44E-14	2.14E-14	6.24E-14	1	1	1	5.88E-14	1.47E-14
H2_ case c_Reg	0.5741	6.86E+00	0.0689	25.3079	3479.5	7.29E+00	0.9961	0.9923	0.9922	6.1059	0.0689
Min NN =	-1.27E-15	1.16E-14	0.00E+00	4.30E-14	9.06E-15	6.20E-18	1.00	1.00	1.00	2.87E-14	0.00E+00
Max NN =	7.99E-14	8.49E-14	1.81E-14	3.77E-13	2.16E-10	7.40E-14	1.00	1.00	1.00	5.88E-14	4.41E-14
Min Reg =	-19.18	1.813	0.0230	9.269	1.067	0.0613	0.9088	0.8258	0.7891	3.223	0.0230
Max Reg =	0.5741	34.73	2.688	257.00	51313.00	18.13	0.9961	0.9923	0.9922	28.20	5.065

Table (1:b): Performance and Error Evaluation of RSM and ANN Methods for Dry Reforming of CH4 Over Ni/MgO Catalyst

Table (1c) presents the relevancy factor *RF* which reflects the effect of the independent variables on the response. The positive relevancy factor of RF_{Temp} (0.7537-0.8940) indicates the prominent effect of the increase of temperature towards the increase of conversion in agreement with Alsaffar [28]. Variation of [CO_2:CH_4] mole ratio has a moderate effect on conversion, RF_{Rt} (-0.5470 - 0.1997) while the space velocity has a negligible value RF_{SV} (−0.0999 – 0.0767), indicating its trivial effect of space velocity on the measured conversion [29]. Table (1a) discloses that the ANN method is more expensive than RSM. This is shown in the larger elapsed time for NN (7.468 - 9.913 sec) compared to that of RSM (0.0335 - 0.0649 sec), because the ANN method performs a series of computationally expensive functions for a single model.

Comp_ Case_Method	χ^2	*MAE*	*MARE*	*AAD*	A_f	B_f	*RV%*	*AFV*	RF_{SV}	RF_{Temp}	RF_{RT}
CH4_ case a_NN	3.75E-29	9.00E-15	1.50E-16	3.40E-32	1.41E-15	3.70E-16	2.26E-14	1.0	0.0672	0.8701	0.1518
CH4_ case a_Reg	2.413	2.85E+00	0.0475	3.12E-03	0.4199	0.0429	6.837	0.9981	0.0687	0.8891	0.1551
CH4_ case b_ NN	2.86E-29	5.49E-17	9.15E-19	2.93E-32	1.33E-15	1.33E-15	2.10E-14	1.0	0.0672	0.8701	0.1517
CH4_ case b_Reg	0.7253	1.16E+00	0.0193	1.08E-03	0.1771	0.0385	4.033	0.9995	0.0726	0.8806	0.1696
CH4_ case c_ NN	7.35E-27	1.23E-12	1.48E-16	1.10E-31	2.44E-15	2.00E-15	4.06E-14	1.0	0.0767	0.8940	0.1543
CH4_ case c_Reg	152.8	1.27E+06	152.8	4.81E-03	0.3542	0.0770	8.490	0.9989	0.0770	0.8977	0.1549
CO2_ case a_NN	9.40E-29	1.58E-14	2.77E-16	1.13E-31	2.89E-15	1.55E-15	3.76E-14	1	-0.0866	0.8157	-0.3903

