

1 Article

2 Developing an ANFIS-PSO Model to Estimate 3 Mercury Emission in Combustion Flue Gases

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15 **Abstract:** Accurate prediction of mercury content emitted from fossil-fueled power stations is of
16 utmost important for environmental pollution assessment and hazard mitigation. In this paper,
17 mercury content in the output gas of power stations' boilers was predicted using adaptive neuro-
18 fuzzy inference system (ANFIS) method integrated with particle swarm optimization (PSO). The
19 input parameters of the model include coal characteristics and the operational parameters of the
20 boilers. The dataset has been collected from 82 power plants and employed to educate and examine
21 the proposed model. To evaluate the performance of the proposed ANFIS-PSO model the statistical
22 meter of MARE% was implemented, which resulted 0.003266 and 0.013272 for training and testing
23 respectively. Furthermore, relative errors between acquired data and predicted values were
24 between -0.25% and 0.1%, which confirm the accuracy of the model to deal nonlinearity and
25 representing the dependency of flue gas mercury content into the specifications of coal and the
26 boiler type.

27 **Keywords:** ANFIS-PSO; air pollution prediction; flue gas, emission, mercury; adaptive neuro-fuzzy
28 inference system (ANFIS); particle swarm optimization (PSO); hybrid machine learning model

30 1. Introduction

31 Intelligent monitoring of the industrial air pollutants is of utmost important to maintain an
32 acceptable air quality [1-4]. Among the numerous industrial pollutants, the mercury contamination
33 has been identified as one of the most acute air pollutants produced by conventional fossil fueled
34 power stations [5-8]. Mercury contamination can cause significant ecological hazard with a
35 considerable effect on human well-being around the world [9-12]. As a lethal and hugely volatile
36 metal, mercury can cause contamination of the surface streams and lakes, as well as groundwater
37 [13]. It is the most dangerous hazard for infants and young adults as it influences the central nervous
38 system, causing utero and severe illnesses [14]. Previous studies, e.g. [7-11] report that a substantial
39 amount of mercury outflows to the earth comes from coal-fired power plants. In 2010, roughly 2000
40 mg mercury outflows to the air from various sections worldwide [15]. Coal burning had a share of
41 24%, which is a relatively high share [16]. Power plants are in charge of around 33% Mercury
42 outflows, and this type of emission is caused by human beings [17], and Elemental mercury emission
43 is about 20-50% of mercury emissions which originate from combustion of coal [18, 19]. Nowadays,
44 mercury emission from coal consumption has become a global concern [12,13,14]. In 2006, total coal
45 consumption in China was about 40.1% of world consumption, which is equivalent to 1238.3 million
46 tons of oil [20]. Thus, some studies suggest that the amount of mercury emission is more likely to

47 increase during the next years because of more uses in developing countries [21]. The environmental
48 protection agency of United States of America announced mercury as one of the most dangerous air
49 pollutants. In 1999, an approximated amount of 45 tons of mercury outflows from coal-consuming
50 plants to the environment (Alto 2000). The developing worry of this contamination in the U.S has
51 incited government and specialists to start endeavors to recognize, estimate, and cut off on the
52 anthropogenic emissions. As a result of the absence of cost-effective, promptly accessible and efficient
53 practical control methodologies in the U.S, discharge of this dangerous contaminant from coal-
54 consuming boilers are not basically under control. It gets worse when the greater of part power
55 supply in a big country such as the United States originates from utility boilers that use coal (EPA
56 2001) and furthermore About 70% of electricity power in China is produced by burning coal, in which
57 50% of this coal is burned in coal-based power plants [22-24].

