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Optimization of Acid Gas Sweetening Plant Based on Least Squares - Support Vector Machine (LS-SVM) Model and Grey Wolf Optimizer (GWO)

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***Abstract*— Natural gas is an energy resource that is widely used as energy and raw material in many industrial processes. It is contaminated some impurities such as CO_2, H_2S and water, hence, removal of the contaminant processes are required. One of the natural gas processing is Acid Gas Sweetening. The purpose of this process is to eliminate H_2S and CO_2 compound from natural gas. H_2S tend to corrosive and CO_2 will reduce the thermal efficiency. In this research, the goal of optimization that had to be accomplished is to minimalize the energy consumption on a condenser and re-boilers in regenerator process. Least Squares - Support Vector Machine (LS-SVM) is used to modeling a $Q_{condenser}$, $Q_{re\text{-}boiler}$ and CO_2 on lean amine, Grey Wolf Optimizer (GWO) is used to find the optimum value of energy consumption in a condenser and re-boilers, based on training process, obtained the value of Root Mean Square Error (RMSE) for $Q_{re\text{-}boiler}$, $Q_{condenser}$ and CO_2 on lean amine respectively are 0.0909, 0.0916 and 0.1011, from validation process, RMSE values obtained for $Q_{condenser}$, $Q_{re\text{-}boilers}$, and CO_2 on lean amine respectively of 0.0680, 0.0587 and 0.0850. The optimum values of energy consumption in a condenser and re-boilers using GWO obtained value are 1.287E+05 kJ/h, the value of Particle Swarm Optimization (PSO) as a comparison are 4.781+05 kJ/h.**

Keywords—Acid Gas Sweetening; Least-Squares Support Vector Machine (LS-SVM); Grey Wolf Optimizer.

I. INTRODUCTION

Natural gas is an energy resource that is widely used as energy and raw material in many industrial processes. It is contaminated some impurities such as CO_2, H_2S and water, hence, removal of the contaminant processes are required [2].

One of the natural gas processing is Acid Gas Sweetening. The purpose of this process is to eliminate H_2S and CO_2 compound from natural gas. H_2S tend to corrosive and CO_2 will reduce the thermal efficiency [1]. Natural gas will be categorized as sour gas if it contains 5.5 mg/m^3 H_2S. Acid Gas Sweetening process is utilized to remove H_2S and CO_2 [2]. In Gas Sweetening absorption process, wide varieties of materials can be used, such as Iron Sponges, Gas Permeation and the composition of Aqueous Amine. The solution of Aqueous Amine is basically divided into several types i.e. Mono Ethanol Amine (MEA), Di Ethanol Amine (DEA) and Tri Ethanol Amine (TEA). In this research, Acid Gas Sweetening absorption process used DEA solution, because this solution rapidly absorbs H_2S and CO_2 with competitive prices [2].

From economical and environmental views, Amine regeneration is required. It process utilize Amine regeneration column to separate CO_2 and H_2S from the rich amine. As well as the common operation of the distillation column, it is required huge energy consumption to boil up CO_2 and H_2S from the rich amine. Hence, the optimization of energy consumption in amine regeneration column is important. In the optimization require three components i.e. model, objective function and optimization technique.

In this research, the model was developed using Aspen HYSYS and Least Squares - Support Vector Machine (LS-SVM), to model non-linear dynamic the behavior of amine regeneration column. The objective function is to minimize energy consumption at reboiler and condenser of the column. Grey Wolf Optimizer (GWO) was used to solve this optimization problem.

II. LITERATURE REVIEW

In this section, it would discuss the theory that is used to perform this research, the scope of discussion are about the principle of Acid Gas Sweetening process, GWO, and LS-SVM.

A. Acid Gas Sweetening

Acid gas sweetening is a gas purification process in which the process is to eliminate the composition of H_2S and CO_2 from natural gas. Since, H_2S is corrosive substance and CO_2 can reduce the combustion efficiency, hence the effort to remove those substances up to allowable content i.e. 3-4 mol% for CO_2 content and 0.25 gr / 100 scf for H_2S content [5].

In this study, DEA is used to absorb these compounds. Absorption process is based on a theory which sulfur and carbon chains will be disjointed by amine solution [6]. The natural gas purification using DEA can be described as follow [7].

