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MODELING OF ODOR SUBSTANCE CONCENTRATION IN A CITY TRANSMISSION PIPELINE VIA MERGING GMDH NEURAL NETWORK AND GENETIC ALGORITHM

Farshid Zare'i [1], *Allahyar Daghbandan* [1], *Sajjad Rezaei* [2], *Amir H. Mohammadi* [3]

[1] *Department of Chemical Engineering, University of Guilan, Rasht, Iran*
[2] *Department of Chemical Engineering, Tarbiat Modares University, Tehran, Iran*
[3] *Discipline of Chemical Engineering, School of Engineering, University of KwaZulu-Natal, Howard College Campus, King George V Avenue, Durban 4041, South Africa*

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Abstract

After production and transmission, natural gas is odorized by the injection of mercaptan substances due to safety issues. Mercaptan concentration distribution in transmission pipelines is sometimes non-uniform which fails to meet safety standards of gas companies. Thus, contributing factors including gas flow velocity, distance of city gas station (CGS), pressure, temperature and mass transfer coefficient in mercaptan concentration distribution were determined to attain a uniform distribution. To obtain the odor substance concentration, first, olfactometry operation was conducted at 147 different points in a pipeline with a length of 72 km, faced with non-uniform odor distribution. Then, experimental and computational data were modeled by merging the group method data handling (GMDH) and genetic algorithm with the aim of obtaining efficient polynomial correlation. The modeling results indicate that gas flow velocity and distance from injection points are among the most effective parameters on odorant distribution. Based on the obtained results, the odor substance concentration can be adjusted to the investigated pipeline with the aim of reaching safety standards.

Keywords: *Odor substance; Concentration distribution; Mercaptan; Genetic algorithm; Neural network.*

1. Introduction

In all chemical plants, there are strict regulations regarding health, safety and environment which are referred to as HSE. These regulations also involve gas distribution networks, and since these networks are generally located in residential areas, the odorization process is vitally important. Odorants with low molecular weights in the forms of synthetic chemicals, such as mercaptans and sulfides with molecular weights of about 60 mg/mol, have been used after the Second World War [1].

The need for a gassy odor was heightened with the development of chemical industry and also the hydrocracking units across the world [2]. The minimum natural gas amount that leads to explosion is a concentration between 0.5% and 4.5% which is defined as explosion threshold. Therefore, the minimum odorants should be a specific amount (the gas concentration should be 1% in air) so that the gas can be easily smelled [1]. The different chemical combinations would be selected based on physical and chemical conditions of flow gas and geographical conditions in order to achieve desirable odorant properties and optimize the odorization process performance [1,3]. A study has previously shown that higher operating pressures could increase the possibility of *tert*-butyl mercaptan (TBM) absorption on iron oxide resulting in an increase and a decrease in odor concentration. In addition, low temperature could cause TBM to fade from gas flow [4]. By investigating the fading smell parameters in gas distribution systems, Saadatmand *et al.* [5] found that the gas average temperature rate, gas pressure and flow rate velocity are effective on odor substances concentration distribution. Moreover, according to a study conducted by National Iranian Gas Company (NIGC), odorants adding

and fading factors are under the influence of two parameters, a- odorants oxidation in pipelines and b- sedimentation of odor substances during transportation via pipelines. In a study, it was indicated that odorants transfer rate in gas flow depends on injection point distance (odorizer station) and odorants carrying velocity in transfer lines [6].

Group method of data handling (GMDH) has several applications such as modeling the complicated systems, forecasting, data mining of multi-variable processes, pattern recognition, diagnostics and clusterization of data sample [7-12]. Additionally, the forecast about systems behavior which is used in engineering, medicine and economics show successful results [8,11,14]. The GMDH neural networks are created by utility of network structures for GMDH algorithm, and hence, have significant effect on its software and conceptual implementation. Therefore, the use of neural self-organized networks in GMDH algorithm leads to success in different scientific areas such as engineering, science, and economics.

According to the NIGC's HSE standards, odorants concentrations must be in the range of 10 to 20 mg/m^3 for city gas pipelines [15]. The concentration non-uniformity has been observed in some transfer pipelines. This non-uniformity causes two major problems: 1- Odorants high concentrations may lead to environmental damages, and 2- the low concentrations of odorants can lead to a lack of odorants detection when gas leakage occurs (the most important scope of odorization). The correlation between odor substances and concentration distribution factors must be determined in order to monitor the odorant behavior integration of odor substance concentration and achieving determined standards.

The main scope of this study was predicting the odor substance behavior in a pipeline located in northern part of Iran with a length of 72 km, which faced the lack of uniform distribution of odor substances, by merging GMDH neural network and genetic algorithm. Moreover, the effect of different parameters were compared in a big scale of length for a period of one year, and the most significant parameters of inappropriate distribution in pipelines were established by neural network.

