

Investigation of the flame temperature for some gaseous fuels using artificial neural network

*Z. Majedi Asl¹, A. Salem²

Chemical Engineering Department Sahand University of Technology, Tabriz, Iran

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ABSTRACT

In the present study the adiabatic temperature of gaseous fuels were calculated and the influence of effective parameters of flame temperature was discussed. Firstly, a new computational program named FTC (Flame Temperature Calculations) was prepared to calculate the adiabatic flame temperature and then the effect of initial temperatures of combustion air and fuel, excess air content and oxygen enrichment on these temperatures was evaluated. The obtained results show that the oxygen enrichment influences the adiabatic temperature, remarkably. Also, FTC is able to estimate the concentration of combustion components such as: carbon dioxide, steam, oxygen, nitrogen, carbon mono oxide and nitrogen oxide. Finally artificial neural networks were presented for estimation of adiabatic temperature. The proper neural networks were trained and tested using obtained data by FTC. The neural network prediction results were compared with those calculated by thermodynamic and chemical equilibrium - based method. It was shown that trained neural networks can provide the adiabatic temperature with reliable accuracy over a wide range of operating conditions.

KEYWORDS

Gaseous fuels, adiabatic flame temperature, combustion, oxygen enrichment, artificial neural network.

1.INTRODUCTION

In any combustion process flame temperature is an important property that controls the rate of chemical reactions and has a specific effect on the designing of combustion equipment [1]. This paper presents the new method developed for adiabatic and real flame temperature calculations. At first, adiabatic flame temperature was calculated based on adiabatic combustion process. Then a new approximation approach for adiabatic flame temperatures estimations using Artificial Neural Network (ANN) is presented . Artificial neural network is one of the most rapidly expanding fields of research and application, and has evolved into a powerful tool in a wide variety of disciplines [2, 3]. There has been considerable interest in recent years in the

use of neural networks for the modeling and control of combustion processes due to their ability to represent non-linear systems and their self-learning capabilities [4]. A preliminary investigation of neural networks to flame temperature prediction has been conducted and encouraging results were achieved. However, the trained network model was applicable for only three hydrocarbon fuels and the prediction accuracy needs to be further improved [5]. In this paper, further investigation of the potential and performance of neural networks for flame temperature prediction are reported. The training process of a number of neural network models for a wider range of applicable fuels and operating conditions are described and the flame temperature prediction accuracy by trained network models is evaluated. It has been shown

*Corresponding author: Z.Majediasl (e-mail:zmajediasl1980@yahoo.com)

that neural networks can provide the flame temperature prediction with a satisfactory level of accuracy for some of fuels i.e. ethane, methane, propane and reforming gas.

2. PART I: FLAME TEMPERATURE CALCULATIONS

Flame temperature was calculated based on adiabatic combustion process. This means that if a fuel-air mixture burns adiabatically at constant pressure, the absolute enthalpy of reactants at the initial state (say, $T=298.15\text{K}$, $P=1\text{atm}$) equals the absolute enthalpy of products at the final state and temperature was calculated in the trial and error method [1].

$$T_{ad} = T_0 + \frac{H'_{\text{Reactant}} - \Delta H_{298}}{C_{p,\text{Products}} \times n_{\text{total}}} \quad (1)$$

$$\Delta H_{298} = \sum_{k=\text{product}} n_k H_{f,k} - \sum_{j=\text{react}} n_j H_{f,j} \quad (2)$$

$$H'_{\text{Reactant}} = \sum_{j=\text{react}} n_j (H_j(T_i) - H_j(T_0)) \quad (3)$$

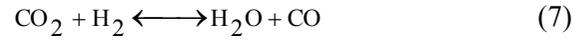
Where H_f is heat of formation in 298K for each pieces and $H_j(T)$ is the enthalpy of components in T that is presented in reference [3]. T_0 is reference temperature and T_i is initial temperature of reactants. N and C_p calculated by:

$$n_{\text{total}} = \sum_{i=\text{products}} n_i$$

$$C_{p,\text{products}} = \left(a + \frac{b}{2}(T + T_0) + \frac{c}{3}(T^2 + T \times T_0 + T_0^2) + \frac{d}{T \times T_0} \right) \quad (4)$$

Where $a = \sum_{i=\text{products}} x_i \cdot a_i$ and b , c and d calculated in the same method. a , b , c and d are the coefficients for heat capacity calculations [3]. x is the mole fraction of product i in total products.