Process in Absorber :

$R_3N + H_2S \rightarrow (R_3NH)^+ + (HS)^-$ (2.1)

$2R_2NH + CO_2 \rightarrow (R_2NH_2)^+ + (R_2NCO_2)^-$ (2.2)

$\{CO_2 + H_2O \rightarrow H_2CO_3\}$ (2.3)

$R_3N + H_2CO_3 \rightarrow (R_3NH)^+ + (HCO_3)^-$ (2.4)

Process in Regenerator :

$(R_3NH)^+ + (HS)^- + \text{Heat} \rightarrow R_3N + H_2S$ (2.5)

$(R_2NH_2)^+ + (R_2NCO_2)- \rightarrow 2R_2NH + CO_2$ (2.6)

$(R_3NH)^+ + (HCO_3)^- + \text{Heat} \rightarrow R_3N + H_2CO_3$ (2.7)

$\{H_2CO_3 + \text{Heat} \rightarrow CO_2 + H_2O\}$ (2.8)

Based on the formula of a chemical reaction of DEA, in acid gas sweetening process, there are two process stage, first natural gas purification in absorber by eliminating H_2S and CO_2 compound, and second is recleaning process of DEA solution in regenerator before it reuses in the absorber. The DEA solution has reversible characteristics, hence, this solution can be cleaned from sulfur and carbon, therefore it can be reused repeatedly [2]. Figure 1 illustrates the process flow diagram of acid gas sweetening.

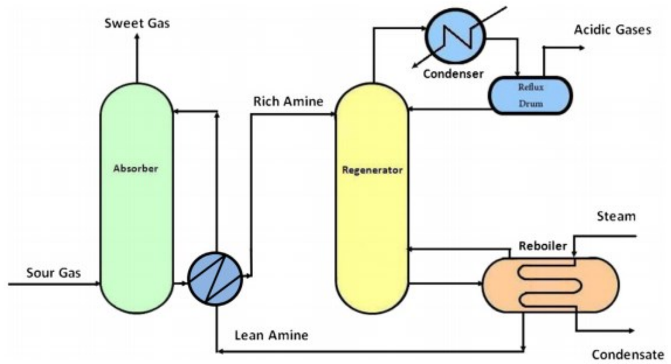

Fig. 1. Acid gas sweetening model [8].

B. Grey Wolf Optimizer

Grey wolf optimizer (GWO) is a swarm intelligence in metaheuristic algorithms. This algorithm inspired by way of life of grey wolf (*canis lupus*). GWO refers to leadership behavior and hunting mechanism of the grey wolf in term of movement strategy of search agents in this algorithm. There are 4 types of wolves based on hierarchical leadership i.e. alpha, beta, delta and omega [9]. Alpha is laid at the top position of leadership in the packs, beta is wolves who give advisors to the alpha, delta and omega are the second class of wolves in the pack, however delta are dominant to omega [9]. Figure 2 illustrate how the grey wolf hunting mechanism.

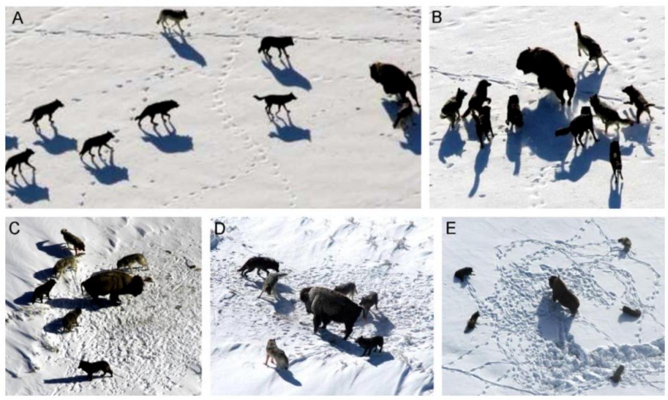

Fig. 2. (A) chasing prey (B–D) pursuing, harassing, and encircling prey (E) stationary situation and assault [9].

The hunting mechanism based on the philosophy of grey wolf in pursuit, harassing, and assault the prey is implemented into the algorithm using a mathematical model. The Mathematical model that described encircling prey and hunting mechanism of grey wolf are shown in equations 2.9 – 2.19 [9].