2. Material and method

2.1. GMDH neural network

Among different identification algorithms, group method of data handling (GMDH) is a self-organized system in which complicated models are formed step by step based on multiple input initial data and evolved output. The GMDH was introduced by Ivakhneko [13] as a multi-analysis method for modeling and identifying complicated and developed systems. The GMDH can be implemented in modeling without technical information about its algorithm. The main scope of GMDH is to establish an analytical function based on feed forward network, which each of its element is a second-degree transfer function and its coefficients are obtained by recursive method.

The GMDH neural network is a unidirectional network made up of several layers including several neurons with a similar structure of two inputs and one output. The input variables of each neuron, output, or estimated values are selected by each two neurons and are placed in previous layer, so that the main system is remodeled for each N output.

Generally, the systems identification problems are presented so that the unknown function, f, with variables {(xip, xiq), i= 1,2,3,…,N} and corresponding values, yi, such as {(yi), i= 1,2,3,…,N} are established. The f function can be estimated so that the sum of error squares for a sample of input and output data in equation (1) are minimized.

$$\sum_{k=1}^{N}\left[\left(\hat{f}\left(x_{ki},x_{kj}\right)-y_k\right)^2\right]\rightarrow Min \qquad (1)$$

It might be linear or non-linear of input variables in equation (1). The map established between input and output variables by GMDH neural network, is a non-linear function as following [16-17]:

$$\hat{y}=a_0+\sum_{i=1}^{m}a_i x_i+\sum_{i=1}^{m}\sum_{j=1}^{m}a_{ij}x_i x_j+\sum_{i=1}^{m}\sum_{j=1}^{m}\sum_{k=1}^{m}a_{ijk}x_i x_j x_k+\cdots \qquad (2)$$

The equation (2) is known as Volterra series functions. The GMDH algorithm is based on decomposition of Volterra series functions to two variables second-degree polynomial. In fact, the scope of this algorithm is finding unknown coefficients (a) in Volterra series functions. Therefore, these coefficients are distributed in decomposed factors by decomposing to two variables second-degree polynomial, so unknown coefficients in this second-degree polynomial are regulated according to equation (3):

$$y_i = f(x_{ip}, x_{iq}) = a_0 + a_1 x_i + a_2 a_i + a_3 {x_i}^2 + a_4 {x_i}^2 + a_5 x_i x_i \quad (3)$$

The y function has 6 variables, so they must be adjusted so that the desired output {(yi), i= 1,2,3,…,N} would be established for all two variables samples depending on system {(xip, xiq), i= 1,2,3,…,N}. For this reason, the G function will be based on minimum square error according to equation (4) [8].

$$\sum_{k=1}^{N} \left[\left(G(x_{ki}, x_{kj}) - y_k \right)^2 \right] \rightarrow Min \quad (4)$$

The equation (5) can be shown as matrix (8) by conditions dominated on problem:

$$Aa = Y \quad (5)$$

$$a = \{a_0, a_1, a_2, a_3, a_4, a_5\}^T \quad (6)$$

$$a = \{y_1, y_2, y_3, \ldots, y_N\} \quad (7)$$

$$A = \begin{bmatrix} 1 & x_{1p} & x_{1q} & x_{1p}^2 & x_{1q}^2 & x_{1p}^2 x_{1q}^2 \\ 1 & x_{2p} & x_{2q} & x_{2p}^2 & x_{2q}^2 & x_{2p}^2 x_{2q}^2 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & x_{Np} & x_{Nq} & x_{Np}^2 & x_{Nq}^2 & x_{Np}^2 x_{Nq}^2 \end{bmatrix} \quad (8)$$

It is necessary to calculate non-square inverse matrix A for solving the equation. So the orthogonal equations solving method is used for calculating non-square inverse matrix A. Therefore, the unknown coefficient vector can be calculated by equation (9).

$$a = (A^T A)^{\pm 1} A^T Y \quad (9)$$

The genetic algorithm as an accidental method in neural network training and linking between the coefficients, has a performance better than methods based on traditional gradient [11].

In most GMDH neural networks, neurons in each layer are connected to same layer's neuron [18]. The encryption scheme in generalizing the neural network GMDH (GS-GMDH) has the ability to express different lengths and sizes in neural networks [12].