58 In 1998, Paying attention to the enormous potential for environmental dangers, EPA proposed
59 a request to ask coal-consuming plants to publish information on the amounts of mercury
60 contaminant outflows from their systems. This request was designed to gather information in three
61 primary stages precisely. The first and principal stage was intended to collect all standard data on
62 coal-burning power plants around the U.S. afterward, as the second stage of the program, analyzed
63 feed data at the entrance of every plant during a year were collected. Eventually, in the third phase,
64 EPA chose 84 out of 1084 plants to gather data of mercury emission in some specified points within
65 the selected plants. This selection was based on some statistic activities on the feed specifications and
66 also the operational structure of each plant. Resulted in information from the third phase of the
67 program was evaluated. Representing correlations were developed to predict the emission of
68 mercury in each plant concerning coal qualities and operating conditions. It was found that the best
69 input data were characteristics of coal, for example, the concentration of mercury, heating value,
70 chlorine sulfur, operating parameters such as temperatures and pressures and also yield parameters
71 in boilers such as the amount of mercury oxidization. Beside abovementioned backgrounds, artificial
72 intelligence approaches are powerful tools to forecast parameters by finding correlations between
73 variables. This kind of networks can see the nonlinear relationship between parameters, so they are
74 valuable method [25].

75 A deep understanding of the power plant is needed to control the amounts of mercury
76 emissions. Therefore, an accurate estimation of emission is of utmost important to control and reduce
77 mercury emission [26]. Numerous investigations were published in the literature regarding
78 applications of artificial intelligence approaches. Computational intelligence has been both used to
79 predict the amount of mercury emission and also to model the elimination of elemental mercury from
80 boilers' outlet gas [27]. Dragomir and Oprea [28] present a multi-agent prediction tool for intelligent
81 monitoring of the pollutants on the power plants. They used a model based on neural networks to
82 predict the amount of SO_2 , NO_x , particulate matters (PMs), and mercury emissions. Jensen et al. [29]
83 presented a study on the relationship between mercury in the flue gas and coal specifications and the
84 type of boiler using a multilayer perceptron model. They derived an accurate model with a
85 correlation coefficient of 0.9750. Antanasić et al. [30] developed a prediction model using neural
86 networks and genetic algorithm (GA) to accurately calculate the amount of PM10 emissions for up to
87 two years ahead. Zhao et al. [31] used support vector machine to develop a model which provided
88 better performance and accuracy. In 2016, Wang et al. [32] worked on the application of GA-back
89 propagation (GA-BP) for predicting the amount of mercury component in flue gases of 20 different
90 coal-fired boilers. Correlation coefficient training data points was as high as 0.895, and they showed
91 that GA-BP is a promising method for this goal. Li et al. [33] employed computational intelligence
92 approach to cut off on the elemental mercury in coal-fired boilers, and finally, they found that the
93 increment of capture efficiency can approximately improve up to 15%.

94 Although, the application of machine learning for prediction of pollutants and mercury
95 emissions is well established within the scientific communities, the potential of the novel machine
96 learning models (e.g., ensembles and hybrids) is still not explored for mercury prediction. In
97 particular a wide range of novel hybrid machine learning methods have been recently developed to
98 deliver higher accuracy and performance [34-36]. For instance, the hybrid model of ANFIS-PSO

99 which is an integration of adaptive neuro-fuzzy inference system (ANFIS) and particle swarm
 100 optimization (PSO) has shown to deliver promising results [37]. The aim of the present study is to
 101 find a reliable relationship between elemental mercury in the output gas, the specification of feed,
 102 and the type of boilers by utilizing an ANFIS-PSO based approach.

103 **2. Model development**

104 The description of the hybrid model of ANFIS-PSO is presented in [37]. Note that, when there is
 105 not enough data on the detailed information of an operating power plant, it is extremely difficult to
 106 build a precise model to predict the amount of mercury outflow. In the present study, an endeavor
 107 has made to develop a model to predict mercury outflows from boilers at some specified testing
 108 locations. In this kind of locations, every single factor that may influence the mercury discharge is
 109 considered and incorporated into the model. A total number of 82 data points were gathered from
 110 literature to train and evaluate the model [29]. The concentration of mercury in the inlet feed, ash
 111 content, chlorine content, the heating value of coal, sulfur content, and temperature were chosen as
 112 the most effective variables. This data bank comprises a total number of 82 data points, from which
 113 75% were used as training, and the rest of them were exploited testing samples. In the developed
 114 ANFIS model, six previously mentioned parameters were considered as input parameters, and the
 115 elemental mercury emission was selected as the target variable. Furthermore, the PSO algorithm was
 116 used to find the optimized Gaussian membership function parameters of the proposed ANFIS model.