Mathematical model of encircling prey:

$$\vec{D} = |C \cdot \vec{X}_p(t) - \vec{X}(t)| \quad (2.9)$$

$$\vec{X}(t+1) = \vec{X}_p(t) - \vec{A} \cdot \vec{D} \quad (2.10)$$

$$\vec{A} = 2\vec{a} \cdot \vec{r}_1 - \vec{a} \quad (2.11)$$

$$\vec{C} = 2 \cdot \vec{r}_2 \quad (2.12)$$

Mathematical model of hunting mechanism:

$$\vec{D}_\alpha = |\vec{C}_1 \cdot \vec{X}_\alpha - \vec{X}| \quad (2.13)$$

$$\vec{D}_\beta = |\vec{C}_2 \cdot \vec{X}_\beta - \vec{X}| \quad (2.14)$$

$$\vec{D}_\delta = |\vec{C}_3 \cdot \vec{X}_\delta - \vec{X}| \quad (2.15)$$

$$\vec{X}_1 = \vec{X}_\alpha - \vec{A}_1 \cdot (\vec{D}_\alpha) \quad (2.16)$$

$$\vec{X}_2 = \vec{X}_\beta - \vec{A}_2 \cdot (\vec{D}_\beta) \quad (2.17)$$

$$\vec{X}_3 = \vec{X}_\delta - \vec{A}_3 \cdot (\vec{D}_\delta) \quad (2.18)$$

$$\vec{X}(t+1) = \frac{\vec{X}_1 + \vec{X}_2 + \vec{X}_3}{3} \quad (2.19)$$

Where:

$\vec{X}_\alpha$: Position vector of alpha

$\vec{X}_\beta$: Position vector of beta

$\vec{X}_\delta$: Position vector of delta

t : Iteration

$\vec{A}$ and $\vec{C}$: Coefficient vector

$\vec{X}_p$: Position vector of prey

$\vec{D}$: Vector of encircling prey

$\vec{a}$: Evaluation component [2 – 0]

$\vec{r}_1$ and $\vec{r}_2$: Random vector [0,1]

GWO concept to find global optimum value in 2D and 3D analogy [9].

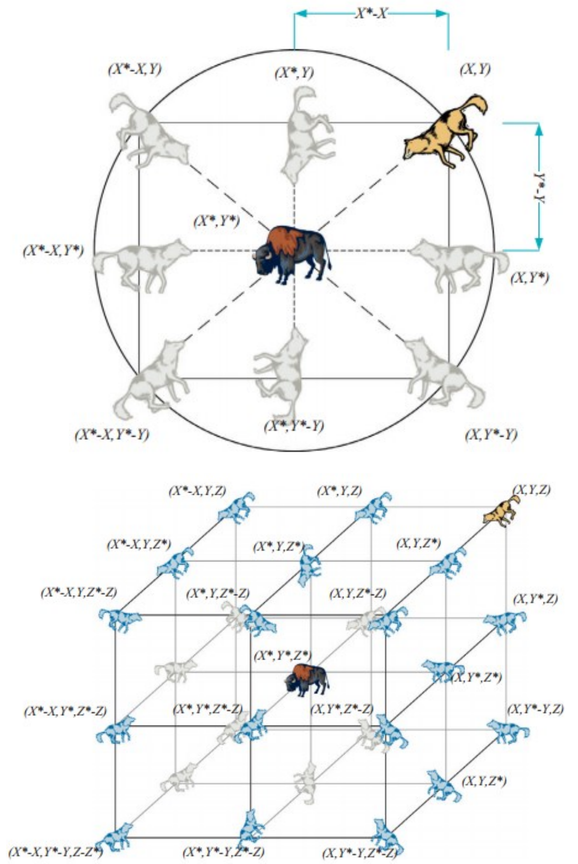

Fig. 3. 2D and 3D position vectors and possibility of next movement [9].

Each search agents will update their position within the search space to reach the global optimum of the objective function. Position update is performed by the magnitude of movement and direction of each search agents with coefficient vectors. At the end of hunting mechanism, the alpha will reach the prey position at the first time. This condition will be defined as best solution and the other wolves will be placed at random points around the best solution [9].