2.2. Effective parameters in odor substance concentration

2.2.1. Odor substance oxidation in pipeline

The thiol compounds oxidation is presented by equation (10). The short chains of mercaptans lead to their oxidation in this chemical interaction. The adsorption and desorption power of odorant by gas pipes depends on molecular weight and odor substances structure [19].

$$2R - SH + O_2 \rightarrow R - S - S - R + H_2O \quad (10)$$

The interaction between odorant molecules and pipelines internal surfaces is shown by equations (11) and (12), in which some odorants will be adsorbed on the internal parts of pipelines. This sweep is continued to achieve a counterpoise, so that the surface adsorption rate and return odorant rate to gas phase are constant. The organosulfurs are more prone to adsorption onto pipe wall in gas flow [19].

$$4Fe + 3O_2 \rightarrow 2Fe_2O_3(s) \quad (11)$$

$$2Fe_2O_3(s) + 2RSH(S) \rightarrow RSSR + Fe_2O_3(s) + H_2O \quad (12)$$

The odorants transfers are based on gas flow velocity in pipelines. This transfer is different based on consumers' consumption and changes in gas flow rates [6].

2.2.2. Modeling of odorant flocculation evaporation in pipeline and its phase change from liquid to gas/vapor

In this model, it is assumed that the odor substances are transported due to high velocity of gas flow and settled in the path due to a decrease in the gas flow velocity, and high molecular weight of mercaptans (about 60 mg/mol) than typical composition of natural gas (about 17.8

mg/mol). If the transfer level is a fraction of the pipe area, which the odorant is settled in it, the odor substance will evaporate in contact with flow gas. Finally, it can be said that C_A (Z, V, Kc (sc, sh)) is calculated in investigated lines. This model has been investigated with the assumption of the rapid reaction in gas and pipe interface C_{Ai}=0, lack of moment interaction, constant mass transfer level at the moment, very low mass transfer between gas mixture components and odor substance concentration in the place of injection C_A, mass transfer coefficient K_d, sectional area of the pipe A, odorant mass accumulation m. Odorant evaporation modeling is shown in Figure 1 and mass transfer equation was solved by equation 13 [6].

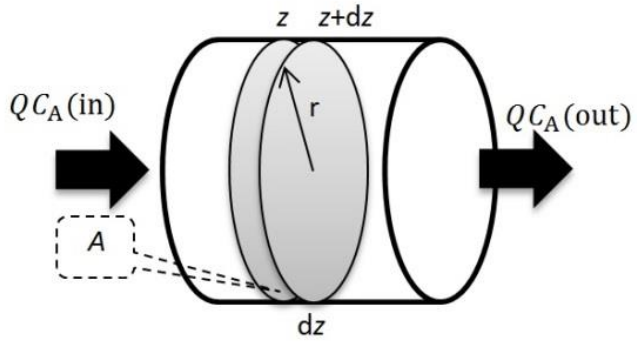


Figure 1. Mass transfer equation in a cross section of pipe with odorant evaporation modeling

$$QC_{A\,in}|_Z - QC_{Aout}|_{Z+\Delta Z} = m = K_d A(C_{Ai} - C_A) \xrightarrow{A=a\pi Ddz} ln\frac{C_{Ai} - C_{A0}}{C_{Ai} - C_A} = \left[\left(\frac{4\alpha K_d}{VD}\right)Z\right] \quad (13)$$

3. Theory and calculations

After extraction and refining for subscribers' consumption, the natural gas is transferred by City Gas Station (CNG). The odor substance injection place is shown in Figure 2 by red circle, which the gas is odorized for subscribers' safety and identifying gas leakage; then the odor gas is obtained to the subscribers by distribution lines.

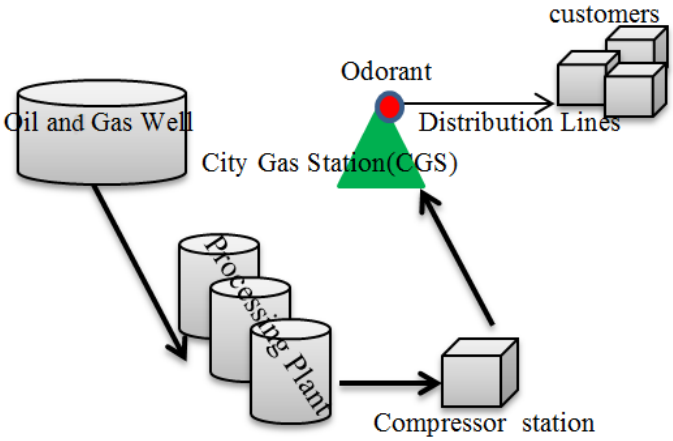


Figure 2. The schematic diagram of natural gas distribution

The gas distribution pipeline, located in a region of the northern part of Iran with a length of 74.4 (km) which was faced with non-uniform mercaptan concentration, is schematically illustrated in Figure 3. This pipeline is between two CGS called feed stations 1 and 2 that are illustrated by green triangles. The electrical pump type odorizer is placed in order for the injecting mercaptan and providing odorant in transfer line. The CGS and TBS stations (gray square) are connected to each other by black lines as pipe; the nominal capacity of the station name is shown at the top of its name. Totally, the investigated line includes 18 stations (12 inches lines are used in stations 4 to 8 and the 16 inches lines are used in other lines). The gas reached to stations in path from both sides of CGS station (indicated by red flash).

