Prediction of Optimal Sulfinol Concentration in Khangiran Gas Treating Unit via Adaptive Neuro-Fuzzy Inference System and Regularization Network

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Abstract

The concentration of H_2S in the inlet acid gas is an important factor that sulfur plant designers must consider when deciding on the right technology or configuration to obtain high sulfur recovery efficiency. Using sterically-hindered solvents such as promoted tertiary amines and various configuration for gas treating unit are several alternatives for acid gas enrichment (AGE) to reduce the concentration of carbon dioxide and heavy aromatic hydrocarbons while enriching the H_2S content of SRU feed stream. The present article uses combinations of Aspen-HYSYS software and two distinct networks (namely, Regularization network and adaptive neuro-fuzzy inference system) to compare the AGE capability of sulfinol-M (sulfolane + MDEA) solvent at optimal concentration to traditional MDEA solution when both of them are used in a conventional gas treating unit (GTU). The simulation outcomes demonstrate that the optimal concentration of Sulfinol-M aqueous solution (containing 37 wt% Sulfolane and 45 wt% MDEA) will completely eliminate toluene and ethylbenzene from the SRU feed stream while removing 80% of benzene entering the GTU process. Furthermore, mole fraction of H_2S in the SRU feed stream increases the conventional 33.48 mole% to over 57mole%. Increased H_2S selectivity of optimal Sulfinol-M aqueous solution will elevate the CO_2 slippage through sweet gas stream at around 4.5mole% which is still below the permissible threshold.

Keywords: AGE, BTEX, Regularization network, MLP, ANFIS

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Introduction

Sour unconventional natural gas often has a higher CO_2:H_2S ratio than conventional gas sources, which results in leaner acid gas feed streams (lower H_2S concentration). Moreover, acid gases from both of these sources frequently contain contaminants such as heavy hydrocarbons (e.g. Benzene, Toluene, Ethylbenzene and xylene (BTEX)), ammonia and methanol which all can cause operating problems in sulfur recovery units (SRUs). Excessive amount of such impurities in acid gas stream entering SRU Claus process drastically decreases the combustion chamber temperature and reduces the overall elemental sulfur recovery efficiency (Chludzinski et al., 1993). A preferential method for reducing the concentration of these contaminants in the acid gas of SRU feed stream is to utilize proper acid gas enrichment (AGE) process at upstream of the sulfur recovery unit.

The recent development and success of applying various kinds of machine learning modeling approaches to tackle various complex engineering problems has attracted much attention to their potential applications in the natural gas industry (Zhou et al., 2013). These powerful tools are traditionally used for their capability of nonlinear mapping and lack of necessity for detailed mechanistic knowledge (Anifowose et al., 2011). The capability of artificial neural networks (ANNs) and adaptive neuro-fuzzy inference system (ANFIS) to model nonlinear and highly complex systems in order to extract underlying truth from noisy data are memorable.

Acid gas enrichment process depends on multiple input variables which possess strong coupling between them with severe uncertainty. Using conventional modeling techniques to model such nonlinear and highly complex systems with large numbers of input and output variables make the application of ANNs along with ANFIS particularly attractive.

The principle of acid gas enrichment process originates from proper selective removal of H_2S at the presence of other impurities (specially CO_2) which can be accomplished in three distinct routes (Seagraves et al., 2011; Palmer et al., 2006):

A) Sterically-hindered amines, controlling the selectivity primarily in the absorber.

B) Various design (configuration) options of gas treating unit (GTU) and absorber internals, affecting the difference in CO_2 and H_2S mass transfer kinetics.

C) Promoted tertiary amines, focusing more on enhanced regeneration and thus leading to lower H_2S loadings.

For selective H_2S absorption in the first route, a molecular structure would be selected which suppresses carbamate formation and, consequently, the rate of CO_2 absorption, without affecting the rate of H_2S absorption. Sterically hindered amines, either primary or secondary amines with large bulky alkyl or alkanol groups attached to the nitrogen (Seagraves et al., 2011), show suitable result for selectively absorbing H_2S in the presence of CO_2. Appropriate molecular configuration leads to an unstable carbamate formed with CO_2 which is readily hydrolyzable, resulting in the formation of bicarbonate as the end product. This phenomenon results in a theoretical ratio of one mole of CO_2 per mole of amine.

The chemistry of acid gas reactions with sterically hindered amines is discussed in some detail by Sartori and Savage (1983) and by Weinberg et al. (1983). Furthermore, Chludzinski and Iyengar (1993) describe the application of sterically hindered amines to AGE units as well as outline the operating conditions and some of the possible unit configurations. FLEXSORB-SE amine, which was recognized by Exxon-Mobil scientists in 1981, is a kind of sterically hindered solvent that was successfully used for selective H_2S absorption purposes (Parks et al., 2010). Different kinds of sterically hindered amines such as amino-2-methyl-1-propanol (AMP), tertiary butyl amino ethanol (TBE), tertiary butyl amino ethoxyethanol (TBEE), MAMP (2-N-methylamino-2-methyl-propan-1-ol), EETB (Ethoxyethanol-t-butylamine), MEEETB (Methoxyethoxyethoxyethanol-tert-butylamine) were tested for their selectivity toward H_2S (Mandal et al., 2004; Lu et al., 2006;

Siskin et al., 2013).

In the second route, necessary modifications can be applied to an existing gas treatment unit (GTU) configuration while using the conventional solvent. Various schemes are used to enhance the selectivity of H_2S over CO_2 (Mak et al., 2015; Al Utaibi et al., 2010; Way et al., 2013).

Finally in the third route, the advanced promoter (e.g. sulfolane) would be added to conventional solvent in order to enhance the selectivity of tertiary amines and also make the release of H_2S from rich amine in the regenerator column easier. Tetra methylene sulfone (TMS) or sulfolane is an excellent industrial solvent with capability of removing H_2S, COS, and CS_2 from various sour gas streams. Aromatic and heavy hydrocarbons such as BTEX and CO_2 are soluble in sulfolane to a lesser degree (Vahidi et al., 2013). Sulfolane is usually blended with alkanol amines (specially methyl diethanol amine (MDEA)) to form adequate mixed solvent (known as sulfinol-M) to capture various impurities, simultaneously (Vahidi et al., 2013; Mokhatab et al., 2012).

Different powerful software along with various mathematical techniques have been used for simulation and modeling of gas treating unit respectively. The results of some recent works will be reviewed in the following section.

Darwish and Hilal (2008) used ANN to detect and diagnose process faults in the dehydration plant. They have concluded that ANN successfully detects the disturbance severity levels in the input variables considered for the contactor. Faults in the stripper–regenerator unit have been perfectly predicted by the ANN for two symptoms (TEG emissions and BTEX emissions in vents).

Fu et al. (2013) developed a neural network to predict overall mass transfer coefficient for carbon dioxide absorption into aqueous diethylenetriamine (DETA). The inlet CO_2 loading, solvent concentration, liquid flow rate, CO_2 partial pressure, and liquid feed temperature were selected as input parameters. They have reported that ANN is a suitable tool for predicting the absorption performance of packed columns.

Angaji et al. (2013) examined the performance of various concentrations of sulfolane in the Sulfinol solvent for GTUs of Khangiran natural gas refinery. They concluded that providing 40.2%wt sulfolane, 21.2% wt H_2O and 37.7%wt MDEA in liquid mixture of Sulfinol-M could increase the capacity of sour gas treatment from 173 to 220 MSCMH. The version of Aspen Plus software which has been used for the entire simulation is unable to provide proper property package for mixtures of MDEA-sulfolane solutions. Limited parameters such as condenser and reboiler duties were investigated in order to optimize sulfolane concentration.

Abdulrahman and Sebastine (2013) used Aspen HYSYS V.7.3 to simulate the Khurmala (Iraqi-Kurdistan region) gas sweetening process. They have tested several amine blends (MEA and MDEA), circulation rate and concentration instead of DEA with flow rate of 400 m^3/hr. Their optimization showed that using DEA 35% is the best recommended process.

Abdulrahman and Sebastine (2013) analyzed the effect of the lean amine temperature on the acid gas content in the sweetened gas and saturated the amine solution by using Aspen HYSYS software. They reported that the optimal temperature for the regenerated amine solution, at which the maximum sweetening of the gas is achieved with minimum amine circulation rate, is within the range 38°C-45°C.

Ghanbarabadi and Karimi (2014) simulated Khangiran gas refinery in order to optimize the concentration and flow rate of MDEA, thermal load of restoration and other operating parameters by using Aspen HYSYS software. They reported that optimum performance of MDEA solvent is 45-50% wt concentration at 55-63˚C.

The superior performances of ANN and ANFIS have been proved in a wide variety of applications (Zhou et al., 2013; Rahmanian et al., 2012).