C. Least Squares - Support Vector Machine (LS-SVM)

Least-Squares Support Vector Machine (LS-SVM) were developed by Suykens *et al.,* [10], LS-SVM is a modification of original Support Vector Machine (SVM) [11], focused on regression tasks and multiclassification modifications. In this research used a toolbox from Suykens *et al.,* [12] to perform regression tasks for the process data that was obtained from plant simulation under Aspen HYSYS.

The basic concept of LS-SVM is based on Nyström Approximation method. This method mapping the process data in the spatial dimension, evaluate data deviation, and perform decomposition based on eigenvectors and eigenvalues of kernel matrix [11]. Radial Basis Function (RBF) kernel is used in this research, RBF kernel can be described in equation 2.20 [13].

$$K(x,x_k) = \exp\left(\frac{-|x_k - x|^2}{\sigma^2}\right) \quad (2.20)$$

Where $K(x,x_k)$ is kernel function that is calculated from two vector x and x_k, σ is kernel parameter to calculated eigenvectors and eigenvalues. Decomposition of the process data is performed using Kentropy algorithm. Kentropy is Quadratic Renyi Entropy for kernel-based estimator [12]. This algorithm computes eigenvectors and eigenvalues decomposition of kernel matrix in order to build a new LS-SVM model based on process data.

The next step is Ridge Regression. It is performed to solve multicollinearity that might occur on modeling based on regression. Multicollinearity is a problem that would produce an error in estimation and bias in the calculation result. Ridge Regression technique provide the best estimation result by centering and scaling methods [14].

It is desired to validate the output from LS-SVM model with actual data. Root Mean Square Error (RMSE) is used to evaluate the accuracy of the model [15]. The mathematical formulation of RMSE can be shown in equation 2.21.

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_1 - \hat{y}_2)^2} \quad (2.21)$$

Where $\hat{y}_1$ is actual data, $\hat{y}_2$ is estimated data and n is a number of data.

III. Methodology

This research begins with plant data collection, acid gas sweetening plant modeling using Aspen HYSYS [16], plant modeling using LS-SVM, objective function, optimization technique using GWO and perform optimization of acid gas sweetening using GWO to obtain minimum energy consumption. The plant model was build using Aspen HYSYS by utilizing process data design and integrate it such as in the real plant. LS-SVM is used to simulate the behavior of plant as per optimization requirement model i.e. fast, robust and accurate. The model will be incorporated with GWO to simulate the optimization of acid gas sweetening plant.

Figures 4 and 5 show the process flow diagram of acid gas sweetening plant under commercial software Aspen HYSYS.

The model was built and validate using plant design data such as tabulated in Table 1. From this model will generate data that will use for training and validation of LS-SVM.