117 The method of ANFIS is proposed by Jang [38, 39] and is a versatile and very intelligent hybrid
 118 system. ANFIS approach can be expressed as a complete collaboration between computing activities
 119 and neuro-fuzzy system [40]. This method integrates natural and neural networks and uses their
 120 strength into its advantage. Such methodology exploits back-propagation calculation from the
 121 information gathering process to make the essential basics of the fuzzy system. Its framework is
 122 related to an arrangement of fuzzy IF-THEN rules which have learning ability to estimate nonlinear
 123 functions. Basics of the ANFIS method are approximately similar to a fuzzy system developed by
 124 Takagi-Sugeno-Kang [41, 42]. In reverse spread learning capability of the ANFIS method, which is
 125 based on the calculation of derivatives of squared errors in a backward manner form output nodes
 126 to the input ones, this method constructs and utilizes robust learning methodology based on gradient
 127 least-squares approach. To determine the consequence factors in the forward section, the least square
 128 approach is utilized. Then the preset parameters will reset by gradient descent in the regressive
 129 advance [43]. The adaptive network is constructed of five layers. Figure 1 shows these layers, their
 130 nodes and connections with the assumption of two inputs to the fuzzy inference system expressed
 131 by "x" and "y" and a single output of "f". As an explanation about the configuration of ANFIS, it
 132 must be noted that two fuzzy 'if-then' rules are utilized which they follow sugeno FIS as:
 133

$$f_1 = P_1 + q_1 y + r_1 \quad \text{assume } x=A_1, y=B_1$$

$$f_2 = P_2 + q_2 y + r_2 \quad \text{assume } x=A_1, y=B_1$$

134 135
 136 Fuzzification layer, which is the first layer of the structure produces all membership grades for
 137 each variable. Node functions in this layer can be defined as follows:

$$O_{1,i} = \mu_{A_i}(x) \quad i=1, 2 \quad (1)$$

$$O_{1,i} = \mu_{B_{i-2}}(x) \quad i=3, 4 \quad (2)$$

138 Memberships of a fussy set are (A_i, B_i) and $O_{1,i}$ represents the resulted value from the i^{th} node of
 139 the first layer. The input signals are generated by the nodes of layer 2.

$$O_{2,i} = w_i = \mu_{A_i}(x) \times \mu_{B_i(x)} \quad i=1, 2 \quad (3)$$

140 The nodes of the third layer are used to compute the following parameter:

$$O_{3,i} = \bar{\omega} = \frac{W_i}{W_1 + W_2} \quad i = 1, 2 \quad (4)$$

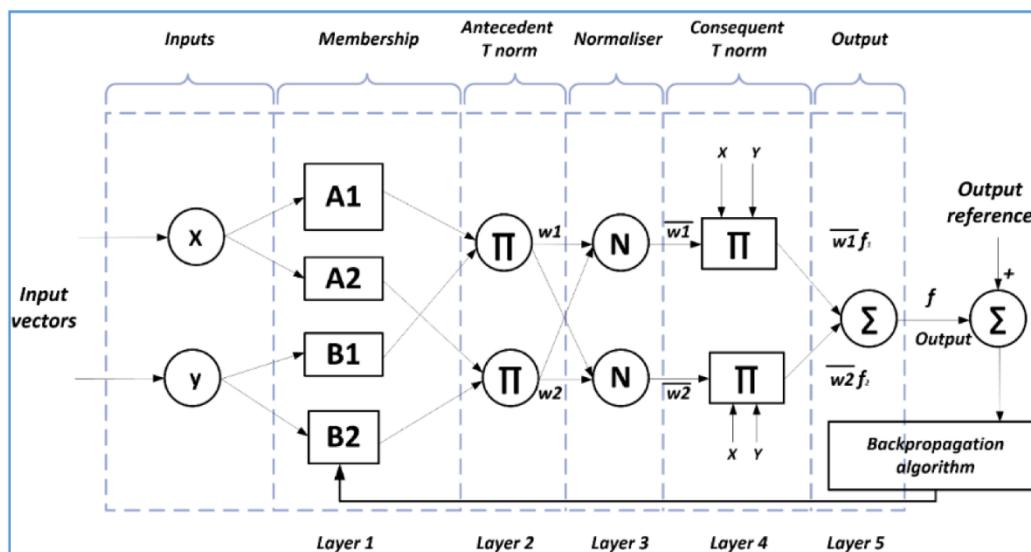
141 Where W_i is ruled firing strengths of node i which has a normalized firing strength of ω_i . Results
142 of layer four can be written as follows:

$$O_{4,i} = \bar{\omega} f_i = \bar{\omega} i(P_i + q_i y + r_i) \quad i = 1, 2 \quad (5)$$