At typical flame temperatures, the products dissociate and the mixture comprises many species. Dissociation of combustion products in flame led to lose of heat from flam. The researchers considered some important equilibrium reactions: dissociation of CO_2 , dissociation of H_2O , CO_2 and H_2O equilibrium reaction and NO formation reactions. Flame temperature calculations are done with or without considering these reactions.



In this program the researchers were able to calculate NO produced from combustion processes with NO formation reactions. Equation constants in the above reactions were calculated from thermodynamic methods. For example for CO_2 dissociation:

$$\tilde{g}^0_{\text{CO}_2} = H_{f,\text{CO}_2} + \Delta H_{\text{CO}_2} - T \cdot \tilde{s}^0_{\text{CO}_2}$$

$$\tilde{g}^0_{\text{CO}} = H_{f,\text{CO}} + \Delta H_{\text{CO}} - T \cdot \tilde{s}^0_{\text{CO}}$$

$$\tilde{g}^0_{\text{O}_2} = H_{f,\text{O}_2} + \Delta H_{\text{O}_2} - T \cdot \tilde{s}^0_{\text{O}_2}$$

$$\Delta G_1^0 = \tilde{g}^0_{\text{CO}_2} - \tilde{g}^0_{\text{CO}} - 0.5 \times \tilde{g}^0_{\text{O}_2} \quad (8)$$

$$K_1 = \exp(-\Delta G_1^0 / R \cdot T) \quad (9)$$

Where H_f and \tilde{s}^0 were found from references for each component [6]. On the other hand for the CO_2 dissociation:

$$K_1 = \frac{P_{\text{CO}_2}}{P_{\text{CO}} \times P_{\text{O}_2}^{1/2}} \quad (10)$$

Where the P for each component is given by:

$$P_{\text{CO}_2} = (n_{\text{CO}_2} / n_{\text{total}}) \times P_{\text{total}}$$

$$P_{\text{CO}} = (n_{\text{CO}} / n_{\text{total}}) \times P_{\text{total}}$$

$$P_{\text{O}_2} = (n_{\text{O}_2} / n_{\text{total}}) \times P_{\text{total}}$$

So the dissociation rate of reaction, x_{CO_2} , is found. With the same method we found, x , for equations 5, 7 and NO formation equations.

2. PART II: ARTIFICIAL NEURAL NETWORK

The second step of this study consists of designing neural networks for estimation of flame temperature. We trained some different networks for different type of fuels. Back propagation networks are used in a large number of working applications as they tend to generalize well. In BP networks, the number of hidden neurons determines how well a problem can be learned. If too many are used, the network will

tend to try to memorize the problem, and thus not generalize well later. If too few are used, the network will generalize well but may not have enough ‘power’ to learn the patterns well. Getting the right number of hidden neurons is a matter of trial and error, since there is no science to it. BP networks are known for their ability to generalize well on a wide variety of problems. BP networks are a supervised type of networks, i.e. trained with both inputs and outputs. In this work the researchers used this type of training algorithm. A trained net work can give us the flame temperature for different conditions of significant fuel combustion with a satisfactory level of accuracy.

3.PART I: RESULTS FROM FTC PROGRAM

There are many parameters that affected on flame temperature. Figures 1 to 6 illustrate effect of variables on the adiabatic flame temperatures. Fig.1 illustrates the effect of fuel temperature on flame temperature in different amounts of excess air. It shows that fuel temperature increasing even to 1000K has no great effect on flame temperature.