CO2_ case a_Reg	11.38	6.51E+02	11.38	2.31E-02	0.9746	0.1054	16.991	0.9910	0.0000	0.8976	-0.4294
CO2_ case b_ NN	7.95E-29	1.21E-18	2.12E-20	1.35E-31	2.52E-15	1.48E-16	4.11E-14	1	-0.0866	0.8157	-0.3903
CO2_ case b_Reg	10.54	6.03E+02	10.54	0.0258	0.8496	0.2423	17.968	0.9920	0.0000	0.8871	-0.4084
CO2_ case c_ NN	2.32E-24	1.41E-10	2.30E-16	1.76E-30	8.51E-15	8.07E-15	1.49E-13	1	-0.0999	0.8221	-0.4362
CO2_ case c_Reg	181354.3	1.11E+11	181354.3	0.5174	2.5489	0.7268	80.4232	0.9829	0.0000	0.8520	-0.4520
CO _ case a_NN	5.75E-29	1.02E-14	4.24E-16	1.35E-31	3.55E-15	3.55E-15	3.95E-14	1	-0.0393	0.8466	0.1727
CO _ case a_Reg	4.09E+00	1.98E+00	8.25E-02	0.0111	0.6838	0.0770	11.3209	0.9932	0.0000	0.9275	0.0000
CO _ case b_ NN	3.69E-29	2.34E-18	9.76E-20	1.05E-31	2.37E-15	-2.96E-16	3.48E-14	1	-0.0393	0.8466	0.1727
CO _ case b_Reg	2.444	1.52E+00	6.31E-02	6.91E-03	0.5336	0.1779	8.929	0.9960	0	0.9202	0
CO _ case c_ NN	1.72E-25	1.36E-11	2.00E-16	1.06E-30	6.22E-15	4.44E-15	1.11E-13	1	-0.0518	0.8857	0.1997
CO _ case c_Reg	20131.6	4.40E+03	6.48E-02	7.88E-02	1.6007	0.5338	30.16	0.9787	0	0.9397	0
H2_ case a_NN	1.20E-28	1.41E-14	4.25E-16	2.57E-31	4.44E-15	4.44E-15	6.21E-14	1	-0.0328	0.7537	-0.5470
H2_ case a_Reg	1.275	1.35E+00	4.07E-02	3.55E-03	0.4358	0.0456	7.2946	0.9979	0.0000	0.7677	-0.5571
H2_ case b_ NN	9.44E-29	3.09E-18	9.32E-20	3.16E-31	3.63E-15	8.14E-16	6.89E-14	1	-0.0328	0.7537	-0.5470
H2_ case b_Reg	0.4053	6.34E-01	1.91E-02	1.17E-03	0.2339	-0.0367	4.1892	0.9995	0.0000	0.7510	-0.5567
H2_case c_ NN	1.20E-28	1.41E-14	4.25E-16	2.57E-31	4.44E-15	4.44E-15	6.21E-14	1	-0.0328	0.7537	-0.5470
H2_ case c_Reg	2702.0	1.92E+03	1.76E-02	9.94E-03	0.7017	-0.1101	12.2111	0.9977	0.0000	0.7488	-0.5680
Min NN =	2.86E-29	1.21E-18	2.12E-20	2.93E-32	1.33E-15	-2.96E-16	2.10E-14	1.00	-0.0999	0.7537	-0.5470
Max NN =	2.32E-24	1.41E-10	4.25E-16	1.76E-30	8.51E-15	8.07E-15	1.49E-13	1.00	0.0767	0.8940	0.1997
Min Reg =	0.4053	0.6340	0.0176	0.0011	0.1771	-0.1101	4.033	0.9787	0.0000	0.7488	-0.5680
Max Reg =	20131.60	1.110E+11	1.814E+05	0.5174	2.549	0.7268	80.42	0.9995	0.0770	0.9397	0.1696

Table (1:c): Performance and Error Evaluation of RSM and ANN Methods for Dry Reforming of CH4 Over Ni/MgO Catalyst

Simulation and Optimization

The graphical presentation of results provides a simple method of optimization and identification of interactions between variables. Each curve represents infinity of combinations between two variables when the third variable is kept constant [30, 31].

Establishing the efficiency of the neural network to predict the response concentration for the various conditions of the experiments, the final optimum ANN architecture was utilized employing Matlab 9.0 for the Prediction of concentration of the various components of the reaction system and to perform the Response Surface plots for the predicted components.