143 In this notation p_i , q_i , and r_i are called consequent parameters. Eventually, the general output
144 can be defined as follows, which is calculated in the nodes of layer 5:

$$O_{5,i} = \sum_{i=1}^2 \bar{\omega}_i f_i = \frac{\omega_1 f_1 + \omega_2 f_2}{W_1 + W_2} \quad (6)$$

145



146

147 **Figure 1.** A schematic view of the ANFIS intelligent system.

148 ANFIS, has shown promising results in a wide range of applications for developing prediction
149 models [44-47]. However, optimization of the model parameters can dramatically improve the
150 quality and accuracy of modeling [37]. For that matter, a huge number of optimization
151 methodologies, such as PSO, are available to reinforce the parameters and answers of the ANFIS
152 system [48]. PSO is extraordinary compared to other approaches with the end goal of optimization.
153 This study takes the benefits of this algorithm.

154 Particle swarm optimization method has been inspired from birds behavior seeking food [49,
155 50]. In this model, particles update their places and pathways based on their and others information;
156 so it was proposed that the particle possess a memory function. The optimization process is based on
157 competition and collaboration between particles. When PSO is used to solve optimization problems,
158 one can follow the particles state by their pathways, and velocities. Three vectors X_i , V_i , P_{best_i} are
159 introduced to explain the properties of a particle: X_i is the current place; V_i the current speed; P_{best_i}
160 the best spatial placement sought by the particle and g_{best_i} is the optimal solution searched by the
161 whole group of particles. The position and pathway of the particle will be updated gradually, based
162 on the following formula:

$$v(k+1) = v(k) + c_1 \text{rand}(0,1) \times [p_{best}(k) - p_{present}(k)] + c_2 \text{rand}(0,1) \times [g_{best}(k) - p_{present}(k)] \quad (7)$$

163

$$164 \text{present}(k+1) = \text{present}(k) + v(k+1) \quad (8)$$

165 Where, $v()$ is particle speed in k th and $k+1$ th iterations; $\text{present}()$ is particle position; c_1, c_2 are
166 learning constants which are greater than zero, and a random number between $[0,1]$ is denoted using
167