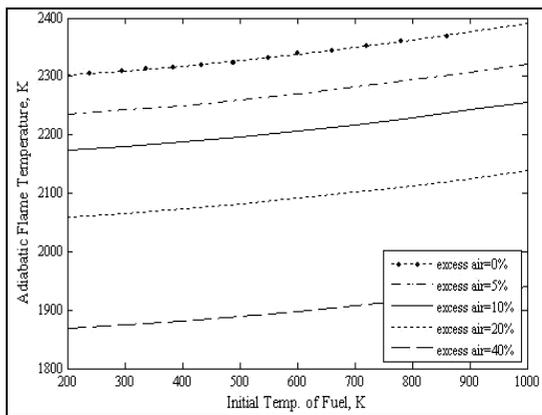


Fig.1:Effect of initial temperature of fuel on the adiabatic flame temperature

As we know both O₂ concentration and preheating of combustion air cause to increase flame temperature. Fig.2 shows that an increase in O₂ concentration will further enhance the adiabatic flame temperature than preheating air. It shows that the effect of increasing O₂ concentration from 21% in normal air to 40% on flame temperature equals preheating combustion air up to 1400K.

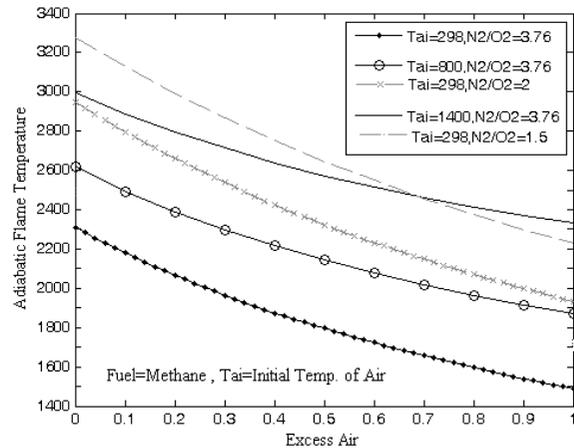


Fig.2: Effect of excess air on the adiabatic flame temperature

Just as Fig.3 shows, the best gas feed composition of the modified O₂ combustion was N₂/O₂≈1.5 or 40%O₂ -60%N₂ and this result agreed with Cheng Chen and Jian-Sheng Huang's

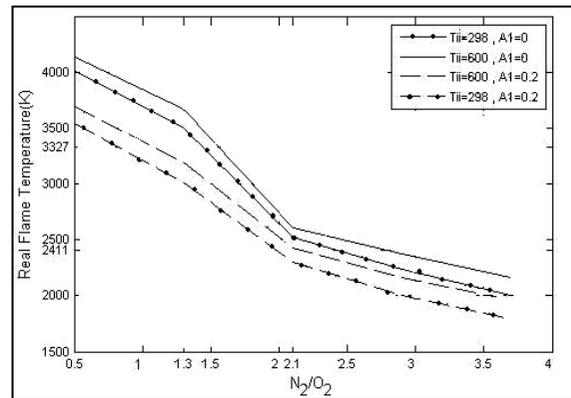


Fig.3:Best ratio of N2/O₂ is 1.5

On the other hand an increase in O₂ concentration led to increasing NO concentration and this is an undesirable matter (Fig. 4). Effect of initial air temperature on flame length for some fuels is shown in Fig.5. It is observed that with the increase in the air temperature, there is no considerable effect on flame length as if air temperature increasing 700K, the flame length decrease from 1.67 to 1.66m that is not so great value.

Fig.6 illustrates the effect of O₂ concentration in combustion air for reforming gas¹ flame.