In the present article, a conventional GTU is simulated by resorting to the powerful Aspen-HYSYS software V.8.3. Instead of using the traditional MDEA solution as solvent, various concentrations of MDEA and sulfolane (known as sulfinol solution) will be used to

predict the concentration of H_2S and BTEX components in the acid gas stream leaving GTU. The above version of Aspen-HYSYS software is capable of providing adequate property package for all mixtures of MDEA-sulfolane solutions. The limited data collected from Aspen-HYSYS simulations using various sulfinol concentrations will be employed as the training data to optimize an adaptive neuro-fuzzy inference system and regularization network. The trained network performances will be initially compared with the performance of conventionally used neural network toolbox of MATLAB software and finally they will be recruited to provide reliable interpolation hyper-surfaces for practical uses.

Importance of AGE and BTEX elimination in a conventional GTU

One of the keys to achieving good Claus plant performance is to maintain a stable flame and high temperatures in the main reaction furnace (>926°C, 1700°F). Higher temperatures increase the conversion of H_2S to elemental sulfur. Contaminants in the acid gas stream can seriously impact the operability and reliability of a sulfur plant. Carbon dioxide and other impurities in the acid gas feed stream to SRU unit acts diluents, reducing reaction furnace temperatures and hence, drastically limit the elemental sulfur capacity. In the worst scenario, excessive amounts of such inert constituents can completely quench the combustion chamber flame.

To achieve high temperatures in the Claus furnace an acid gas feed stream typically requires at least 50 mole percent H_2S. If the H_2S concentration in the acid gas from the acid gas removal unit is lower than 50%, several Claus plant design options are available out of which the most common is the split flow design (Mokhatab et al., 2012; Kidnay et al., 2006). Although other options such as split flow design, acid gas or air preheat plus oxygen enrichment are available to increase the overall sulfur recovery efficiency none of them is as preferable as the acid gas enrichment process.

Effective elimination of carbon dioxide from acid gas streams via a successful acid gas enrichment scenario can dramatically decrease the size of a conventional Claus unit in the design stage or significantly increase the plant throughput for an existing SRU facility.

Two significant problems occur when high concentrations of BTEX are passed through SRU. The first is general deactivation of the catalyst in the catalytic chamber due to accumulation of carbon and/or carsul (a variety of heavy carbon-sulfur compounds) in the pores of the catalyst due to coking of the hydrocarbons (Kidnay et al., 2006; Zarenezhad et al., 2008). This problem affects all Claus catalysts, both alumina and titania. The second problem with BTEX is rapid deterioration of hydrolysis catalysis in titania catalysts. Nowadays, titania catalysts are used in many plants that require high sulfur recovery efficiency, because it is proved that this catalyst significantly improves the degree of COS and CS_2 hydrolysis over that of alumina catalysts, especially at lower temperatures.

Unfortunately, field experience and recent laboratory testing have shown that titania catalysts are especially prone to rapid decline in the amount of hydrolysis they catalyze when exposed to BTEX. It is therefore crucial to oxidize and recover energy from BTEX completely in the combustion chamber. Incomplete destruction of such aromatic compounds can result in contamination of the final elemental sulfur product (production of dark yellowish sulfur) and deactivation of the catalysts. Several studies have shown that catalyst coking has been tied directly to aromatic content of acid gas stream with toluene being the primary contributor (Crevier et al., 2001; Zarenezhad, 2011).

Installing proper acid gas enrichment process or using suitable adsorption system such as carbon active is an available alternative to mitigate BTEX content of SRU feed stream at upstream section.

Various mixtures of sulfolane and MDEA solutions (sulfinol solvent) will be considered for their performances of the enrichment efficiency in the Khangiran refinery GTU. Effective AGE increases the H_2S content of SRU feed stream and alleviates SRU existing complications such

as flame temperature and BTEX issues.

Characteristics of Sulfinol solvent

Mixed or hybrid (or composite) solvents composed of a non-aqueous physical solvent and an aqueous amine take advantage of both physical and chemical absorptions. The best known example of such mixed solvents is the Sulfinol solvent which was initially introduced by Shell Company in 1963. It is a mixture of Sulfolane ($C_4H_8O_2S$), water and diisopropanolamine (DIPA, $C_6H_{15}NO_2$) or MDEA known as Sulfinol-D or Sulfinol-M, respectively.

The sulfinol-M solution is mainly used for the selective absorption of H_2S from natural gas in the presence of CO_2. As it was mentioned before, solubility of aromatic hydrocarbon and carbon dioxide are in a lesser degree compared to the sulfur compounds (Mokhatab et al., 2012).

The advantages of sulfinol-M are higher acid gas loading, lower energy requirements for regeneration, lower corrosion rates, relatively poor hydrocarbon selectivity and lower foaming tendency. Thermodynamic modeling of aqueous sulfolane solutions (in the absence of alkanolamines) for prediction of their thermal and physical properties have well received remarkable attention in numerous studies (Zong et al., 2011; Shokouhi et al., 2013).

Optimization of sulfolane concentration in the proposed sulfinol-M solvent instead of MDEA solvent in the Khangiran natural gas refinery treating unit via Regularization network and ANFIS is the essence of this work. In the following section, brief review of RN and ANFIS will be presented.

Intelligent Systems

Modern computer hardware technology together with intelligent software solutions makes it possible to process the large amount of data at low cost. Some well-known analysis methods and tools that are used for data mining are statistics (regression analysis, discriminant analysis, and principal component analysis), time series analysis, decision trees, cluster analysis, neural networks, fuzzy models and neuro-fuzzy models. These approaches are particularly useful when data are abundant and modeling knowledge is missing (Zhou et al., 2013).

Adaptive neuro-fuzzy inference system (ANFIS)

The learning ability of neural networks combined with fuzzy modeling has created the adaptive network based fuzzy inference system (FIS). ANFIS is a rule-based fuzzy logic model whose rules are developed during the model training. In general, rule based models can be classified into four categories: fuzzy relational, linguistic, neural network based, and Takagi–Sugeno–Kang (TSK) fuzzy models. ANFIS is the combination of low level calculation of ANN along with the high reasoning ability of a fuzzy logic system (Rahmanian et al., 2012). At the computational level, ANFIS can be regarded as a flexible mathematical structure that can approximate a large class of complex nonlinear systems to a desired degree of accuracy. Appendix A contains a detailed review of ANFIS rules and related structure. Figure 1 shows block diagram representation of training algorithm for optimized ANFIS used in the present article.

The ANN method, either alone or in combination with the least squares method, is employed for tuning of the adjustable parameters for obtaining an optimized ANFIS structure during the training phase. For a fixed value of consequent parameters, back-propagation (BP) ANN based on gradient descent method finds the optimal value of premise parameters. The output of the ANFIS is calculated first by employing the consequent parameters. Next, the output error is used to adjust the premise parameters by means of a standard BP algorithm. When both the premise and consequent parameters need tuning, the combination of least squares and gradient descent method based BP-ANN is adopted for parameter optimization. The least squares method is used to optimize the consequent parameters by forward pass keeping the value of premise parameters fixed. Once the optimal consequent parameters are found, the backward pass starts immediately to optimize the premise parameters using the

gradient decent BP-ANN. In the present article, a Sugeno-type FIS using subtractive clustering is generated using *genfis2* function to provide an initial set of membership functions for the training of ANFIS. Figure 2 shows our training algorithm for optimizing ANFIS (Rahmanian et al., 2012).

Artificial neural networks

Artificial Neural Networks (ANNs) are aptly suited for investigating of ill-understood problems with imprecise data which can successfully model and predict various complex and highly non-linear processes. ANNs have been widely applied in many fields such as process modeling, control, optimization, estimation and forecasting (Haykin, 1999). Many neural networks have been constructed to perform approximation of multi-dimensional function by solving the hyper-surface reconstruction problem. This form of learning is closely related to classical approximation techniques such as regularization theory. The solution of multivariate regularization theory leads to a class of three-layer networks called Regularization networks which is reviewed in the following section (Haykin, 1999).