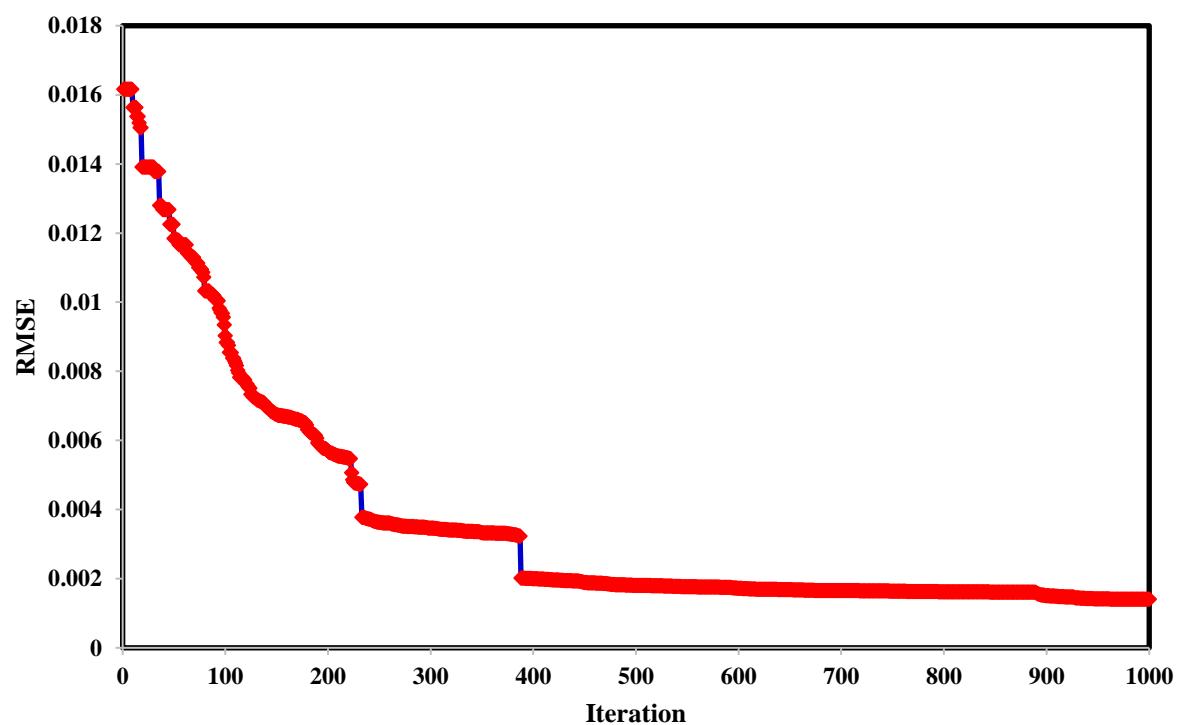
168 $rand()$. Formula (7) represents the updating process of the particle's speed, which includes a particle's
 169 historical velocities and personal and global best positions [51].

170 **3. Results**

171 The amount of mercury emission was estimated using an ANFIS approach. Emission of mercury
 172 into the environment generally is a strong function of mercury six previously mentioned variables.
 173 We used MATLAB software to construct our model. A Gaussian function was used to optimize the
 174 parameters. In addition to that, the total number of 10 clusters were utilized in the ANFIS hybrid
 175 system. Optimization was conducted on a total number of parameters that were determined by:

$$176 \quad N_T = N_c N_v N_{mf} \quad (9)$$

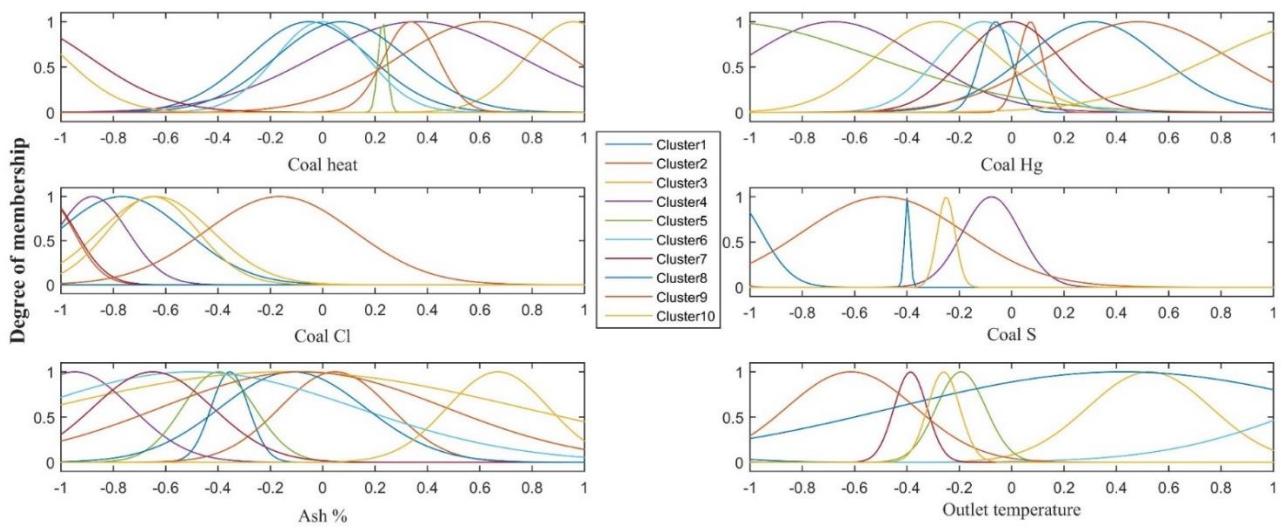
177 Where the number of parameters for undergoing optimization is denoted by N_T , and N_{mf} is used to
 178 show the number of Gaussian membership functions that are used, N_v and N_c show how many
 179 variables, and clusters are used in the model, respectively. It is noteworthy to state that in this study,
 180 two membership functions, seven input and output variables, and 10 clusters are used. Eventually,
 181 using a PSO algorithm, optimization was conducted for 140 tuning parameters. As is shown in Figure
 182 2, to evaluate the functionality of the PSO algorithm, a root means square error (RMSE) analyze was
 183 used. Results show that in a total number of 1000 iterations, the minimum value of RMSE is touched.
 184 Figure 3 indicates train membership function parameters for each input variables. It is seen that the
 185 results of the presented model are in good agreement with the obtained data, which is the result of
 186 great learning capability of the developed ANFIS model. Figure 4 illustrates the obtained data of
 187 mercury emissions versus the test and training of ANFIS hybrid system.