¹ . CH₄=0.224, C₂H₆=0.276, C₃H₈=0.224, C₄H₁₀=0.072, C₅H₁₂=0.074, C₂H₄=0.03, H₂=0.049

Considering Fig.6, we find that decreasing in N_2/O_2 ratio from 3.76 to 2.5, flame length decrease 25%.

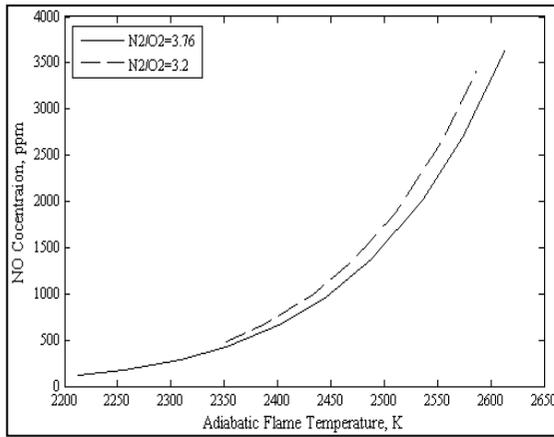


Fig.4: Increasing NO concentration with increasing adiabatic flame temperature

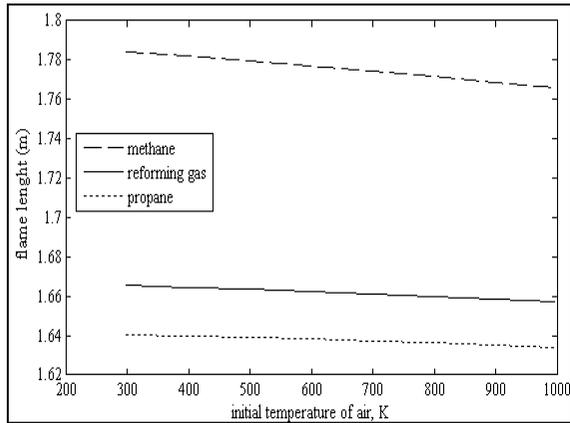


Fig.5: Effect of air temperature on flame length, fuel=reforming

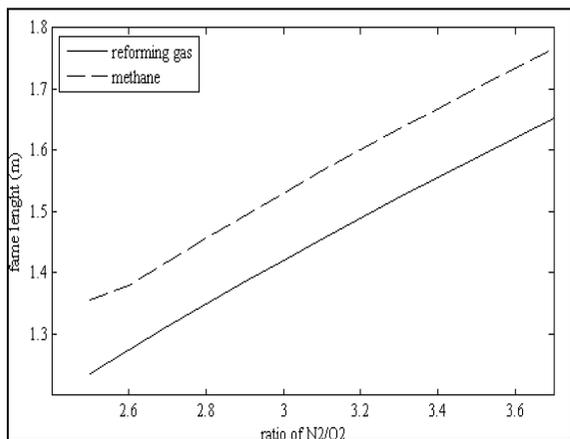


Fig.6: Effect of N_2/O_2 ratio on flame length, fuel=reforming gas

4. ARTIFICIAL NEURAL NETWORK RESULTS

In the current study, the following four neural network models were built and trained for the following different cases:

Model 1: to predict the adiabatic flame temperature of a single fuel.

Model 2: to predict the adiabatic flame temperature of communicate fuels.

Model 1: Methane (CH_4) fuel was selected for the training and evaluation of Model 1. Four variables, Initial temperature of air T_{ai} , initial temperature of fuel T_i , percentage of excess air A_1 and the ratio of N_2/O_2 in combustion air A_2 , were considered as input data. The training data of each input variable were chosen according to table 1:

A total of 750 rows of input data together with their corresponding desired outputs were used as the training data set. A feed-forward network with two hidden layers was used to produce the network Model 1. Each hidden layer has 3 and 15 neurons, respectively (i.e., the network size is 4–3–15–1). The logistic function was used for all layers. The error is defined as $|(t'-t)/t|$, where t is calculated by the FTC code developed by author in this study and t' is the predicted temperature. The maximum error for training data was 4.8×10^{-3} .