This has been accomplished by dividing each factor into 20 intervals and performing the simulation versus two coded variables while keeping the third at zero coded value. Therefore, a total of 400 situations were evaluated. The simulation results are presented in Figure (1-4) along with the experimental data. The three-dimensional concave curved response surfaces in these figures designate the probability of obtaining a maximum value of the measured concentration within the chosen factors' levels beside the interactive relationships among the factors and the response [32, 33].

The contour plots along with the experimental data of Figures (1:4b) consider the individual and cumulative influence of the variables and the mutual interaction between the independent and dependent variables [34]. The oval shape of the contour plots points to a significant interaction between the independent variables. The smallest ellipses in the contour plots denote the maximum predicted values [7]. When there is no interaction between the parameters, the 3d contour plot shows a circular or round shape [35]. The maximum concentration response and its corresponding input variables have been obtained by a grid search investigating the simulated results exploring the region defined by the experimental design limits. Table 2 shows the maximum predicted ANN & the previously published RSM concentration [19] together with the corresponding experimental ones which reflect the excellent ability of ANN for prediction.

component	zero space velocity			zero coded temperature			zero coded mole ratio		
	NN	Exp	RSM	NN	Exp	RSM	NN	Exp	RSM
CH_4	89.948	89.948	95.629	80.899	80.899	85.175	99.05	99.050	99.752
CO_2	86.091	86.091	87.2	76.912	76.912		80.181	80.181	
CO	39.224	39.224	41.293	38.033	38.033		41.928	41.928	
H_2	48.32	48.320	48.309	42.906	42.906	41.621	44.278	44.278	44.193

Table 2: Experimental and predicted Values of Maximum Responses of Various Components

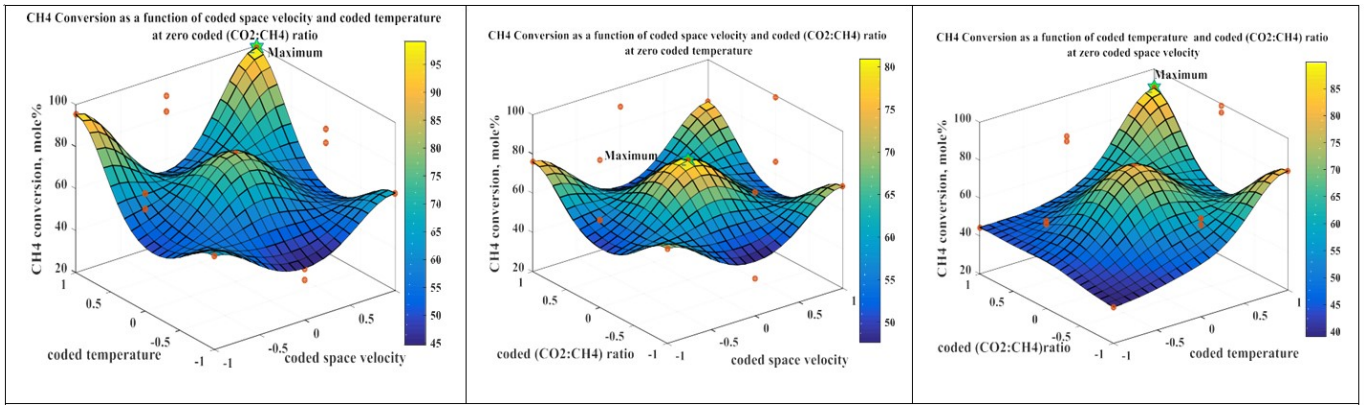

Figure (1: a): NN Surface plots for CH_4 conversion of methane dry reforming over Ni/MgO Catalyst