A. Simulation on Aspen HYSYS

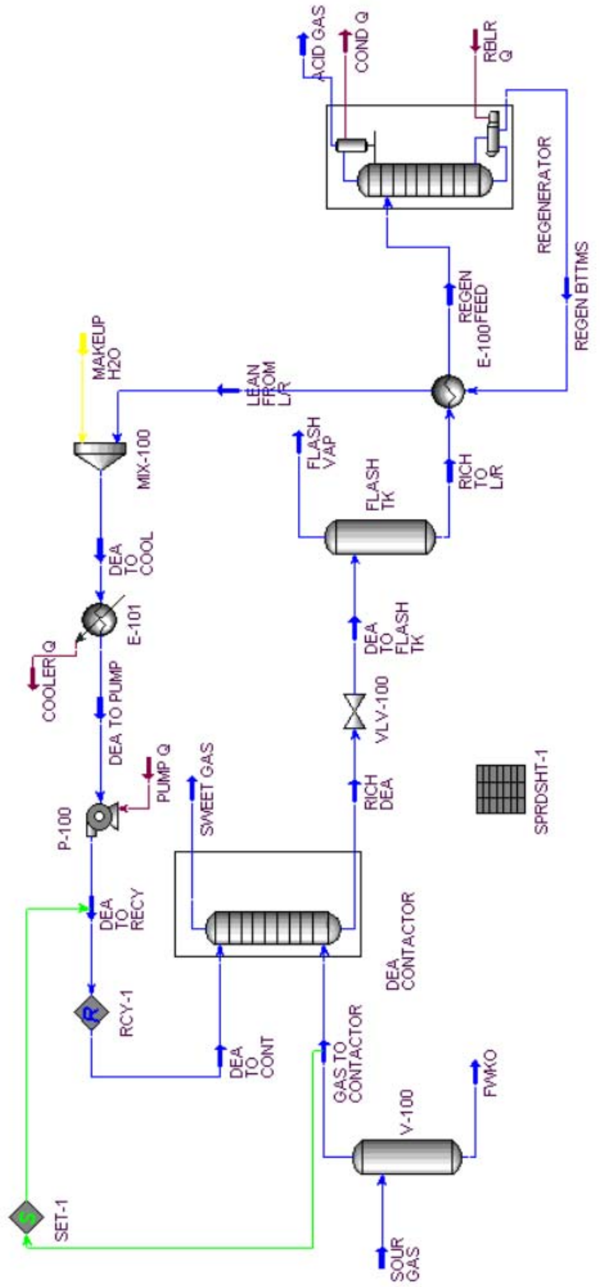

Fig. 4. Model plant of acid gas sweetening developed on Aspen HYSYS [15].

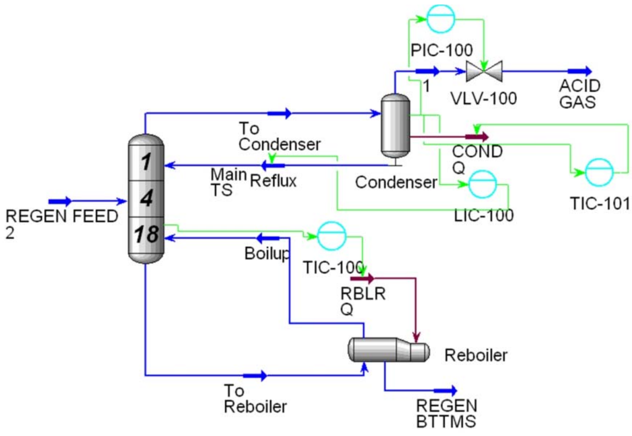

Fig. 5. Process flow diagram of regenerator process.

Data regarding the initial operating conditions that put on the process which refer to [16].

TABLE I. INITIAL OPERATION DATA OF MODEL

Data	Value
Temperature sour gas	30 °C
Pressure sweet gas	6927 kPa
Mass flow sour gas	1472 kg mol/h
Mole fraction CO_2 on sour gas	4.1 %
Mole fraction H_2S on sour gas	1.7 %
Mole fraction DEA on sour gas	0 %
Mole fraction Methane on sour gas	86.92 %
Mole fraction Ethane on sour gas	3.93 %
Mole fraction Propane on sour gas	0.93 %
Mole fraction Nitrogen on sour gas	0.16 %
Mole fraction i-Buthane on sour gas	0.26 %
Mole fraction n-Buthane on sour gas	0.29 %
Mole fraction i-Penthane on sour gas	0.14 %
Mole fraction n-Penthane on sour gas	0.12 %
Mole fraction n-Hexane on sour gas	0.18 %
Mole fraction n-Heptane on sour gas	0.72 %
Mole fraction H_2O on sour gas	0.5 %

B. Objective function

The objective function that used in this study is minimized energy consumption in reboiler and condenser of amine regeneration column, and it is shown in equation 3.1.

$$J = \frac{(Q_{Re-boiler} + Q_{Condenser} * \eta)}{\dot{m}_{Feed}} \tag{3.1}$$

Where:

$Q_{Re\text{-}boiler}$ = Heating energy on re-boiler in regenerator (kJ/h).
$Q_{Condenser}$ = Cooling energy on condenser in regenerator (kJ/h)
$\dot{m}_{Feed}$ = Total mass flow sour gas (kg/h).
η = Efficiency of heating / cooling.

IV. Result and Discussion

A. *Training data using LS-SVM*

On modeling stage, data from acid gas sweetening plant under Aspen HYSYS is used to update the coordinate of the data of LS-SVM that provided accurate prediction output. The result of training for $Q_{condenser}$ and $Q_{re\text{-}boiler}$ under training stage it can be shown in Figures 6 and 7, respectively. The accuracy of the model under training stage is indicated as RMSE value in Table 2.