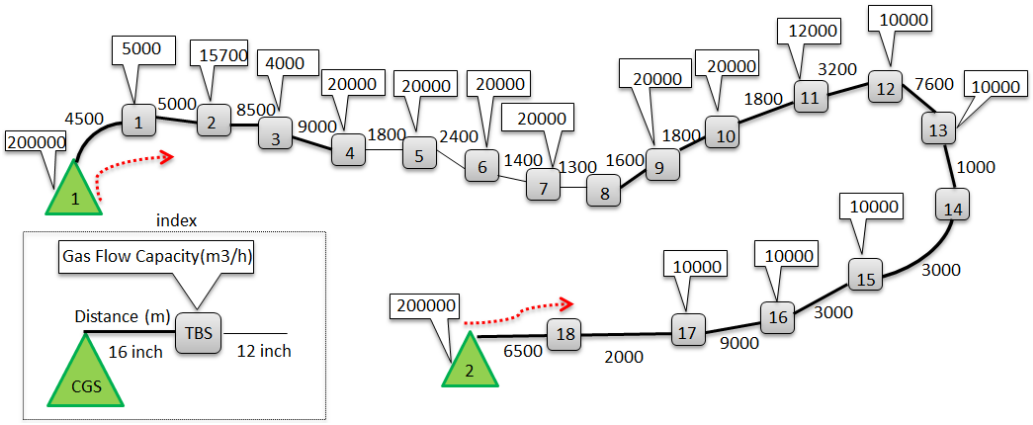


Figure 3. Investigated Nod map in the pipeline

Different points are selected based on possible velocity change in pipe (around TBS station) and different distances to injection point in order to investigate and measure odor substance concentration by an odor handy device. At the beginning of the path in CGS stations, the input temperature and pressure are measured by gage and flow meter, respectively. The mentioned data are entered with gas mixture percentage, distance of measured concentration point (point 2 or exit pipe (i+1)), the pipe effective coefficient (0.9), and pipe diameter as input to system. The velocity , temperature ,density ,reduced pressure, mass transfer coefficient in gas lines, pressure at point 2, Sherwood numbers, Schmidt numbers, Reynolds, fraction coefficient, mass transfer coefficient at the exit are calculated after entering inputs and using equations of Appendix A (Figure 4).

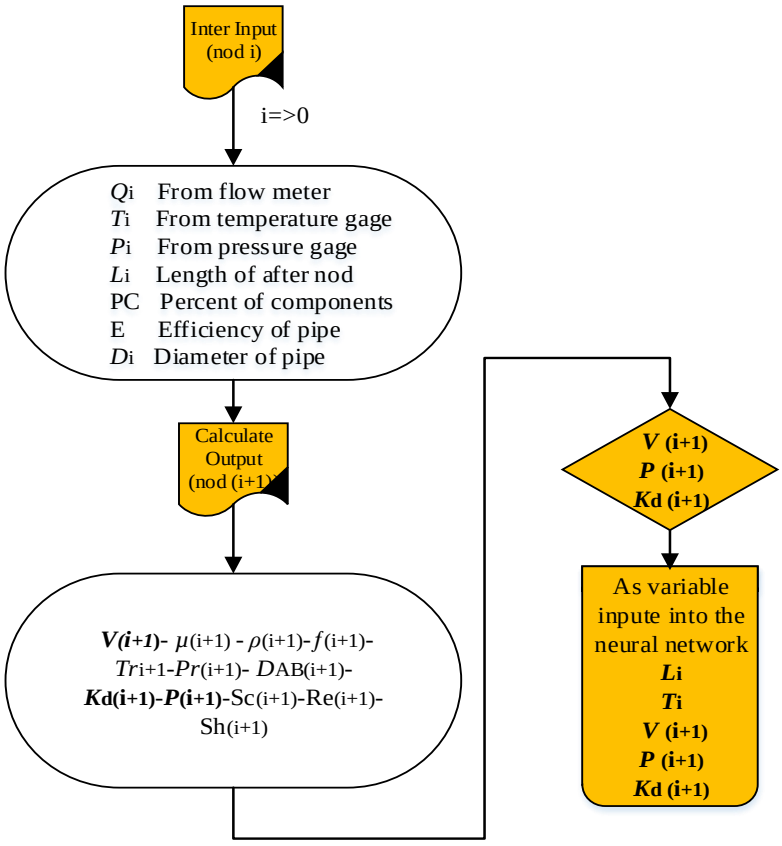


Figure 4. Computation steps of input data to neural network

According to effective parameters on gas concentration distribution in section 2.2, the flow gas velocity, pressure, and mass transfer coefficient variables in measured concentration points with gas average temperature and distance to odor substance variables are effective parameters on odorization. The calculations are done in all 148 investigated systems by entering inputs and calculating outputs, so the input data to neural network is formed. Data are gathered during a year from the hot season (low gas consumption), June and September, to the cold season (high gas consumption), November, December and January. A set of these data is used as input data set to neural network.