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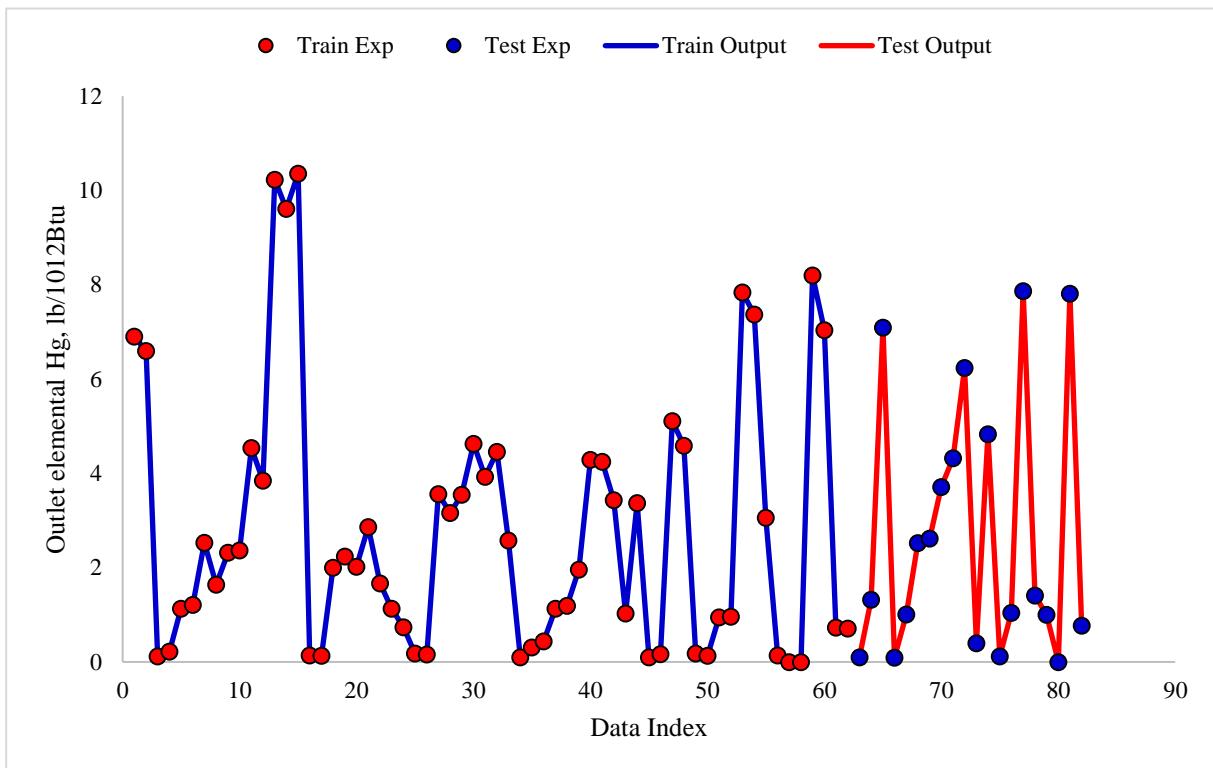
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Figure 2. Root mean square errors versus number of iterations.