A brief review of Regularization networks

Poggio and Girosi proved that the ultimate solution of the ill-posed problem of multivariate regularization theory could be represented in the concise form of (Poggio et al., 1990; Shahsavand, 2000):

$$\left(G+\lambda I_N\right)\underline{w}_\lambda = \underline{y} \tag{1}$$

where G is the N×N symmetric Green's matrix which usually is factorizable isotropic Gaussian basis function with certain spread , λ the regularization parameter, I_N is the N×N identity matrix, $\underline{w}_\lambda$ is the N×1 linear synaptic weight vector and $\underline{y}$ is the real response values corresponding to input vector $\underline{x}_i = 1,2,\ldots,N$. The structure of RN and Gaussian basis function parameters are elaborated in Appendix B. Figure 2 depicts the Flow diagram representation of our in-house optimal training algorithm for a Regularization network. The performance of

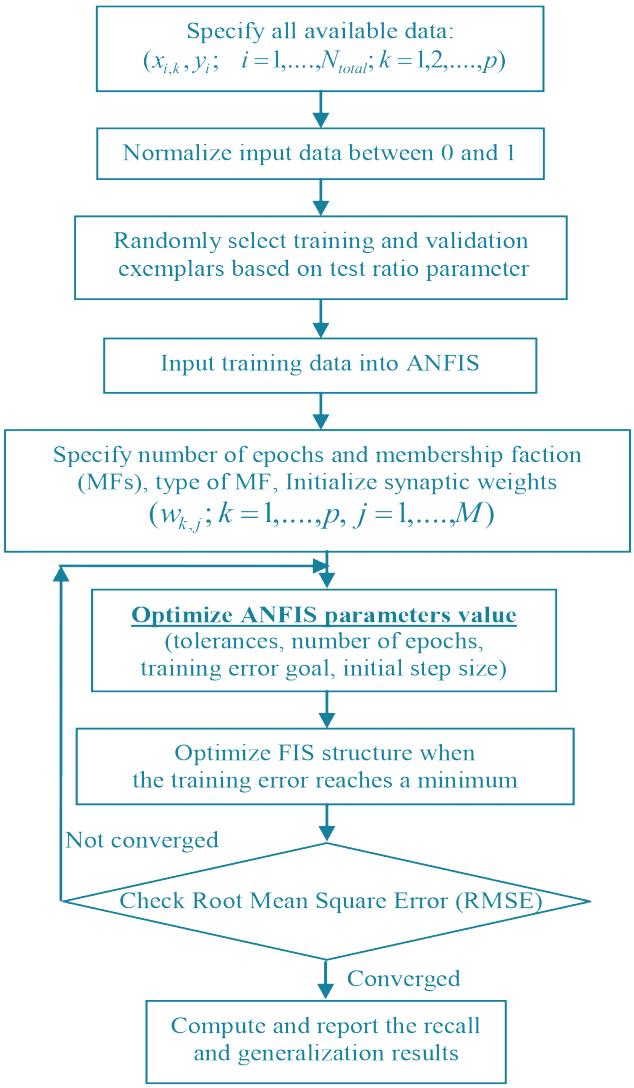

Figure 1. Block diagram representation of training algorithm for optimized ANFIS.

Regularization network strongly depends on the appropriate choice of the isotropic spread and the proper level of regularization which is described in Appendix B. In the following figure, e_k is the N×1 unit vector in which all elements (except the k^{th} one) are zero.

Simulation case study: GTU of Khangiran (Or Hasheminejad) natural gas refinery

Khangiran is the major gas field in North East of Iran, near the Turkmenistan border, and it supplies gas to six north eastern provinces through Khangiran (Hasheminejad) refinery which has been operational since late 1970s

with around 50 sour gas wells. According to recent reports, total gas intake of the refinery, whether sour or sweet, amounts to 57 MMSCMD and by completion of underway development projects, the gas sweetening capacity of the refinery will increase by 10 MMSCMD to reach 67 MMSCMD. Sulfur production capacity of Khangiran gas refinery stands at 2,600 tons a day while the actual production is 2,000 tons. At present, it consists of five sour gas treating units (GTUs) along with four sulfur recovery units with maximum total sulfur production capacity. All sweetening units were designed using 34wt% DEA in water as the solvent (Shahsavand et al. 2010; Moaseri et al., 2013; Shahsavand et al., 2011). Since 2006, 47 wt% MDEA solution in water was replaced for DEA solution, to decrease amine circulation rate and hence save energy in regenerator reboilers and provide extra sweetening capacity for sour gas treatment. The wet sour gas analysis for the contactor feed of the Khangiran GTUs has been presented in our previous article (Shahsavand et al. 2010).

The acid gas leaving Khangiran refinery's GTU contains about 35% hydrogen sulfide. Such low quality SRU feed stream requires split flow with pre-heat scheme for 500 tons per day production of elemental sulfur by each sulfur recovery unit. In the absence of sufficient pre-heat, serious operational problems will be encountered, such as combustion chamber low flame temperature (around 860 0C), unburned BTEX components, low quality and impure produced elemental sulfur with dark yellowish color.

Low acid gas quality combined with the premature catalyst deactivation rapidly decreases the overall efficiency of the entire Claus process from the standard value of 97% to less than 90%.

The entire Khangiran GTU process was initially simulated using Aspen HYSYS version 8.3 simulator (Aspen HYSYS V.8.3 contains a special acid gas property package which supports various Sulfolane-M solutions.) using the actual operating conditions which has been described in full detail in our previous article (Shahsavand et al. 2010). The simulation was initially calibrated by validation with real plant data. The most important operating conditions are summarized in Table 1. Figure 3 shows the simplified schematic diagram of Khangiran gas refinery showing all output parameters of artificial neural network (*in italic fonts*). Both ANFIS and in-house RN are used to investigate the effects of inputs (sulfolane and MDEA weight percent in the lean amine solution) on actual operational variables such as benzene, toluene and ethylbenzene (BTE) escape factors (Defined as: (moles of BTE escaping from regenerator to SRU / total BTE moles entering GTU)×100), H_2S mole fraction and total moles

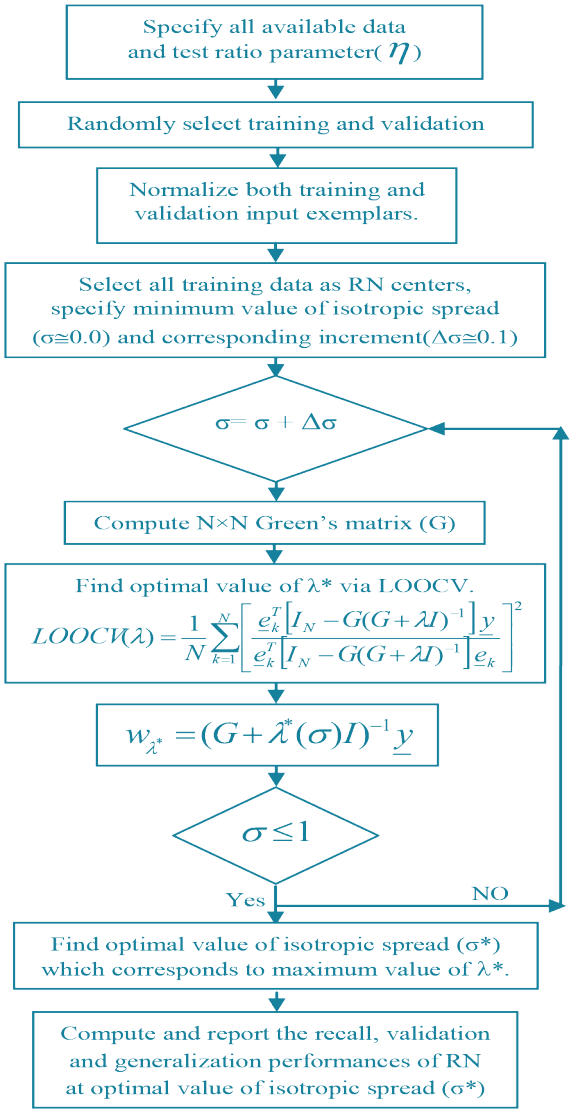

Figure 2. Flow diagram representation of our in-house optimal training algorithm for a Regularization network

of SRU feed, reboiler temperature and mole fraction of CO_2 in sweet gas.

Networks predictions

Figure 4 maps the entire input domain of the ANN and illustrates 37 concentration pairs used as training exemplars for MDEA and sulfolane in the range of (25-47 wt%) and (0-37 wt%), respectively.

The training data of appendix C is used to train networks including conventional MATLAB ANFIS Editor Toolbox and exact fit networks (which is equal to RN, but λ=0) along with Regularization network and optimized ANFIS. After training, the trained network can be used for predicting outputs for one or some of the training data (recall) or computing outputs for some exemplars outside the training set but inside the training domain (generalization).

Figure 5 presents typical recall performances of all above four networks for benzene escape factor (%) (out of six other recall performances) which is significantly appropriate. A person unfamiliar with the over-fitting concept may take proper recall performance as a reliable basis to accept all predictions of such network. Figure 6, which shows the corresponding generalization performances over 100×100 mesh, clearly

Table 1: Some operational conditions of Khangiran GTUs.