4. Results and discussion

Figure 5 presents the measured concentrations of odor substances at different gas temperatures and velocities. Gas temperatures indicate the temperature of the pipeline. The higher gas temperature indicates the lower gas consumption and vice versa. The highest concentration is measured at 293 K, which is in the range of gas velocity in pipeline from 0.58 to 1.59 m/s, which seems to be a low velocity. Moreover, it can be seen that, at low temperatures of 279 and 283 K, the distribution of mercaptan concentration is roughly uniform. This suggests that at velocities between 1.77 and 4.7 m/s, a lower amount of odorants sedimentation through the pipeline meet NIGC standards.

Figure 6 depicts the concentrations of odorants at various temperatures and distances from the injection point, CGS. The highest odorants concentrations are measured at 291 K. At a distance of about 6.8 km from the injection site, mercaptan concentration peaks. This is due to the TBS, which transmits a large volume of gas to the city pipelines reducing its velocity, and increases the time for sedimentation of odor substance. At lower temperatures the effect of distance is insignificant.

According to the influence hypothesis in Section 2.2.b, the odorants mass transfer and its conversion from liquid to gas/vapor is of importance. The distribution of the odorants mass transfer coefficients at different gas concentrations are shown in Figure 7. These data were calculated from the liquid to gas mass transfer equations. Sherwood and Reynolds numbers, diffusion coefficients and other parameters in Appendix A are calculated in order to obtain mass transfer coefficients. This diagram shows that the temperature has a reverse relation with the rate of mass transfer of odor substances.

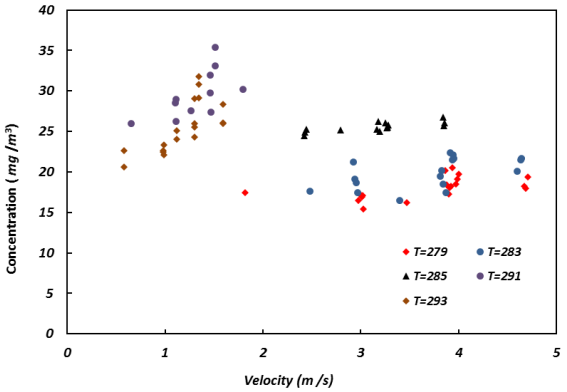


Figure 5. Mercaptan concentrations at various gas temperatures and velocities at real conditions

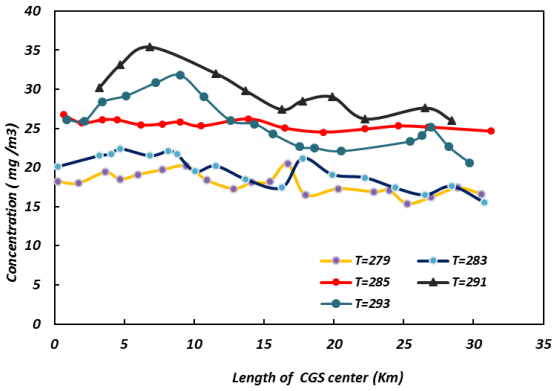
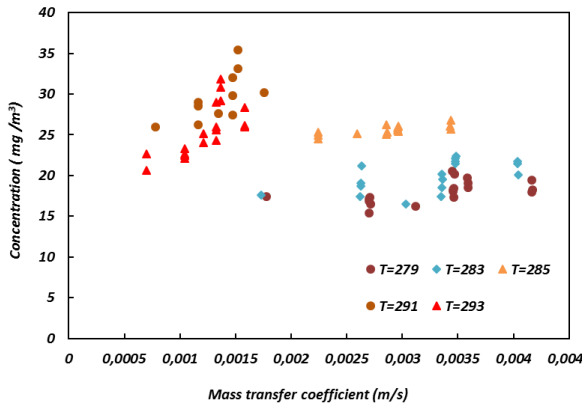


Figure 6. Mercaptan concentrations at different temperatures and distances from CGS.



In Table 1, the maximum, minimum and average of training data (103) and experiment data (45) are indicated.

The genetic parameters, according to Figure 8, are considered in optimization stage for investigated systems. The network forecasting is done in 3 layers to obtain output model.