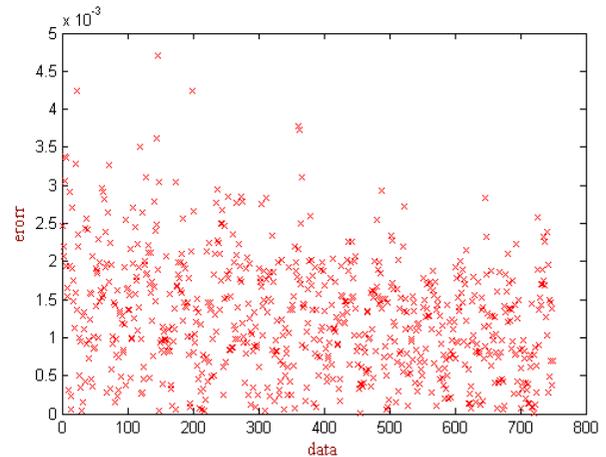


Fig.7: Errors of model 1 for training data

Table 1: input variable for model1

Variable	symbol	From	to	step
Initial air temperature, K	T_{ii}	213	1200	170
Initial fuel temperature, K	T_i	221	1200	200
Excess air	A_1	0	3.5	0.8
The ratio of N ₂ /O ₂ in air	A_2	0	3.76	0.75

To evaluate the accuracy of neural network1 predictions, the following two test data sets corresponding to different operating conditions were arbitrarily selected for the result comparison. Tabell1 and table 2 show these data sets.

As Fig.8 A and B show, the average errors range with the two test data sets is from 0.1 to 0.28%, and the maximum error is 0.6%.

Model 2: the wide range of fuels combustion condition was trained in model2. Initial temperature of air T_{ai} , initial temperature of fuel T_i , percentage of excess air A_1 and the ratio of N₂/O₂ in combustion air A_2 and volume percentage of each fuel in communicated fuel were considered as input data. The training data of each input variable were chosen according to table 4:

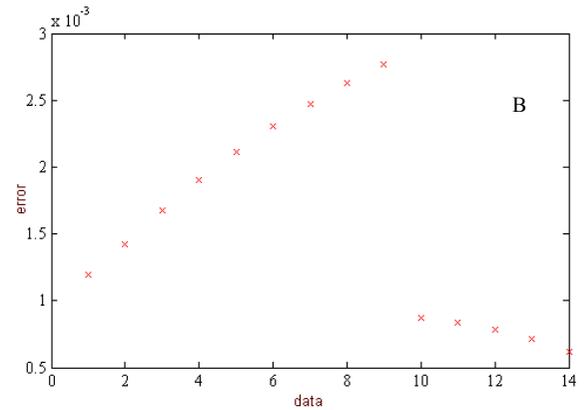
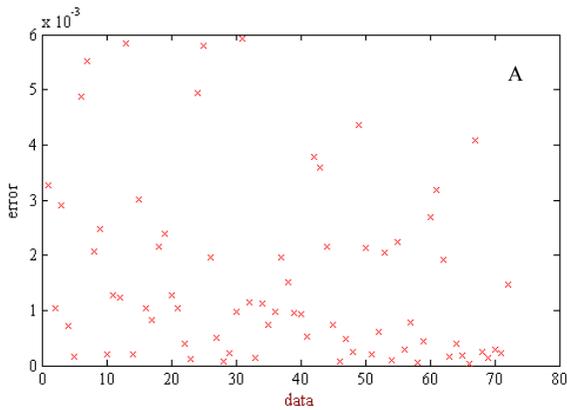


Fig 8: Prediction errors of Model 1 for two different data tests under various operating conditions, A. data test1, B. data test2