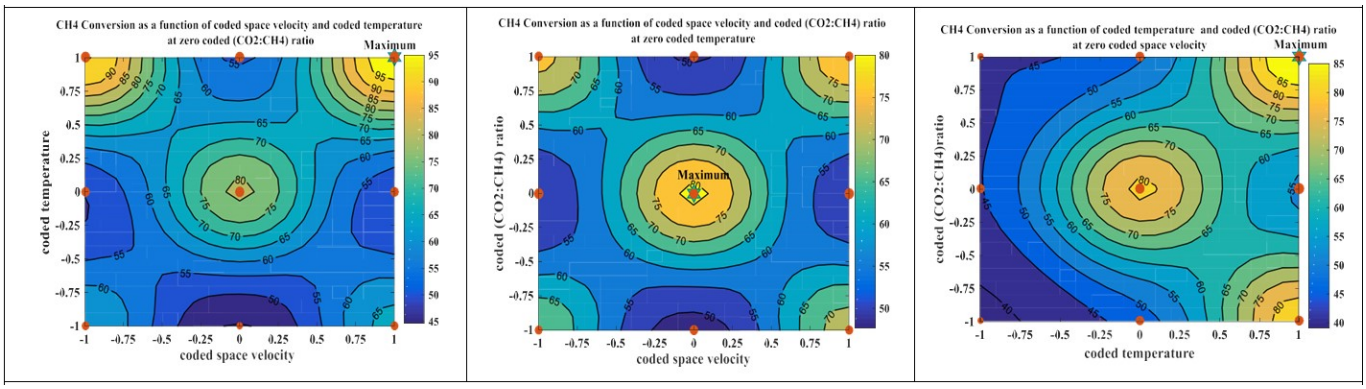

Figure (1: b): NN Contour plots for CH_4 conversion over of methane dry reforming over Ni/MgO Catalyst

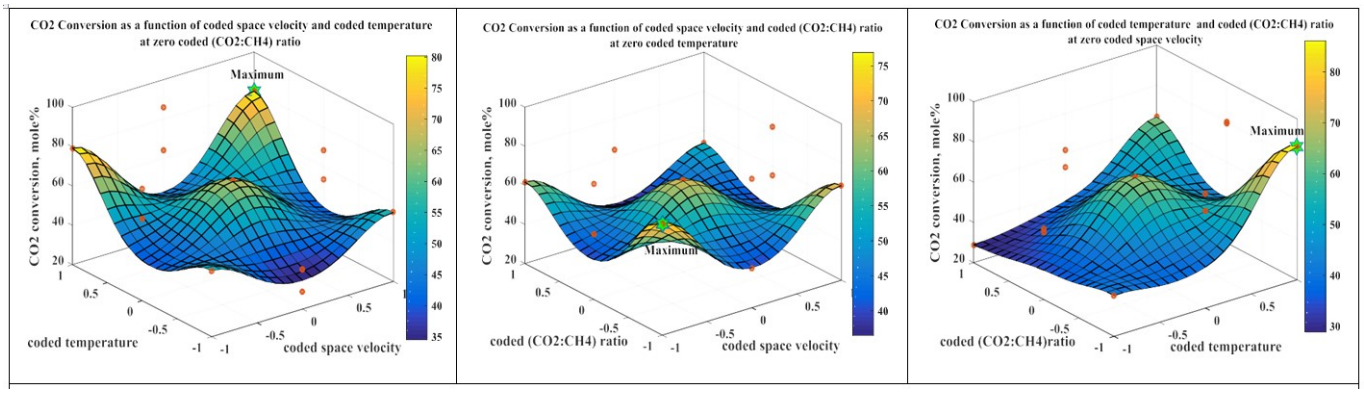

Figure (2: a): NN Surface plots for CO_2 conversion of methane dry reforming over Ni/MgO Catalyst