Figure 7. Calculated mercaptan mass transfer coefficients for the conversion from liquid to gas/vapor at various gas concentration

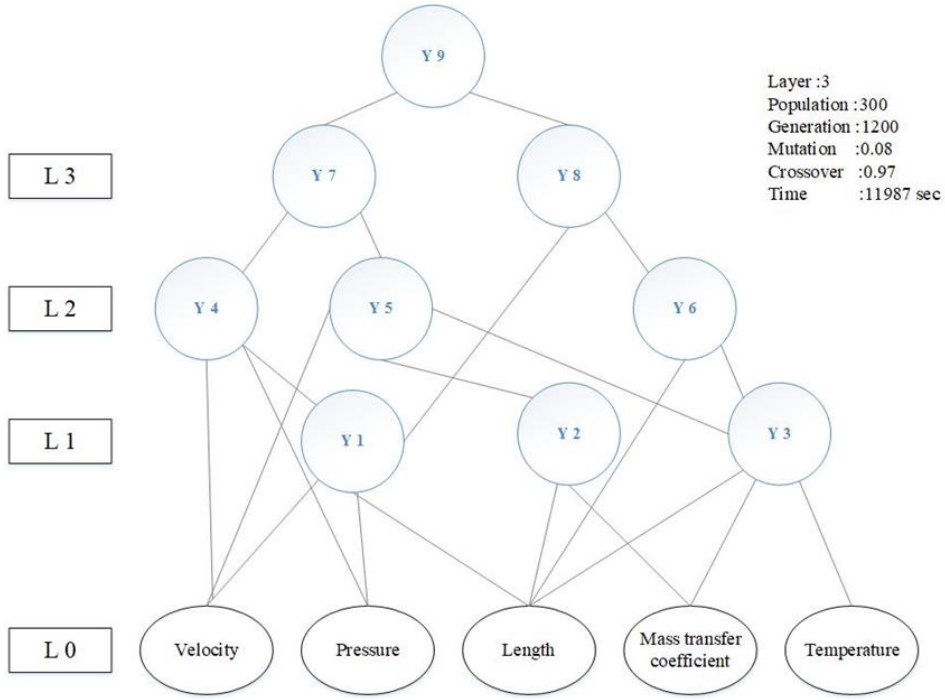


Figure 8. The proposed structure of the GMDH Multi-purpose neural network for estimation of the concentration of odor substance

Table 1. Descriptive statistics of variables used to develop the GMDH

Variable		Train (103 data set)			Test (44 data test)		
		Maximum	Mean	Minimum	Maximum	Mean	Minimum
Input	*V(m/s)*	4.703064	2.01229	0.039014	3.999188	2.057561	0.107756
	P(kPa)	1825.125	1794.037	1651.777	1823.673	1788.2	1655.625
	L(km)	39.99542	16.0355	0.214043	0.399	10.868	23.509
	*K*c(m/s)	0.004267	0.001829	0	0.003658	0.001829	0.000305
	T(K)	293.15	286.14	279.15	293.15	285.7722	279.15
Output	*C*A(mol/L)	47.200	23.548	14.000	40.8	23.19027	14.7

The evolutional scheme of neural network structure is used by genetic algorithm with the purpose of designing GMDH network. The genetic algorithm is used for producing initial population, which leads to producing new chromosome. Among these chromosomes the one with less training error and better forecast is selected in order to evaluate the power of obtained

model. The error values are indicated in Table 2, which show that the model is reliable (obtained using the equations in Appendix B). After selecting the best chromosome for forecasting model, its polynomial graph is formed based on Table 3 that its value is calculated based on genetic data. The data are divided in two groups in Figure 9 that training data are validated by experimental data, and it is shown that results are acceptable according to formed model.

Table 2. Statistical results for odor substance concentration

	RRSE	AADP (%)	NRMSE	RMSE	MSE	R^2
train	1.219	10.553	0.1107	3.676	13.5157	0.9773
test	1.683	11.561	0.1789	4.671	21.825	0.9618
total	0.367	10.894	0.1204	3.999	15.996	0.9727

Table 3. Model multi-substant equal GMDH (Volttera Series) for estimating odor substant concentration

Basic regression polynomial (Volttera Series)

Y=Y9(Y8(Y6(Y3(5,3),3),Y1(3,2)),Y7(Y5(Y3(5,3),Y2(4,3)),Y4(Y1,1)))