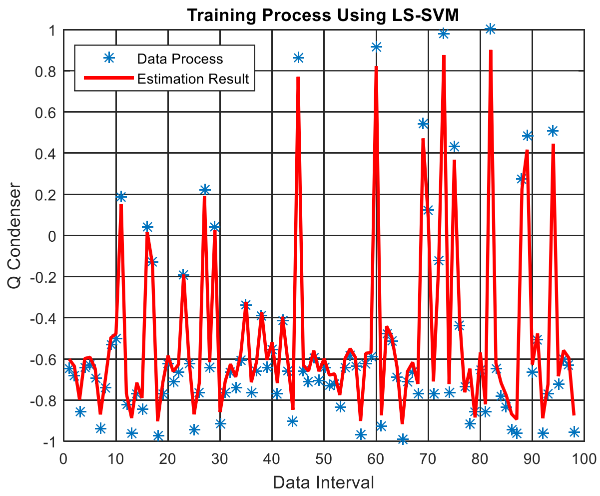

Fig. 6. The result of training $Q_{condenser}$ data based on LS-SVM.

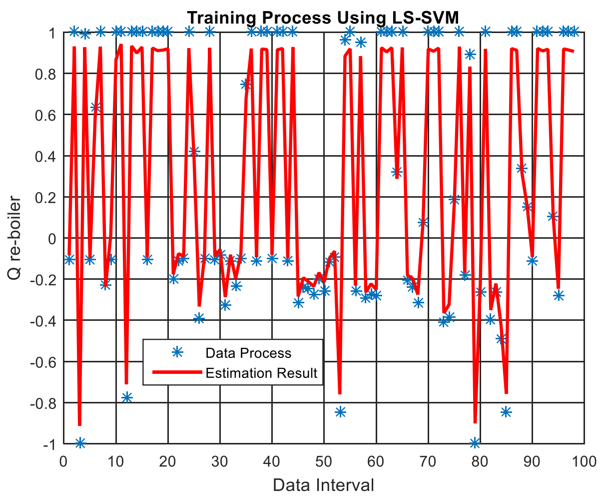

Fig. 7. The result of training $Q_{re\text{-}boiler}$ data based on LS-SVM.

TABLE II. RMSE CALCULATION OF TRAINING PROCESS

No.	Variable	RMSE Value
1	$Q_{condenser}$	0.0916
2	$Q_{re\text{-}boiler}$	0.0909

B. *Validation process using LS-SVM*

The validation process is performed by simulate the different process data. This process is utilized to avoid overlearning model. The result of validation stage can be shown in Figures 8 and 9. RMSE under validation process is tabulated in Table 3. It is shown the RMSE under training and validation stage slightly different or in another word, the LS-SVM model is suitable to use in optimization process in the next stage.

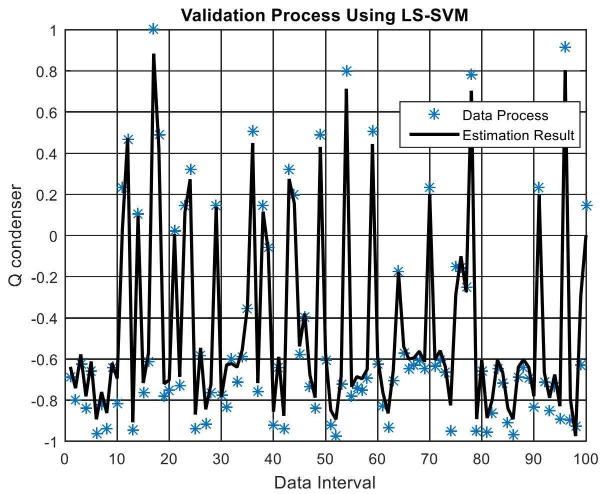

Fig. 8. The result of validation $Q_{condenser}$ data based on LS-SVM.