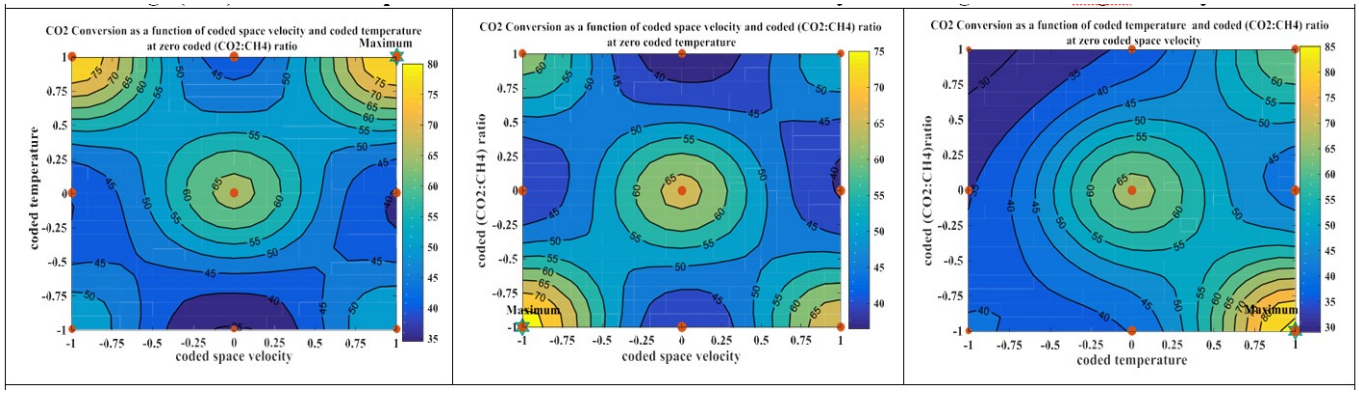

Figure (2: b): NN Contour plots for CO2 conversion of methane dry reforming over Ni/MgO Catalyst

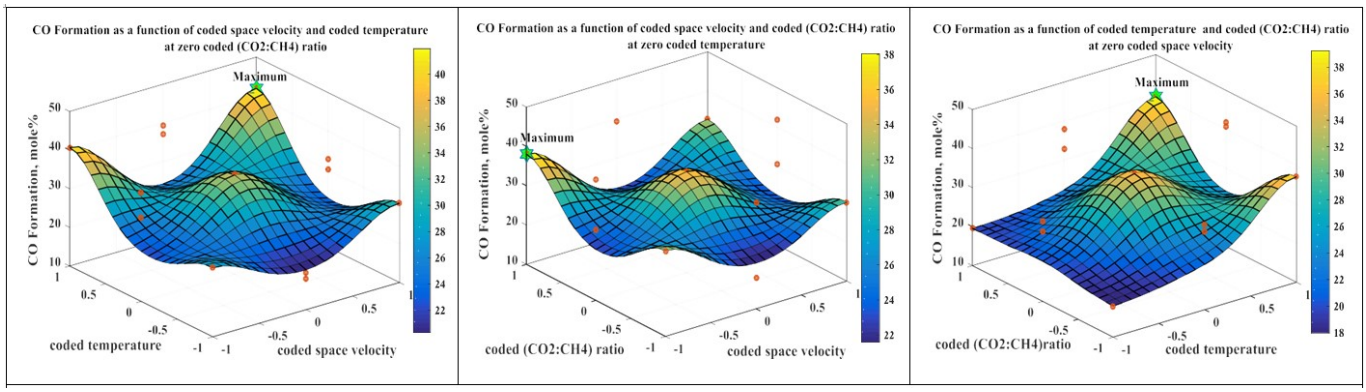

Figure (3: a): NN Surface plots for CO formation of methane dry reforming over Ni/MgO Catalyst