Yi(zj,zk)=a0(i)+a1(i) zj+a2(i)zk+a3(i) zjzj+a4(i) zkzk+a5(i)zjzk

i	a0	a1	a2	a3	a4	a5
1	8.875754	0.475174	1.328846	-0.02348	-0.0067	-0.01743
2	0.191467	-2.88694	36.28694	0.011272	-0.07802	-0.13145
3	47.32473	-0.14197	-4532.79	-0.03862	179084.6	59.23848
4	10.04962	0.191445	-0.14456	0.015436	0.000573	0.006022
5	-15.9467	1.845944	2.108465	0.070071	-0.00816	-0.14609
6	5.664134	-0.06307	0.568644	-0.0478	-0.0707	0.13018
7	22.81855	-0.68887	-0.20673	-0.01632	-0.02877	0.083305
8	22.81855	-0.68887	-0.20673	-0.01632	-0.02877	0.083305
9	-9.20191	4.517381	-2.59854	0.026331	0.161005	-0.20983

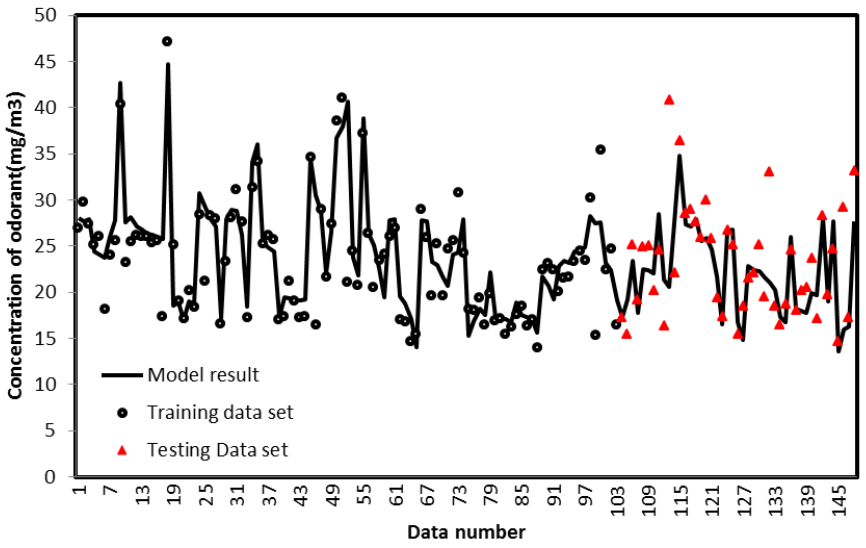


Figure 9. Odor substance amount graph based on the data number. (●) Training data. (▲) Testing data. (—) Data model by combining neural network and genetic algorithm

5. Conclusion

This study was conducted in order to evaluate and forecast the odorization process by the GMDH network. Forecasting results, based on relationship among neurons, show that the most effective parameters on mercaptan concentration distribution are distance from injection point and gas flow velocity. The most significant part of the study indicates that velocity reduction beside TBS stations due to catching a part of flow gas volume (subscribers' consumption) leads to non-uniformity of odor substance concentration, which can be explained by modeling the odor substance flocculation evaporation on pipeline ground. This phenomenon is increased in the hot seasons due to a sharp drop in gas velocity. The selection of odorizers considering stations distance, flow gas capacity, and number of stations must be attained due to non-uniform distribution of odor substances. It was also observed that the problem points in mercaptan distribution path can be identified and increasing or decreasing odorization and achieved safety can be helped by forecasting. Studying the gas pipeline in the region and different temperatures during years can have a significant role in more accurate evaluation of odor substance behavior forecast.

Acknowledgment

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Nomenclature

ρ	*density(g/m^3)*	P_{pr}	*sub-critical pressure(kPa)*
m	*mass and weight(g)*	Q	*volume flow(m^3/s)*
v	*volume(m^3)*	u	*velocity (m/s)*
G	*specific gravity*	Re	*Reynolds number*
M	*molecular weight(g/mol)*	D	*diameter(cm)*
ν	*viscosity(m^2/s)*	C_A	*odor substance concentration(mol/L)*
T	*temperature(K)*	D_{AB}	*diffusion coefficient(cm^3/s)*
P	*pressure(kPa)*	V_A	*atomic volume per molecule($m^3/kg.atm$)*
T_r	*reduced temperature*	Sc	*Schmidt number*
P_r	*reduced pressure*	Sh	*Sherwood number*
T_c	*critical temperature*	K_d	*mass transfer coefficient(m/s)*
P_c	*critical pressure*	E	*efficiency pipeline*
Z	*compressibility factor*	Le	*length of the section(km)*
T_{pr}	*sub-critical temperature(K)&(Rankin)*		