P	Temp.(°C)	Pres. (psia)	Flow (Kgmole/hr)	H_2S(mol%)	CO_2(mol%)
Sour gas (To contactor)	52	1050	7319	3.57	6.43
Treated Gas	36	1050	6574	0	0.66
Lean Amine (To Contactor)	57	1050	18650	0.03	0.01
Rich Amine (From Contactor)	72	1050	19380	1.35	2.21
Lean Amine (To Flash Drum)	57	90	70	0.03	0.01
Rich Amine (To Regenerator)	99	90	19445	1.35	2.19
Lean Amine (From Regenerator)	121	27	18670	0.03	0.01
Acid Gas (From Flash Drum)	69	90	28.5	0.04	6.81
Acid Gas (From Regenerator)	55	27	755	33.48	56.05

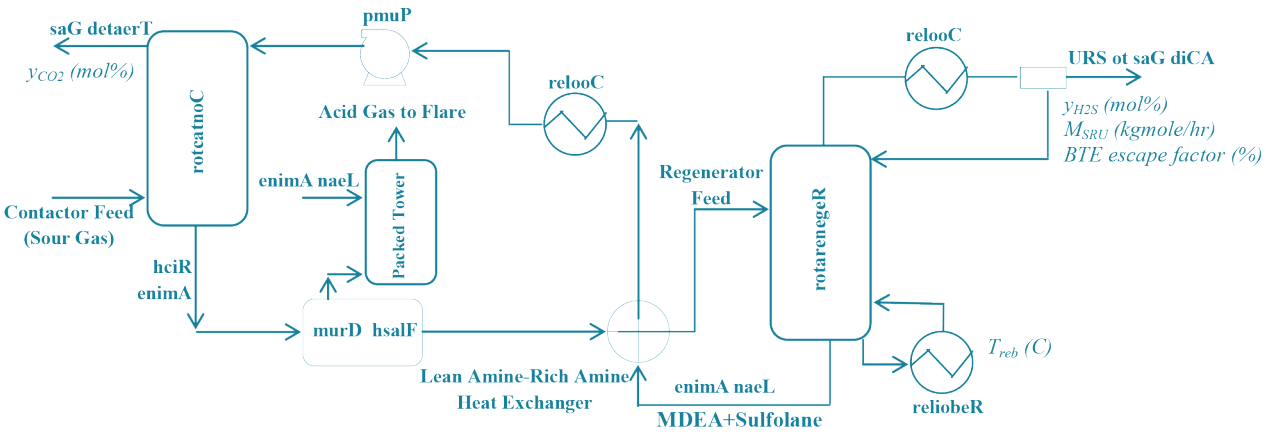

Figure 3. Simplified schematic diagram of Khangiran gas refinery unit.

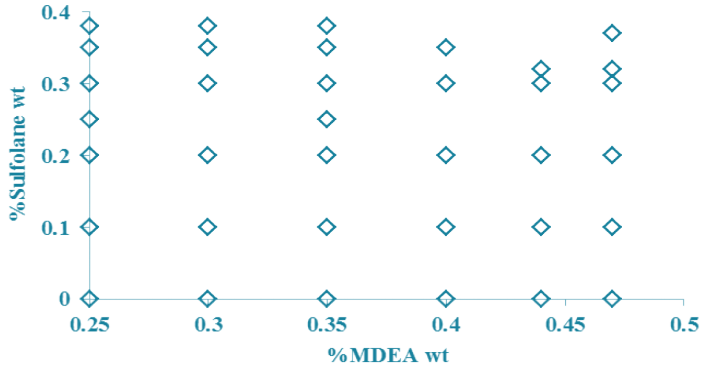

Figure 4. Sulfolane and MDEA input data for training our in-house optimal RN and optimized ANFIS.

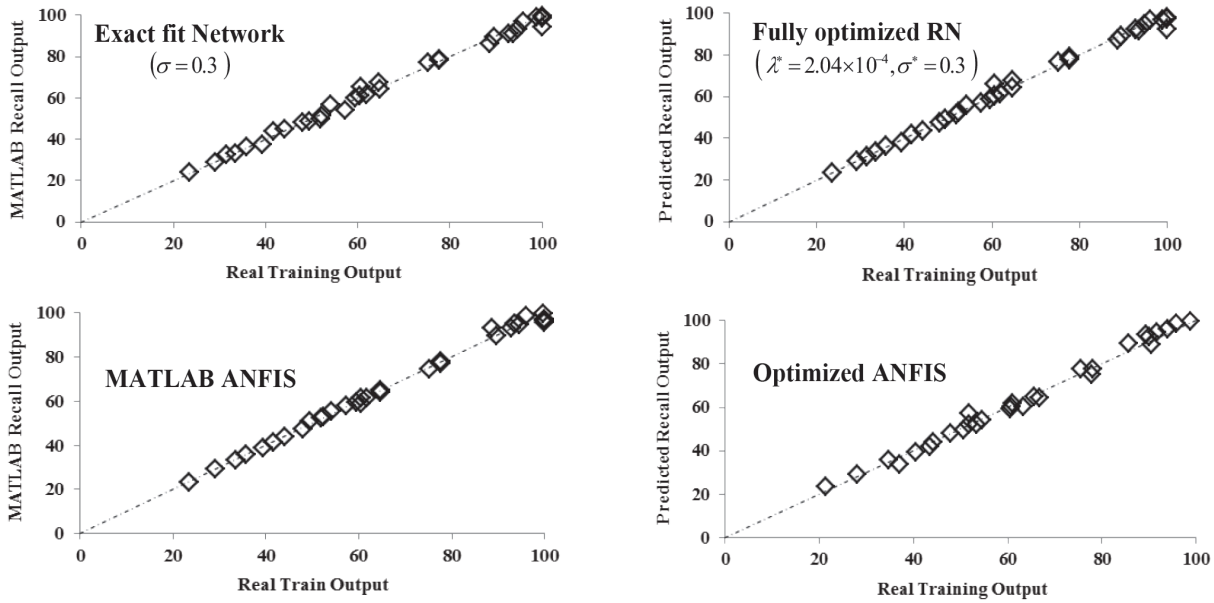

Figure 5. Typical recall performances of various ANN and ANFIS for Benzene escape factor.

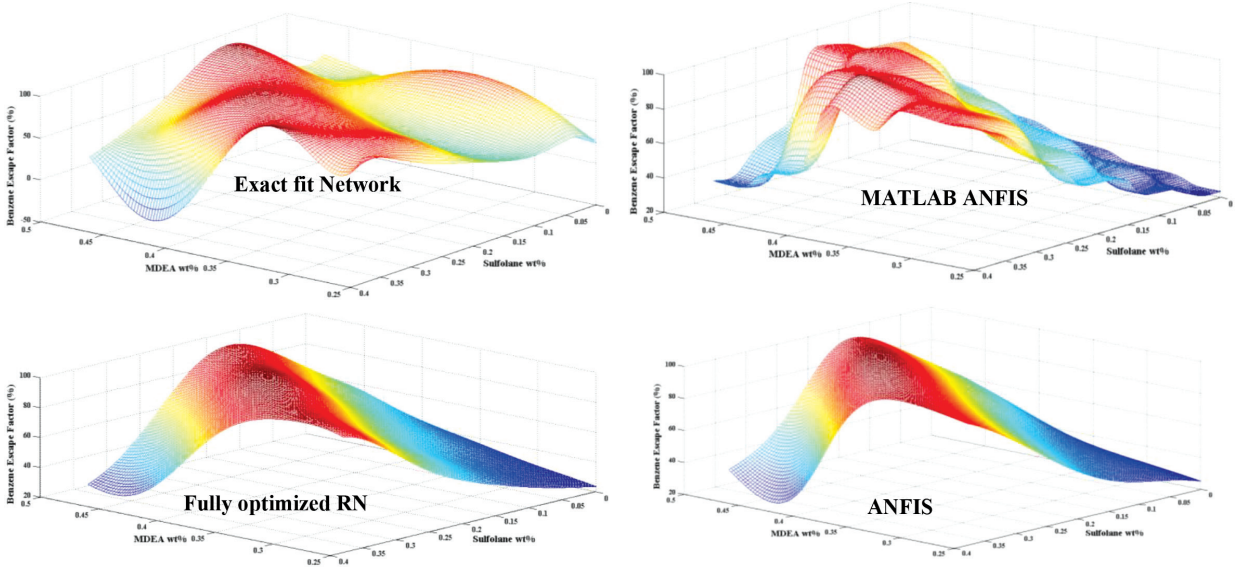

Figure 6. Typical generalization performances of Benzene escape factor (%) in SRU feed stream versus MDEA and sulfolane (wt%) variation in lean amine for various networks.

illustrates that such a naive presumption can lead to catastrophic results when the trained network is used for generalization purposes.