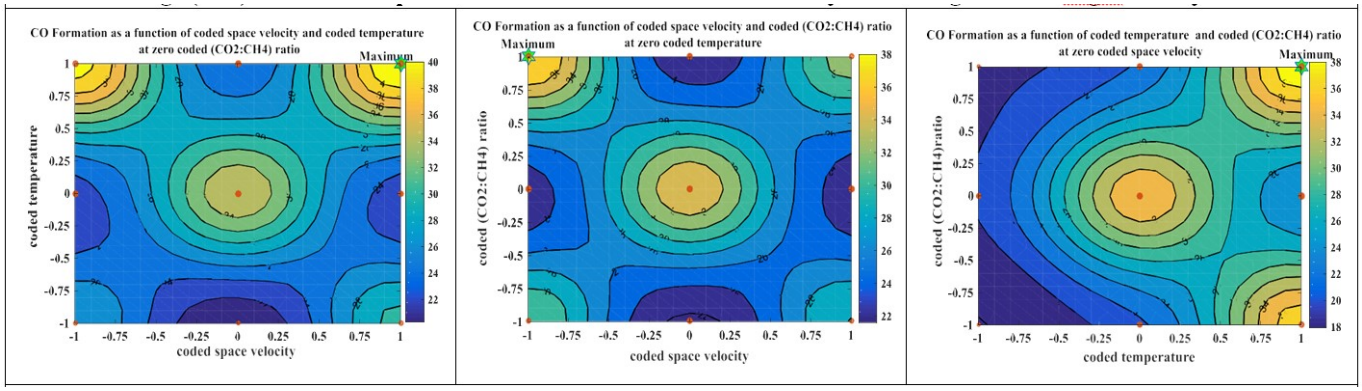

Figure (3: b): NN Contour plots for CO formation of methane dry reforming over Ni/MgO Catalyst

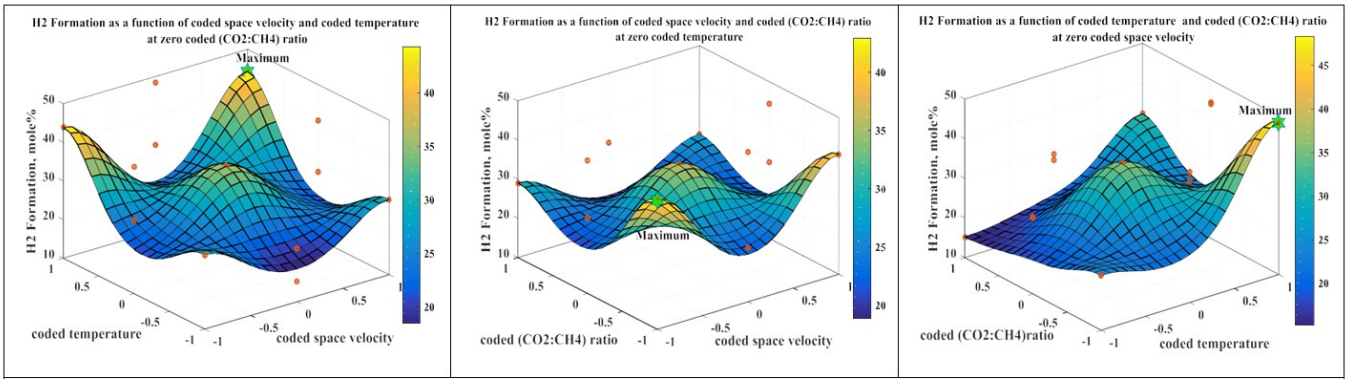

Figure (4: a): NN Surface plots for H2 formation of methane dry reforming over Ni/MgO Catalyst