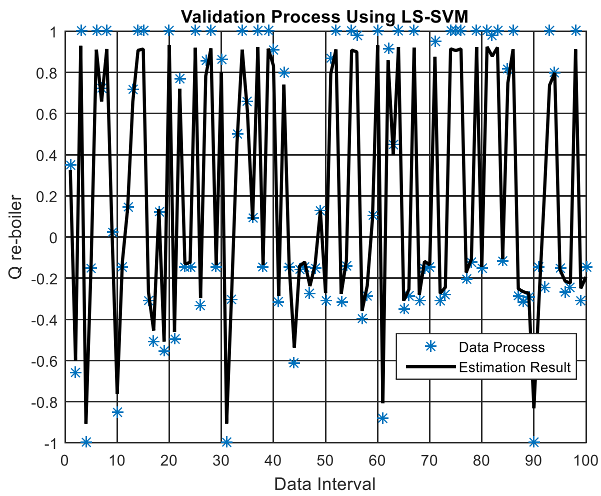

Fig. 9. The result of validation $Q_{re\text{-}boiler}$ data based on LS-SVM.

TABLE III. RMSE CALCULATION OF VALIDATION PROCESS

No.	Variable	RMSE Value
1	$Q_{condenser}$	0.0680
2	$Q_{re\text{-}boiler}$	0.0587

C. *Energy minimization using GWO*

GWO was used to obtain the minimum energy consumption on acid gas sweetening that developed based on Aspen HYSYS. The parameters of GWO are tabulated in Table 4. By incorporating LS-SVM model, GWO will seek the minimum energy consumption by changing reflux and reboiler heat duty. In order to measure the performance of GWO, Particle Swarm Optimization (PSO) is used as a comparison.

TABLE IV. ALGORITHM PARAMETERS

No.	Parameters	Value
1	GWO search agents	50
2	PSO search agents	50
3	Sum of iteration	1000
4	Dimension of problem	2 ($Q_{condenser}$ + $Q_{re\text{-}boiler}$)