Table 2: input data test1 for model

Variable	Symbol	From	to	step
Initial air temperature, K	T_{ai}	200	1200	75
Initial fuel temperature, K	T_i		Constant value 298	
Excess air	A_1	0	2	0.75
The ratio of N ₂ /O ₂ in air	A_2	0.6	3.76	0.55

Table 3: input data test2 for model

Variable	Symbol	From	to	Step
Initial air temperature, K	T_{ai}	200	1200	75
Initial fuel temperature, K	T_i		Constant value 298	
Excess air	A_1		Constant value 0.05	
The ratio of N ₂ /O ₂ in air	A_2		Constant value 3.76	

Table 4: Input variable for model 2

Variable	Symbol	from	to	step
Initial air temperature, K	T_{ii}	213	1200	170
Initial fuel temperature, K	T_i	221	1200	200
Excess air	A_1	0	3.5	0.8
The ratio of N ₂ /O ₂ in air	A_2	0	3.76	0.75
Methane volume percent	F1	0	1	0.5
Ethane volume percent	F2	0	1	0.13
Propane volume percent	F3	0	0.5	0.21
Butane volume percent	F4	0	0.1	0.041
Pentane volume percent	F5	0	0.1	0.041
Ethene volume percent	F6	0	0.2	0.1
Propene volume percent	F7	0	0.1	0.041
Butene volume percent	F8	0	0.2	0.15
Acetylene volume percent	F9	0	0.02	0.01
Hydrogen volume percent	F10	0	0.1	0.041

Table 5: Input variable for model2

Variable	Symbol	From	to	step
Initial air temperature, K	T_{ai}	200	1200	75
Initial fuel temperature, K	T_i	Constant value 298		
Excess air	A_1	Constant value 0.05		
The ratio of N ₂ /O ₂ in air	A_2	Constant value 3.76		

A total of 18720 rows of input data together with their corresponding desired outputs were used as the training data set. A feed-forward network with three hidden layers was used to produce the network Model 2. Each hidden layer has 5, 15 and 8 neurons, respectively (i.e., the network size is 14–5–15–8–1). The logistic function was used for all layers.

The maximum error for training data was 2.55×10^{-2} . Fig.9 shows the error of network 2 trained for model 2.

Two test data sets corresponding to different fuels were arbitrarily selected for the result

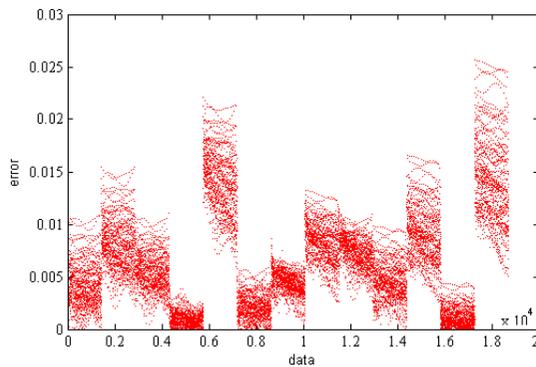
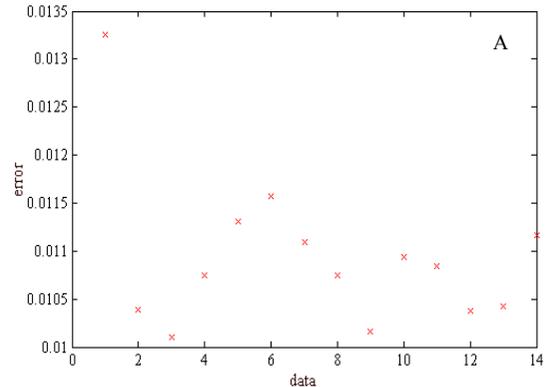


Fig.9:Errors of model 2 for training data

comparison. Data test 1 was reforming gas with following component: CH₄=0.224, C₂H₆=0.276, C₃H₈=0.224, C₄H₁₀=0.072, C₅H₁₂=0.074, C₂H₄=0.03, C₃H₆=0.0, C₄H₈=0.0, C₂H₂=0.0, H₂=0.049 and operating conditions according to table 5. Data test 2 was Refinery gas with following component: CH₄=0.36, C₂H₆=0.182, C₃H₈=0.197, C₄H₁₀=0.019, C₅H₁₂=0.0, C₂H₄=0.054, C₃H₆=0.0, C₄H₈=0.075, C₂H₂=0.0, H₂=0.033 and operating conditions same as data test1.