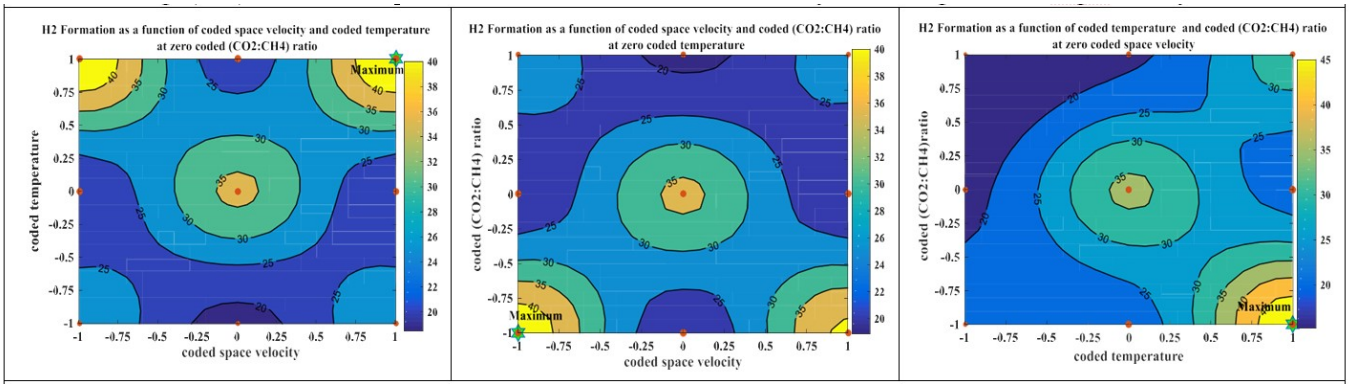

Figure (4: b): NN Contour plots for H2 formation of methane dry reforming over Ni/MgO Catalyst

Comparative Evaluation of RSM and ANN

The performance of RSM is easier compared to ANN and its sensitivity analysis is more precise so it is recommended for modeling a new process. ANN is best suited for nonlinear systems that include interactions higher than quadratic as it has excellent prediction and optimization abilities besides it does not require any prior specification for a suitable fitting function [7, 36]

ANN model offers little information about the contribution of the factors and their influence on the response if further analysis has not been done. The quadratic predicting equation of RSM reveals the factor's contributions and their significance from the coefficients of the regression models and, therefore, can reduce the complexity of the models [37, 38]. The greater prophetic accuracy of the ANN is attributed to its ability to process multi- dimensional. Non-linear, and clustered information via a multi--step calculation process that is reiterated until an appropriate error is attained providing better validation of new technological strategies. RSM is restricted to the use of a second-order single-step polynomial calculation [28].

Therefore, using RSM-ANN modeling resolves the shortcomings of RSM, and the actual association between independent and response parameters can be studied through experimental data [39].

Conclusion

A generalized, properly fit, robust feed-forward artificial neural network model with 10 neurons using radial basic function was successfully established, trained to utilize the data from the experimental laboratory, tested to predict the responses of the various components comprising the reaction system, and compared to RSM. The study indicated that the properly trained ANN model has consistently performed more accurate prediction in all aspects compared to those of RSM expressed in the very high values of R^2 and F ratios and the very low value of error indicators for the ANN results compared to RSM ones despite the small number of training data available. A simulation process was performed within the studied input variables and the results have been portrayed in three and two dimensions together with the predicted responses of the various components and maximum along with the experimental data. The predicted maximum of the various components was in very good agreement with the experimental ones. The study revealed the prominent effect of the increase of temperature towards the increase conversion whereas the variation of (CO_2:CH_4) mole ratio has moderate effect while the space velocity has a negligible effect. It could be concluded that ANN modeling is more appropriate in predicting the output response than empirical modeling so it can be used to economize material and time in designs.

Availability of data and materials

The datasets during and/or analyzed during the current study are available from the corresponding author upon reasonable request.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

Prof. Dr. Tahani S. Gendy: Conceptualization, methodology, software, writing original draft, data curation

Prof. Dr. Radwa A. El-Salamony: formal analysis, investigation, validation. Resources

Prof. Dr. Salwa A. Ghoniem: formal analysis, validation.

Prof. Dr. Seham A. El-Temtamy: Project administration, conceptualization writing –review, editing, supervision.

Prof. Dr. Dalia Radwan: Investigation, formal analysis. Prof. Dr. Mohamed A. Ebied: Investigation, formal analysis. Prof. Dr. Ahmed El-Naggar: Investigation, formal analysis

Supplementary Information

https://www.annexpublishers.com/articles/JNT/2101-Supplementary-Information.pdf

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