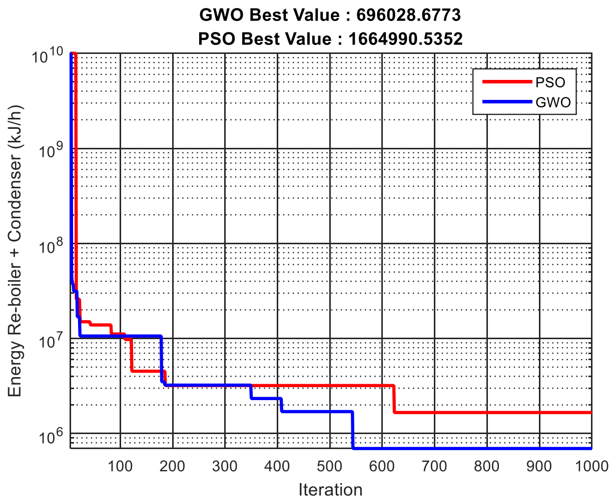

Fig. 10. Result of first running

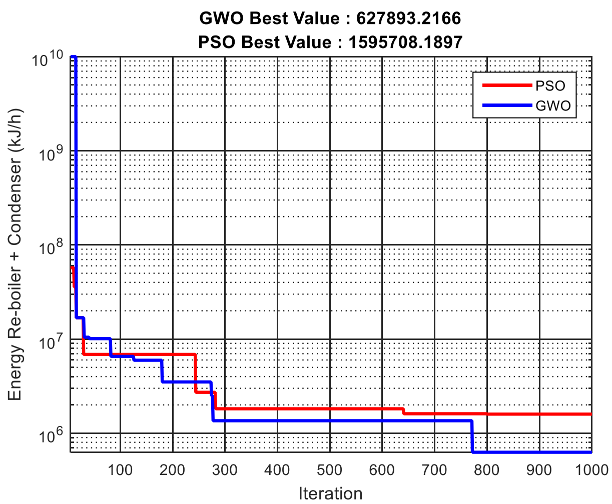

Fig. 11. Result of second running

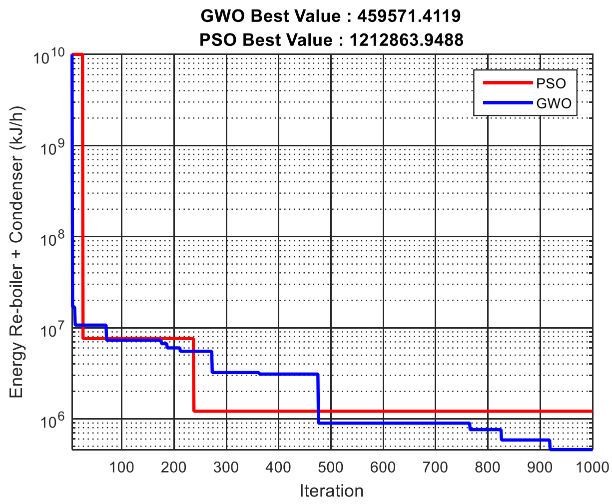

Fig. 12. Result of third running

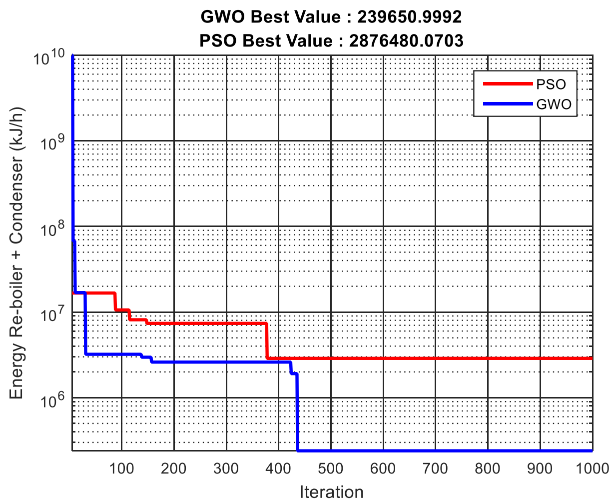

Fig. 13. Result of fourth running

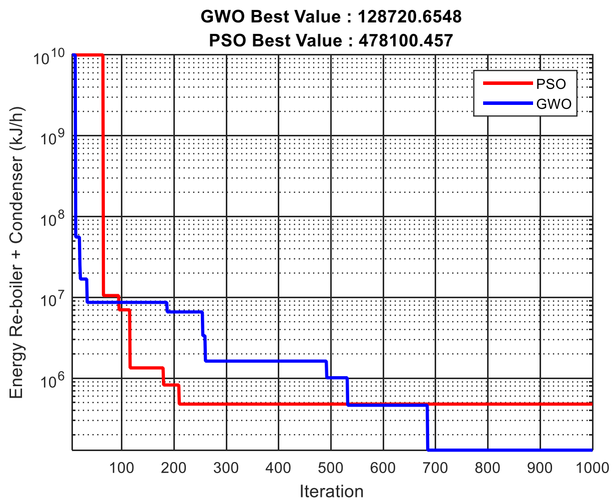

Fig. 14. Result of fifth running

TABLE V. RESULT OF RUNNING

No.	GWO	PSO
1	6.960E+5 (kJ/h)	16.649E+5 (kJ/h)
2	6.278E+5 (kJ/h)	15.957E+5 (kJ/h)
3	4.595E+5 (kJ/h)	12.128E+5 (kJ/h)
4	2.396E+5 (kJ/h)	28.764E+5 (kJ/h)
5	**1.287E+5 (kJ/h)**	**4.781E+5 (kJ/h)**

The optimization result using GWO and PSO under 5 times repetition, it is shown in Figures 10 – 14 and tabulated in Table 5 that GWO surpass PSO optimization performance in term of speed and value of global optimum. The energy consumption before and after optimization is tabulated in Table 6. The energy consumption was reduced a half of value before optimization.

TABLE VI. COMPARISON OF PREVIOUS AND THEREAFTER OPTIMIZATION BASED ENERGY MINIMIZATION

No.	Component	Before Optimization	After Optimization using GWO
1	$Q_{condenser}$	367668 (kJ/h)	18108 (kJ/h)
2	$Q_{re\text{-}boiler}$	25132320 (kJ/h)	138070 (kJ/h)
	Total (kJ/h)	**2.55E+10**	**1.287E+5**

V. CONCLUSION

Aspen HYSYS was used to developed acid gas sweetening process and LS-SVM was provided an accurate model and it is used in the optimization process. The GWO has better performance than PSO in term of speed and global value. Optimization result provided reducing energy consumption a half of value before optimization.

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