Appendix A. Relations used for calculations in pipelines

$Q = 737\mathrm{E}\left(\frac{\mathrm{T_b}}{\mathrm{P_b}}\right)^{1.02}\left(\frac{{P_1}^2 - \mathrm{e}^s {P_2}^2}{\mathrm{G}^{0.961} T_f L e Z}\right)^{0.51} D^{2.53}$	(A .1)
$u = 0.002122\left(\frac{Q_b}{D^2}\right)\left(\frac{P_b}{T_b}\right)\left(\frac{ZT}{P}\right)$	(A .2)
$P_{\mathrm{avg}} = \frac{2}{3}(P_1 + P_2 - \frac{P_1 \times P_2}{P_1 + P_2})$	(A .3)
$\mu_g = 10^{-4} K\, exp\left(X\left(\frac{\rho_g}{62.4}\right)^Y\right)$ $K = \frac{(9.4 + 0.02M_a)T^{1.5}}{209 + 19M_a + T}$ $X = 3.5 + \frac{986}{T} + 0.01M_a$ $Y = 2.4 - 0.2X$	(A .4)
$\mathrm{T_r} = \frac{\mathrm{T}}{\mathrm{T_c}}$	(A .5)
$\mathrm{P_r} = \frac{P}{P_c}$	(A .6)
$\mathrm{T_{pr}} = \frac{T}{T_c}$	(A .7)
$\mathrm{P_{pr}} = \frac{P}{P_c}$	(A .8)
$T_{\mathrm{pc}} = \Sigma \mathrm{y_i} T_{\mathrm{c}}$	(A .9)
$P_{\mathrm{pc}} = \Sigma \mathrm{y_i} \mathrm{P_c}$	(A.10)
$Z = \frac{1}{\left(\left[1 + \frac{\left((P_{avg} \times 344400 \times (10)^{1.785\mathrm{G}}\right)}{T_f^{3.825}}\right]\right)}$	(A .11)
$D_{AB} = \frac{.001\, T^{1.75}}{P\left[(\sum V_A)^{\frac{1}{3}} + (\sum V_B)^{\frac{1}{3}}\right]}\left(\frac{1}{M_A} + \frac{1}{M_B}\right)^{\frac{1}{2}}$	(A .12)
$\frac{D_{AB(1)}}{D_{AB(2)}} = \left[\frac{T_1}{T_2}\right]^{\frac{3}{2}}\left[\frac{P_2}{P_1}\right]$	(A .13)
$T_c' = \sum x_i T_{ci}$	(A .14)
$P_c' = \sum x_i P_{ci}$	(A .15)
$Sc = \frac{\mu}{\rho \mathrm{D_{AB}}}$	(A .16)
$0.5 \le \mathrm{SC} \le 2000$ $3000 \le \mathrm{Re_d} \le 5 \times 10^6$ $\mathrm{f} = [1.82 \log(\mathrm{Re}) - 1.64]^{-2}$	(A .17)
$K_{\mathrm{d}} = \frac{\mathrm{Sh}\, \mathrm{D_{AB}}}{\mathrm{d}}$	(A .18)

Appendix B. Statistical analysis

1- Mean Squared Error

$$\mathrm{MSN} = \frac{1}{n}\sum_{i=1}^{n}\left(Y_{(i,exp)} - Y_{(i,model)}\right)^2 \quad \text{(B .1)}$$

2-Root-Mean Squared Error

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}\left(Y_{(i,exp)} - Y_{(i,model)}\right)^2} \quad \text{(B .2)}$$

3- Normalized Root-Mean Squared Error

$$\mathrm{NRMSE} = \left[\frac{1}{n}\sum_{i=1}^{n}\left(Y_{(i,exp)} - Y_{(i,model)}\right)^2\right]^{0.5} \Big/ \left(Y_{(i,exp)} - Y_{(i,model)}\right) \quad \text{(B . 3)}$$

4-Average Absolute Deviation Percent

$$\mathrm{AADP}(\%) = \frac{100}{n}\sum_{i=1}^{n}\left|\left(Y_{(i,model)}/Y_{(i,exp)}\right) - 1\right| \quad \text{(B . 4)}$$

5-Root relative-squared error

$$\mathrm{RRSE} = \sum_{i=1}^{n}\sqrt{\left(\frac{\left(Y_{(i,exp)} - Y_{(i,model)}\right)^2}{\left(Y_{(i,model)} - \overline{Y}\right)^2}\right)} \quad \text{(B . 5)}$$

6-Coefficient of Determination

$$R^2 = 1 - \left[\sum_{i=1}^{n}\left(Y_{(i,exp)} - Y_{(i,model)}\right)^2 \Big/ \sum_{i=1}^{n}\left(Y_{(i,exp)}\right)^2\right] \quad \text{(B . 6)}$$

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To whom correspondence should be addressed: Mr. Farshid Zare'i, Department of Chemical Engineering, University of Guilan, Rasht, Iran E-mail farshidzarei@msc.guilan.ac.ir
Professor Amir H. Mohammadi, Discipline of Chemical Engineering, School of Engineering, University of KwaZulu-Natal, Howard College Campus, King George V Avenue, Durban 4041, South Africa E-mail amir_h_mohammadi@yahoo.com