As Fig.10 A and B show, the average errors range with the two test data sets from 1.01 to 1.08%, and the maximum error is 1.32%.



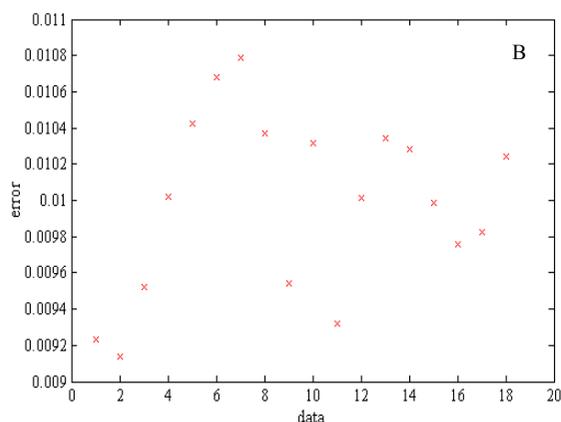


Fig.10: Prediction errors of Model 2 for two different data tests under various operating conditions, A. data test1, B. data test2

5. CONCLUSION

There are some different parameters that effected on flame temperature such as initial temperature of fuel, initial temperature of combustion air, amount of excess air and the ratio of N₂ per O₂ in air that used for fuel complete combustion. The effect of each of these parameters were investigated with a new computational program named FTC (Flame Temperature Calculations) was prepared in MATLAB to calculate the flame temperature. Just as results show, the fuel initial temperature

has not large effect on flame temperature. The initial temperature of air increased the flame temperature but we found that the ratio of N₂ per O₂ has an important effect on the flame temperature. Investigated parameters illustrated that O₂ concentration has an important rule for increasing adiabatic flame temperature. Optimum O₂ concentration was 40%. As a result of this program we find that if the minimum flame length with maximum temperature were desired, modified O₂ combustion is a good method than preheating air combustion. Use of developed air for combustion of fuels led to save energy in many industries such as cement industry.

In this study, an artificial neural network is used for prediction of flame temperature. This paper

has demonstrated the usefulness and effectiveness of applying neural networks in modeling combustion reactions for gaseous fuels. Neural networks usually used for complex issues such as problems which have complex equations usually driven from experimental data. In combustion problems there are many of these types of equations. Each of the equations has regression errors. Furthermore they have errors resulting from calculations. Errors will be larger if the number of experimental equations increased or the calculations are more complicated. Maximum error for two trained neural network was 1.3%. This degree of accuracy shows that the proposed ANN can be used to obtain the flame temperature very fast and exactly. Trained neural networks can provide the adiabatic temperature with reliable accuracy over a wide range of operating conditions.

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7. BIOGRAPHIES



Zohre Majedi Asl is employed at the Research & Technology Company of Iranian National Petrochemical Company. She studied chemical engineering at the Esfahan university, Iran and received her Diploma in 2005. She received her Msc. degree in Sahand university of technology, Iran. Her field of interest is the application of alternative fuels in the industries, olefin plants and their problems, furnaces, cement industries. She is the author of 4 conference papers.



Dr. Amin Salem is the professor of Sahand university of technology. He received a Diploma in Chemical Engineering and his PhD all in elm- o- sanaat university, Tehran, Iran. His areas of interest include the design, development and analysis of ceramic production processes, combustion phenomena and cement industries. He has published more than 10 papers and he is the author or co author of 20 conference papers. He has also some pat