It should be emphasized that un-regularized networks (Exact fit network) tend to follow (fit) the noise (or measurement errors associated with real data) and lead to severely oscillatory generalization performances as shown in Figure 6. A similar oscillatory trend can be observed at MATLAB ANFIS toolbox generalization performance.

The optimum level of regularization eliminates the ill-conditioning problem and leads to a more reasonable generalization performance. It is quite clear that LOOCV criterion is relatively successful to stabilize the generalization performance. Both Regularization network and optimized ANFIS provide almost similar generalization performance over the entire domain. From now on, only the generalization performances of these two networks will be presented.

According to both fully optimized RN and optimized ANFIS networks of Figure 6, sulfolane and MDEA concentrations of (0,0.25) and (0.37, 0.47) can be considered as the optimal choices based on minimization of benzene escape factor entering SRU, which only permits 20% of the total inlet benzene entering GTU passing to the SRU feed stream. Evidently, the first point (i.e. 0 & 0.25) seems much more attractive from both economical and operational view points. However, other considerations (as will be discussed in the following sections) will indicate that the other optimal point will be more appropriate for sustainable production.

Figure 7 depicts the generalization performances of toluene escape factor versus MDEA and sulfolane (wt%) variation in lean amine via Regularization and optimized ANFIS networks. As before, the generalization performances of both networks are practically the same and no distinct difference can be distinguished. Both generalization performances indicate that at the global optimum point of (0.37, 0.47), almost the entire toluene content of SRU feed stream has been eliminated. Evidently, the other suboptimal point of (0, 0.25) will lead to the relatively high concentrations of toluene.

Similarly, Figure 8 shows that the optimal point of (0.37, 0.47) provides minimum Ethylbenzene escape factor and practically removes all Ethylbenzene from GTU feed stream. In light of the above results, a mixture of 37 wt% sulfolane, 47 wt% MDEA and 16 wt% H_2O provides minimum escape factors for all BTE components. Small fluctuations observed in predictions of optimally tuned RN for Ethylbenzene escape factor indicate that LOOCV criterion relatively fails to totally filter the noise embedded in the training exemplars. Other techniques such as modified U curve method can lead to more stable hyper-surfaces.

Figure 9 depicts two similar generalization

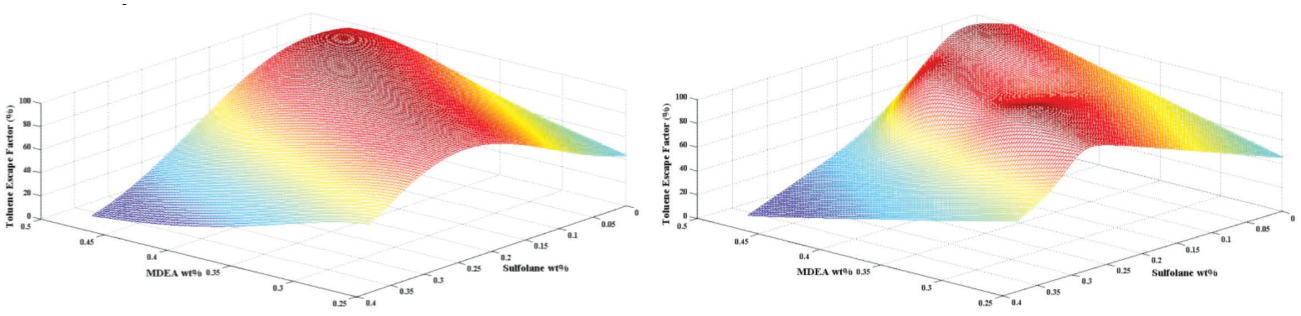

Figure 7.Generalization performances of Toluene escape factor (%) in SRU feed stream versus MDEA and sulfolane (wt%) variation in lean amine (Left: RN, Right: ANFIS)

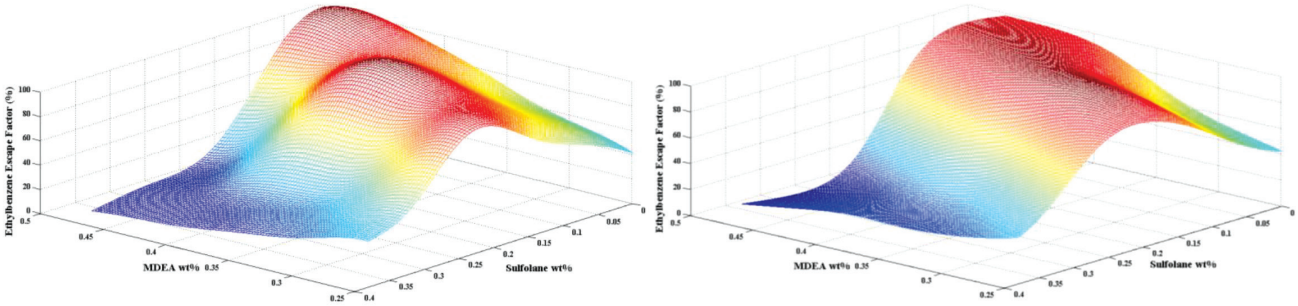

Figure 8.Generalization performances of Ethylbenzene escape factor (%) in SRU feed stream versus MDEA and sulfolane (wt%) variation in lean amine (Left: RN, Right: ANFIS)

performances for the total molar flow rates (kgmole/hr) entering SRU versus MDEA and sulfolane (wt%) variation in lean amine solution. Evidently, lower molar flow rates are more desirable since they indicate higher levels of acid gas enrichments due to efficient CO_2 rejection. Both Figures indicate that as before, the optimal point of (0.37, 0.47) provides minimum molar flow rate of 415 kgmole/hr for the SRU feed stream. About 43% drop in the total molar flow rate of SRU inlet stream (compared to 725 kgmole/hr at (0 & 0.47)) will dramatically reduce the size of a conventional Claus unit in the design stage or significantly increase the plant throughput at an existing SRU facility.

Figure 10 illustrates two similar generalization

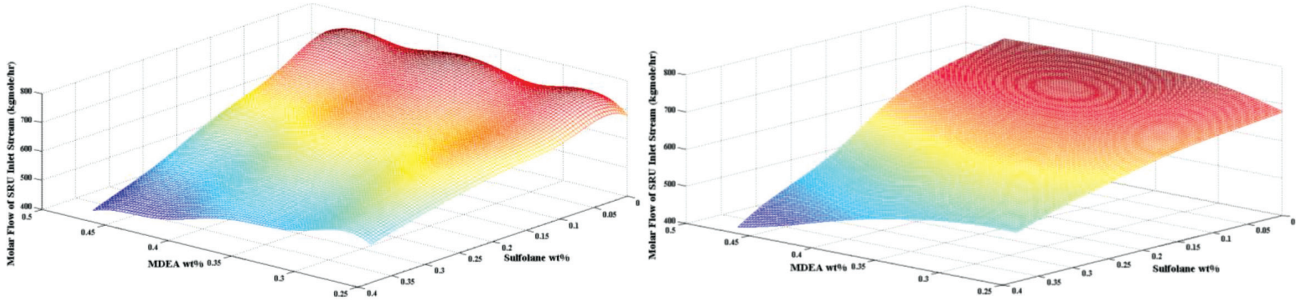

Figure 9. Generalization performances of SRU feed stream molar flow (kgmole/hr) versus MDEA and sulfolane (wt%) variation in lean amine (Left: RN, Right: ANFIS)

performances for hydrogen sulfide mole fractions of SRU feed streams versus MDEA and sulfolane concentrations in lean amine solutions. Figure 10 clearly shows that the H_2S mole percent in SRU feed stream increases more rapidly when sulfolane wt% increases. In an original GTU with no AGE (which uses a solvent containing 47 wt% MDEA and 52 wt% H_2O), the SRU feed stream contains around 34 mole% H_2S while, by using a solvent containing 37 wt% sulfolane, 47 wt% MDEA and 16% H_2O, the H_2S content of acid gas stream entering SRU will raise to more than 57mole% which indicates around 62% H_2S enrichment. It is anticipated that such a high amount of H_2S mole fraction in SRU inlet stream, which is due to large slippage (rejection) of CO_2 and other impurities such as BTE, can severely increase the furnace temperature of Claus unit and alleviate the catalytic deactivation while increasing the sulfur recovery efficiency.