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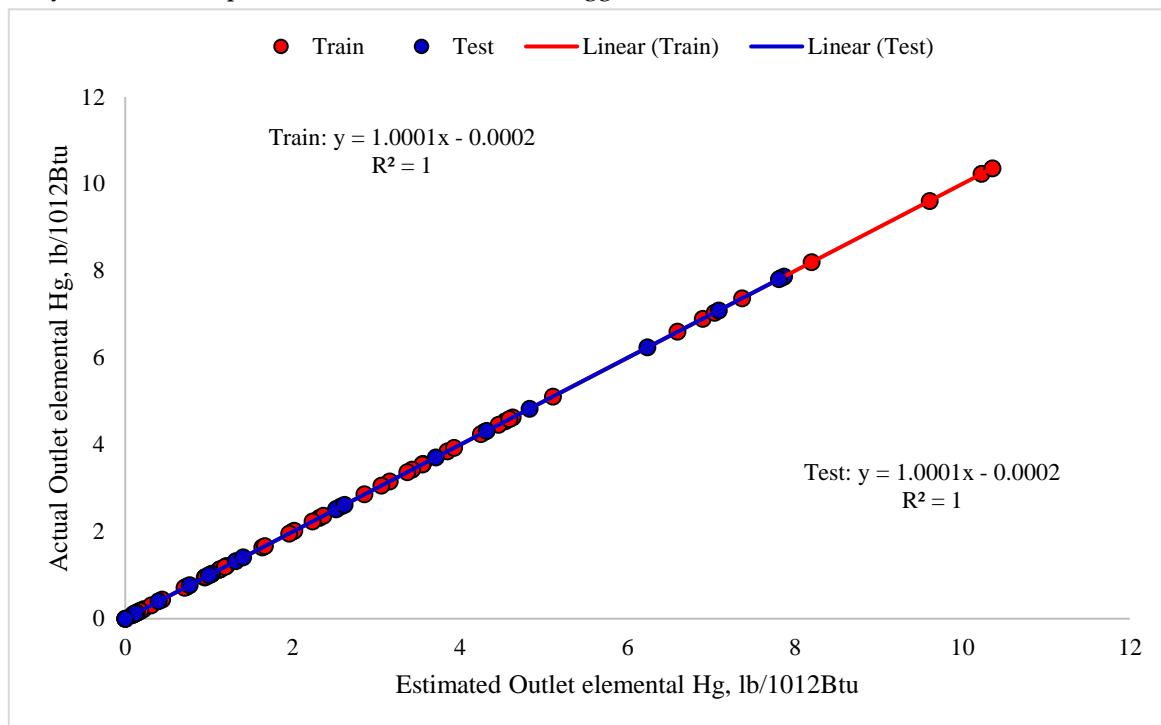
Figure 3. Trained membership function parameters.

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193
194**Figure 4.** Obtained data from plants and ANFIS values for mercury emissions in the stages of training and testing.195
196
197
198
199
200
201

As is shown in Figure 5, actual and predicted mercury emissions are located on a straight line with an approximate slope of 1 (45° line) which indicates that the obtained information and ANFIS predicted ones are in good agreement. The obtained cross-fit line in both test and training data sets have an R^2 Equal to 1, which shows the accurateness of the model. To compare the results of the model and evaluate its precision, the method of mean absolute relative error is used. For training and testing steps, using mean absolute relative error percentage (MARE %) method, percentage values of 0.003266 and 0.013272 are calculated, respectively. Resulted relative deviations are presented in the

202 Figure 6. Low relative deviations are observed due to accurately-predicted values. Different statistical
 203 analyses were also presented in Table 1 for the suggested model.