Two 3D plots shown in top of Figure 11

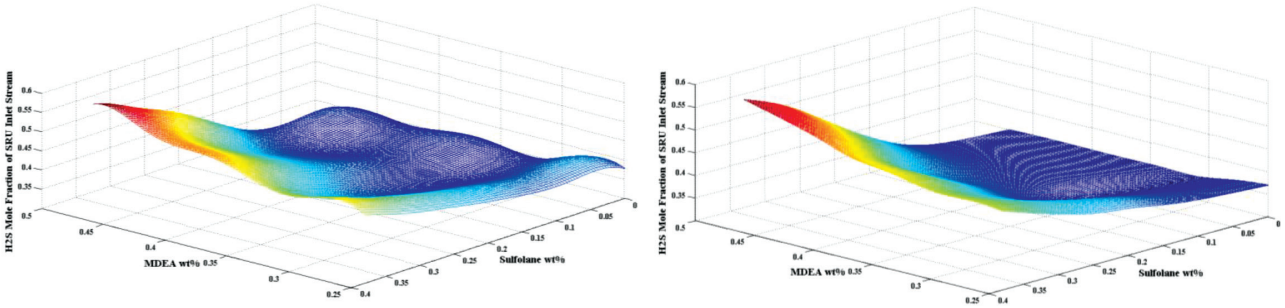

Figure 10.Generalization performances of hydrogen sulfide mole fraction in SRU inlet feed stream versus MDEA and sulfolane (wt%) variation in lean amine (Left: RN, Right: ANFIS)

depict the generalization performances of the optimally regularized and optimized ANFIS networks for reboiler temperature of GTU regenerator column versus MDEA and sulfolane concentrations. Severe oscillations are still revealed in the generalization performance of the regularization network. Evidently, LOOCV criterion fails to provide the optimal level of regularization parameter for the regularization network. Hence, it cannot successfully filter out the noise and extract the true underlying trend embedded in the noisy data set. Our previous work (Niknam Shahrak et al., 2013) summarized various techniques (such as visual, L-curve, modified L-curve, U-curve and modified U-curve methods) for automatic selection of the optimum ridge regression or regularization parameter.

In the absence of a reliable method for successful estimation of the optimal regularization level, the computed values for the optimal spreads has no practical meaning and both the optimal values of the isotropic spread and the regularization level should be recomputed using one of the above techniques. The bottom-left 3D plot of Figure 11 clearly shows that visual optimization of regularization level dramatically fails when improper value is selected for the Gaussian isotropic spread (note the value of vertical axis). On the other hand, the bottom-right 3D plot of Figure 13 illustrates that visual optimization of regularization level successfully captures the true underlying trend embedded in the training data when proper value of (σ=1.0) is selected for the Gaussian isotropic spread.

It is proved that maximum recommended skin temperature (tube wall temperature) for MDEA is 178 ˚C (350 F) and the temperature when MDEA degradation starts is advised as 182 ˚C (360 ˚F) (Reza et al., 2006; Chakma et al., 1997). However, lots of parameters can affect the degradation process and must be taken into account. Amine solutions are prematurely degraded by reaction with CO_2, oxygen, organic sulfur compounds, and other gas impurities to form heat-stable salts and amine degradation products. Most scientific literature agree that MDEA thermal degradation temperature starts at 127˚C (260 ˚F) in the presence of H_2S and CO_2. In other words, to achieve a reliable and steady operating system, it is recommended that the maximum amine temperature should be kept below127 ˚C (260 ˚F).

Both right 3D plots of Figures 11 indicate that the reboiler temperature essentially remains independent of MDEA concentration, especially for extremely low sulfolane concentrations. The previously found optimal solution containing 37 wt% sulfolane and 47 wt% MDEA still leads to rebolier temperature of around 129 ˚C which can cause excessive degradation of MDEA. To ensure more sustainable operation, the sulfinol solution of 37 wt% sulfolane and 45 wt% MDEA may be recommended.

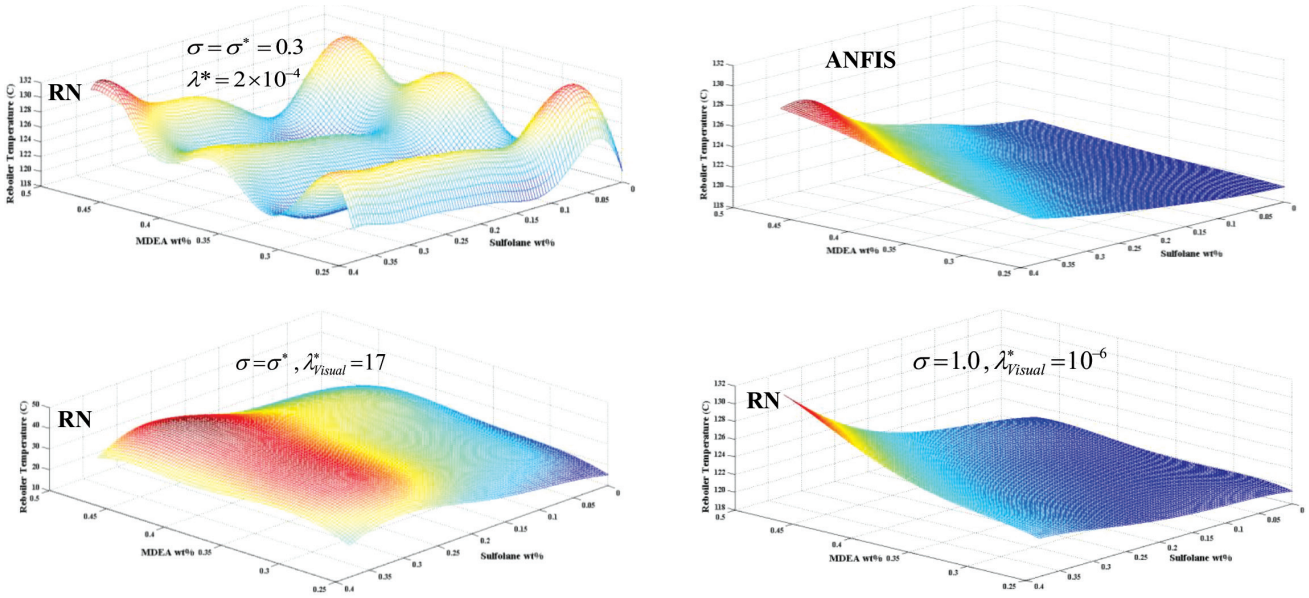

Figure 11.Generalization performances of reboiler temperature (0C) of regenerator column versus MDEA and sulfolane (wt%) variation in lean amine.

Figure 12 shows two nearly equal generalization performances of both networks for carbon dioxide mole fraction in sweet gas stream (mole%) leaving the contactor. Conventionally, the carbon dioxide content of the sweet gas entering the trunk line should be around 2-5 mole percent (Mokhatab et al., 2012; Kidnay et al., 2006). As it is anticipated, high concentrations of sulfolane will reject the carbon dioxide from acid gas stream and increase the mole fraction of CO_2 inside the sweetened gas stream. Therefore, the previously determined optimal concentrations of 37 wt% sulfolane and 45 wt% MDEA can lead to excessive CO_2 rejection rate. Fortunately, Figure 12 shows that the CO_2 mole fraction of the contactor overhead is around 4.5 mole% which is still well within the permissible range. Table 2 summarizes all simulation results including various escape factors and different constituents molar flow and compositions for several locations of the GTU process operating with optimal concentration of Sulfinol-M solution (37 wt% Sulfolane, 45 wt% MDEA).

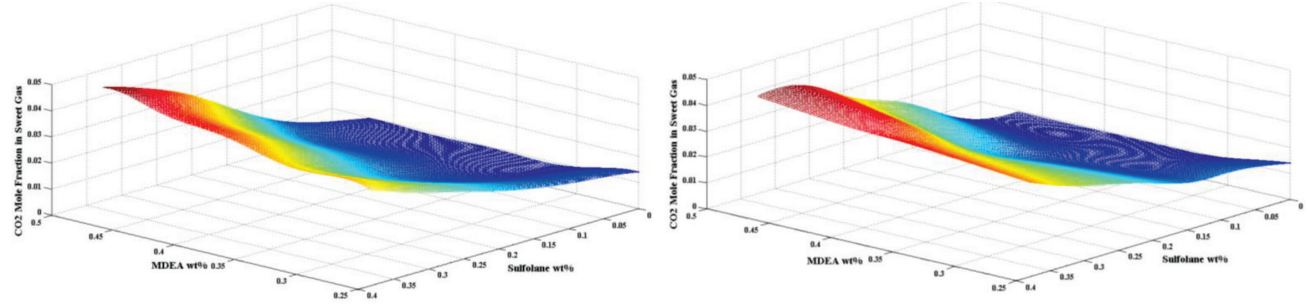

Figure 12 .Generalization performances of carbon dioxide mole fraction in sweet gas stream (mole%) versus MDEA and sulfolane (wt%)variation in lean amine (Left: RN, Right: ANFIS)

Table 2: Summery of simulation results at optimal concentration of Sulfinol-M solution. (37 wt% Sulfolane, 45 wt% MDEA)

Benzene Escape Factor	Toluene Escape Factor	Ethylbenzene Escape Factor	SRU Molar Flow	H_2S mole% in SRU feed	Reboiler Temp.	CO_2 mole% in sweet gas
%	%	%	kgmole/hr	%	^0C	mol%
20	0	0	415	57	129	4.5

Conclusion

Contaminants in the acid gas stream can seriously impact the operability and reliability of a sulfur plant. Therefore, designers must determine the most economical means of removing or destroying these contaminants so that they do not negatively affect the performance of the facility. Selective removal of H_2S in the presence of CO_2 and other impurities provides better-quality Claus process feed stream for attaining proper sulfur recovery efficiency.

Various mixtures of sulfolane and MDEA solutions (Sulfinol solvent) were used to simulate the conventional GTU process of Khangiran natural gas refinery via Aspen-HYSYS V.8.3 and their performances for the H_2S enrichment efficiency were evaluated. Optimized ANFIS network and its recall and generalization performances were compared with our previously developed in-house Regularization network and two other networks borrowed from conventional MATLAB neural network toolbox (ANFIS Editor and exact fit networks). It was clearly shown that two fully optimized ANFIS and RN networks provided more reliable interpolation hyper-surfaces for ten outputs in order to find optimal sulfolane concentration in the sulfinol-M solvent.

The outstanding generalization performance of the RN network is the result of its strong theoretical backbone due to the powerful multivariate regularization theory coupled with the efficient technique of leave one out cross validation (CV) criterion. Also, strong noise filtering capabilities of ANFIS network via minimization of error provide a distinguished performance. The optimal concentrations of 37 wt% sulfolane and 45 wt% MDEA were selected for the GTU process of Khangiran refinery which can successfully eliminate the entire toluene and ethylbenzene from the SRU feed stream while removing 80% of benzene entering the GTU process. The mole fraction of H_2S in the SRU feed stream also increased from 33.48 mole% to over 57mole% when using the optimal Sulfinol-M aqueous solution.

Acknowledgment

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Appendix A

A schematic structure of an ANFIS network which has five distinct layers is shown in Fig. 1.A. For simplicity, it is presumed that the fuzzy inference system has two inputs (x, y) and just one output (f). The following rules can be written for a first order Sugeno fuzzy model:

Rule 1: If x is A_1 and y is B_1, then $f_1 = p_1 x + q_1 y + r_1$

Rule 2: If x is A_2 and y is B_2, then $f_2 = p_2 x + q_2 y + r_2$

In the above rules: p_1, q_1, r_1 and p_2, q_2, r_2 are the consequent parameters. Also A_1, B_1, A_2, and B_2 are the linguistic labels. As shown in figure 1, fuzzy inference system consists of five distinct layers which are described below:

Layer 1 (or Fuzzification layer):

The fuzzy part of ANFIS is mathematically incorporated in the form of membership functions (MFs) to divide dimensions of each input. In most practical applications, Gaussian function presented in equation 1, because of minimum training and testing errors compared to the other shapes, was chosen as the best membership function ($\mu_{Ai}(x)$):

$$\mu_{Ai}(x) = \exp\left[-\left(\left(\frac{x-c_i}{a_i}\right)^2\right)^{b_i}\right] \qquad (1.A)$$

Where a_i, b_i and c_i are a constant (referred to premise parameters) that define the bell-shaped of membership function. Every node i in this layer is an adaptive node with a node function:

$O_{1,i} = \mu_{Ai}(x)$ for i = 1, 2 or

$O_{1,i} = \mu_{Bi-2}(x)$ for i = 3, 4 (2.A)

Generally, X (or y) is the input variable of node i and A_i (or B_{i-2}) is a linguistic label associated with this node. Therefore, $O_{1,i}$ is the membership grade of a fuzzy set (A_1,A_2,B_1,B_2).

Layer 2 (Rule layer):

Every node in this layer is a fixed node labeled as π and the output of nodes in this layer is the product of all the incoming signals:

$$O_{2,i} = w_i = \mu_{Ai}(x) \cdot \mu_{Bi}(y) \qquad i = 1, 2 \qquad (3.A)$$

Every node in this layer computes the multiplication of the input values and gives the product as the output. The membership values represented by $\mu_{Ai}(x)$ and $\mu_{Bi}(y)$ are multiplied in order to find the firing strength of a rule where the variables x and y have the linguistic values A_i and B_i, respectively.

Layer 3 (Normalization Layer):

Each node in this layer normalized the related firing strengths (w_i). The ratio of firing strength of each rule to the sum of all rules firing strength is calculated according to the following equation:

$$O_{3,i} = \overline{w}_i = \frac{w_i}{w_1 + w_2} \qquad i=1,2 \qquad (4.A)$$

where O_{3i} is the output of layer 3 and $\overline{w}_i$ is the normalized firing strength.

Layer 4 (Defuzzification Layer):

Every node in this layer is an adaptive node with a node function, indicating the contribution of each rule towards the overall output.

$$O_{4,i} = \overline{w}_i f_i = \overline{w}_i (p_i x + q_i y + r_i) \quad i=1, 2 \qquad (5.A)$$

Layer 5 (Output Layer):

The single node in this layer is a fixed node labeled sum, which computes the overall output as the summation of all incoming signals:

$$\text{Overall output} = O_{5,i} = \sum_i \overline{w}_i f_i = \frac{\sum_i w_i f_i}{\sum_i w_i} \quad i=1,2 \qquad (6.A)$$

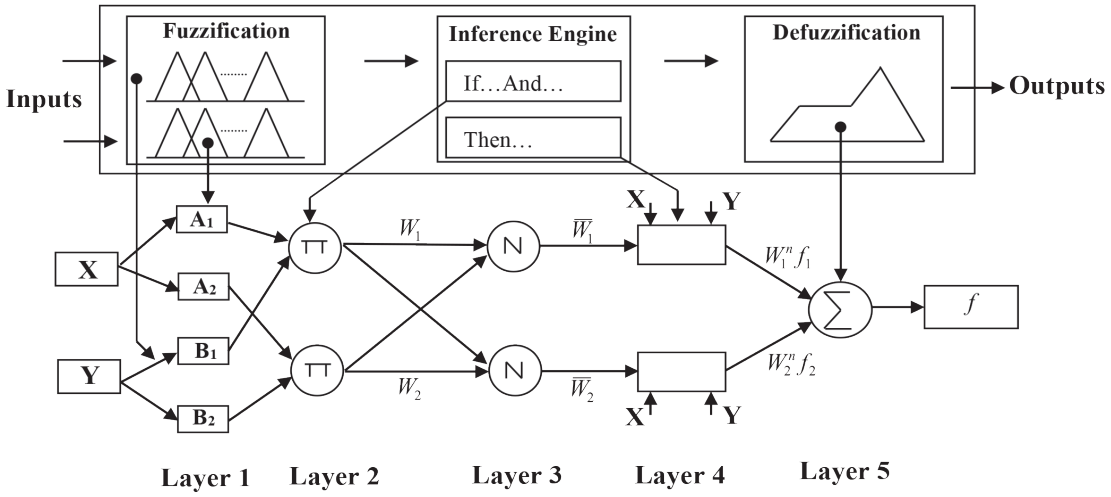

Figure 1.A ANFIS structure for a two-input Takagi-Sugeno model

Appendix B

Generally, Regularization refers to a process of introducing additional information in order to solve an ill-posed problem or to prevent over-fitting phenomena. This information is usually of the form of a penalty for complexity, such as restrictions for smoothness or bounds on the vector space norm. Many regularization techniques correspond to imposing certain prior distributions on model parameters.

Poggio and Girosi showed that regularization principles lead to approximation schemes which are equivalent to networks with one hidden layer which are called Regularization Networks (RN). In particular, they have described that a certain class of radial stabilizer (associated priors in the equivalent Bayesian formulation) lead to subclass of Regularization Network which is already known as a Radial Basis Function (Shahsavand et al., 2007).

Figure 1.B illustrates the equivalent network (known as the Regularization network (RN)) for the above equation with N being the number of both training exemplars and neurons of RN. These neurons (or centers) should be positioned exactly at the locations of training exemplars.