204

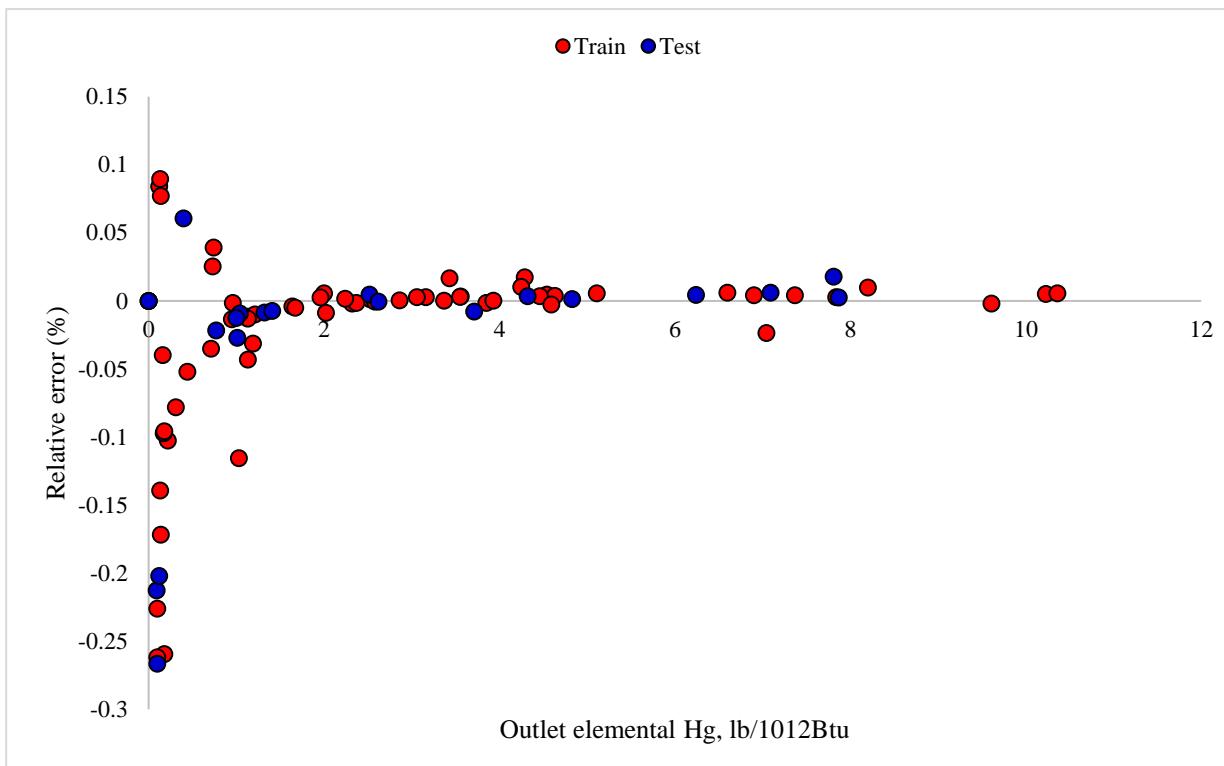
205 **Figure 5.** Regressions derived between estimated and collected data of mercury emissions.

206

Table 1. Statistical analysis of the model for all phases.

	Train	Test
R²	1.000	1.000
MSE	1.40E-07	1.39E-07
MRE (%)	0.037	0.044

207



208

209 **Figure 6.** Deviation between the obtained data from plants and predicted mercury emissions.210 **4. Conclusions**

211 Emission of mercury is known as one of the most perilous environmental contamination. In this
 212 study, a comprehensive literature review was done, and a predictive model was built to predict the
 213 amount of mercury emission based on the characteristics of the coal supply, operational conditions,
 214 and so forth. The presented model is based on the ANFIS system, which utilizes a PSO algorithm to
 215 estimate the amount of mercury emission to the environment. Data from 82 power plants have been
 216 used to train and develop the ANFIS model. The MARE% for training and testing were 0.003266 and
 217 0.013272, respectively. Furthermore, relative errors between acquired data and predicted values were
 218 between -0.25% and 0.1%, which confirm the accuracy of PSO-ANFIS model. It was seen that for both
 219 training and testing parts, the coefficient of determination was calculated to equal to unity, which
 220 reflects the accuracy of the proposed ANFIS-PSO based model.

221 **Author Contributions:** For research articles with several authors, a short paragraph specifying their individual
 222 contributions must be provided.

223 **Conflicts of Interest:** The authors declare no conflict of interest.

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