For a special choice of stabilizing operator, the Green's function reduces to the following multidimensional factorizable isotropic Gaussian basis function with infinite number of continuous derivatives (Shahsavand et al., 2005).

$$G(\underline{x},\underline{x}_j)=\exp\left[-\frac{\|\underline{x}-\underline{x}_j\|^2}{2\sigma_j^2}\right]=\prod_{k=1}^{p}\exp\left[-\frac{(x_k-x_{j,k})^2}{2\sigma_j^2}\right] \quad (1.B)$$

In the above equation, σ_j denotes the isotropic spread of the j^{th} Green's function and is assumed to be identical for all input dimensions. The network consists of a single hidden layer with N neurons and the activation function of the j^{th} hidden neuron is a Green's function $G(\underline{x},\underline{x}_j)$ centered at a particular data point $\underline{x}_j$. The influence of the regularization parameter λ is embedded in the unknown synaptic weights w_js. The performance of Regularization network strongly depends on the appropriate choice of the isotropic spread and the proper level of regularization. Small values of λ lead to oscillatory solutions due to fitting of the noise, while excessively large levels of regularization parameter will over-smooth the Regularization network predictions (Shahsavand et al., 2007). The leave one out cross validation technique (LOOCV) is frequently used for automatic selection of optimal ridge regression level. A detailed comparison of LOOCV with other techniques such as Generalized cross validation (GCV), L-curve, modified L-curve, U curve and modified U-curve method have been presented

in our recent article (Niknam Shahrak et al., 2013). The optimal value of ridge regression parameter is case dependent and as before, the LOOCV criterion (among many others) can be used to provide the best value of l for the problem at hand. Our fully optimized in-house training algorithm for the isotropic Regularization network has been discussed in sufficient detail elsewhere (Shahsavand et al., 2009).

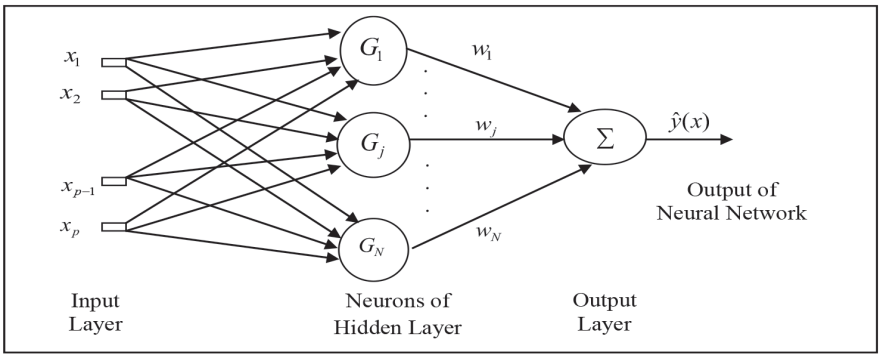

Figure 1.B. Schematic representation of Regularization network with single hidden layer

Appendix C

MDEA Conc.	Sulfolane Conc.	Benzene Escape Factor	Toluene Escape Factor	Ethylbenzene Escape Factor	SRU Molar Flow	H_2S mole% in SRU feed	Reboiler Temp.	CO_2 mole% in sweet gas
wt%	wt%	%	%	%	kgmole/hr	mol%	°C	mol%
0.47	0	59.5	98.8	100	729	0.35	120.9	0.009
0.47	0.1	89.5	99.9	100	687.5	0.36	121.9	0.0157
0.47	0.2	99.9	50.9	29.2	591.1	0.42	123.6	0.0292
0.47	0.3	54.1	26.8	13.4	481.8	0.52	126.7	0.0437
0.47	0.32	48.0	23.3	11.3	464.9	0.54	127.7	0.044
0.47	0.37	39.3	3.3	6.7	413.2	0.57	128.3	0.045
0.44	0	52.3	93.8	98.9	730.7	0.35	120.7	0.0093
0.44	0.1	77.7	99.9	100	697	0.36	121.6	0.0142
0.44	0.2	99.8	94.0	38.7	616.5	0.41	122.9	0.0257
0.44	0.3	64.6	32.8	17.2	507.1	0.50	125.4	0.0405
0.44	0.32	57.4	28.9	14.7	489.2	0.51	126.2	0.0429
0.4	0	44.1	82.5	88.6	730.7	0.35	120.3	0.0091
0.4	0.1	64.7	99.7	100	704.6	0.36	121.1	0.0129
0.4	0.2	96.0	99.5	81.1	640.1	0.39	122.2	0.0223
0.4	0.3	99.9	41.9	23.7	541.9	0.46	124.1	0.036
0.4	0.35	60.5	31.1	16.1	493.6	0.51	125.7	0.0424
0.35	0	35.8	68.4	70.7	728.2	0.35	120	0.0092
0.35	0.1	51.9	94.2	99.1	704.8	0.36	120.7	0.0124
0.35	0.2	77.7	99.8	98.9	654.2	0.38	121.6	0.0199
0.35	0.25	94.6	97.4	51.3	617.4	0.41	122.2	0.0253
0.35	0.3	99.8	60.5	33.8	574.8	0.44	123	0.0314
0.35	0.35	99.9	42.1	23.8	529	0.48	124	0.0377
0.35	0.38	88.7	35.5	19.0	503.5	0.50	124.9	0.0412
0.3	0	29.1	56.1	55.1	716.6	0.35	119.8	0.0101
0.3	0.1	41.7	80.0	86.4	693.1	0.36	120.3	0.0133
0.3	0.2	61.8	99.4	99.9	651.8	0.39	121.1	0.0196
0.3	0.3	93.6	83.8	46.0	589.3	0.43	122.1	0.0289
0.3	0.35	99.7	55.1	33.6	549.8	0.46	122.9	0.0345
0.3	0.38	99.9	46.7	27.5	528.2	0.48	123.5	0.0376
0.25	0	23.5	45.0	41.9	678.8	0.37	119.5	0.014
0.25	0.1	33.5	65.1	68.0	657.6	0.38	119.9	0.0174
0.25	0.2	49.4	91.9	98.4	626.2	0.40	120.6	0.0223
0.25	0.25	60.5	99.1	99.7	603	0.42	121.1	0.0259
0.25	0.3	75.1	95.5	60.5	579.7	0.43	121.5	0.0294
0.25	0.35	92.7	68.6	45.0	551.8	0.46	122.1	0.0336
0.25	0.38	98.7	58.7	37.6	533.2	0.47	122.5	0.0363

پیش بینی غلظت بهینه سولفینول در واحد تصفیه گاز پالایشگاه خانگیران از طریق سیستم استنتاج تطبیقی عصبی- فازی و شبکه رگولاریزاسیون

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چکیـــــــده

غلظت سولفید هیدروژن در گاز اسیدی ورودی به واحد بازیافت گوگرد از جمله پارامترهای مهم و تاثیرگذار می باشد که باید طراحان آن واحدها در هنگام تصمیم گیری برای انتخاب فرآیند یا ساختار درست جهت بدست آوردن بیشترین بازده بازیافت گوگرد در نظر داشته باشند. استفاده از حلال های ممانعت فضایی شده مانند آمین های نوع سوم ارتقاء یافته و همچنین ساختارهای متفاوت برای واحد تصفیه گاز، از جمله گزینه های مختلف برای غنی سازی گاز اسیدی (AGE) که به منظور کاهش غلظت دی اکسید کربن و هیدروکربن های آروماتیکی سنگین و افزایش غلظت سولفید هیدروژن در جریان خوراک ورودی به واحد بازیافت گوگرد انجام می گیرد، خواهد بود. در مقاله حاضر با استفاده از تلفیق نرم افزار اسپن-هایسیس و دو شبکه مجزا (به نام های شبکه رگولاریزاسیون و سیستم استنباط فازی- عصبی تطبیقی) نسبت به مقایسه توانایی غنی سازی گاز اسیدی حلال سولفینول-M (سولفولان+MDEA) در غلظت بهینه و حلال رایج MDEA، هنگامی که هر دوی آن ها به عنوان حلال واحد تصفیه گاز مورد استفاده قرار می گیرند، اقدام شده است. نتایج حاصل از شبیه سازی حاکی از آن بود که در غلظت بهینه حلال سولفینول-M (شامل ۳۷% وزنی سولفولان و ۴۵% وزنی MDEA) تمامی تولوئن و اتیل بنزن و همچنین ۸۰% از بنزن ورودی به واحد تصفیه گاز، از خوراک ورودی به واحد بازیافت گوگرد حذف خواهند شد. علاوه بر این، کسر مولی سولفید هیدروژن در خوراک ورودی به واحد بازیافت گوگرد از مقدار فعلی ۳۳/۴۸% به بالای ۵۷% افزایش پیدا خواهد کرد. افزایش انتخاب پذیری حلال سولفینول-M باعث افزایش کسر مولی دی اکسید کربن در جریان گاز شیرین به حدود ۴/۵% خواهد شد که کماکان زیر مقدار مجاز می باشد.

واژگان کلیدی: غنی سازی گاز اسیدی، بنزن- تولوئن-اتیل بنزن، شبکه رگولاریزاسیون، سیستم استنباط فازی- عصبی تطبیقی

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