Modelling and Optimization of Primary Steam Reformer System (Case Study : the Primary Reformer PT Petrokimia Gresik Indonesia)

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Abstract

Steam reforming of hydrocarbons has been in use as the principal process for the generation of hydrogen and synthesis gas needed in the Ammonia production in petrochemical industries. Optimal operation of existing steam reformers is crucial in view of the high energy consumption and large value addition involved in the process. The economic objective of the process is determined by the cost of gas (Methane), the cost of steam and additional fuel. An optimum steam to gas ratio is expected from an optimum process control. This can be applied on ratio control parameter for natural gas feed. In addition, steam Carbon Ratio is used to decrease coke formation in catalyst reformer. This paper presents the model identification and optimization of reforming control system of an industrial Primary Reformer at PT. Petrokimia Gresik (One of the fertilizer petrochemical industry in Indonesia). The reformer model has been approximated in the form of Takagi-Sugeno-Kang fuzzy inference system, with architecture in neural-network model. ANFIS (Adaptive Neuro-Fuzzy Inference System) has been utilized to determine NARX or ARX parameters model describing the dynamic of Industrial operational data have been used for training and validating the model. The optimization problem has been addressed through the utilization of Constrained Nonlinear Programming. The aim is to find the optimal process and ratio controller parameters to achieve the maximum Hydrogen formation. For a maximum fixed production rate of hydrogen produced by the unit, minimization of methane feed rate is chosen as the objective function to meet processing requirements.
Keywords: Hydrocarbons, Model identification, ANFIS

1 Introduction

Steam reforming of hydrocarbons has been in use as the principal process for the generation of hydrogen and synthesis gas needed in the Ammonia and Urea production in petrochemical industries. Today, natural gas is the most common feedstock for steam reforming. In Primary Reformer, natural gas (assumed to be pure methane in this study) is mixed with appropriate quantities of steam and recycle hydrogen before entering the reformer furnace. The main important catalytic reaction is taking place [1]:

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2, \Delta H_R(298) = -2.061 \times 10^5 \text{ kJ/mol} \quad (1)$$

The extent of the endothermic reforming reactions is controlled largely by the rate of heat transfer from the furnace to the catalyst pellets and reacting gases inside the reformer tubes. Optimal operation of existing steam reformers is crucial in view of the high energy consumption and large value addition involved in the process. The economic objective of the process is determined by the cost of gas (Methane), additional fuel and the cost of steam. An optimum steam to gas ratio is expected from an optimum process control. This can be applied on ratio control parameter for natural gas feed. In addition, steam carbon ratio is used to decrease coke formation in catalyst reformer.

This paper presents the model identification and optimization of reforming control system of an Industrial Primary Reformer at PT. Petrokimia Gresik. The reformer model has been approximated in the form of Takagi-Sugeno-Kang, input-output fuzzy inference system, with architecture in neural-network model [2]. ANFIS (Adaptive Neuro-Fuzzy Inference System) has been utilized to determine NARX [3] or ARX parameters model describing the dynamic of Industrial operational data have been used for train and validate the model.

The optimization problem has been addressed through the utilization of Constrained Nonlinear Programming [4]. The aim is to find the optimal process and ratio controller parameters to achieve the maximum hydrogen formation. For a maximum fixed production rate of hydrogen produced by the unit, minimization of methane feed rate is chosen as the objective function to meet processing requirements. The aim in this level is to find the optimal process and controller parameters to achieve the maximum hydrogen formation. If the strategy is infeasible, new set of parameters will be introduced to the outer level and iteration continues until a feasible control giving the highest hydrogen yields is obtained. For a fixed production rate of hydrogen produced by the unit, minimization of methane feed rate is chosen as the objective function to meet processing requirements, and heat integration.

The modelling scheme has been implemented as a real time control software developed using graphical-based programming language LabVIEW [5] and calculation of steam-gas optimal ratio using Matlab [6] and these are run on personal computer.

2 Neuro Fuzzy (ANFIS) based Modelling

Since all calculation is based on the process model, it is very important to have a reliable and efficient process model. Ideally, the process model should be derived from physical and chemical consideration. However, in many cases, this approach of modelling is not favourable as the lack of process knowledge contributes mostly to the difficulties. Therefore an empirical process modelling approach is used in many cases in which the plant dynamic can be inferred from the measured plant data directly. A parametric model for process identification is favourable to be used in industrial practice. Since most of the process models in industrial control show a strongly nonlinear behaviour, a popular Nonlinear Auto Regressive with eXogeneous Variable (NARX) parametric model form is widely used to represent nonlinear systems. In this model, the output is a nonlinear function of previous outputs and inputs of the systems [3], or

$$y(k) = F(y(k-1),\ldots,y(k-n),u(k-d-1),\ldots,u(k-d-n)) + e(k) \quad (2)$$

Here *y(k)* and *u(k)* are the sampled process output and input at time instant k respectively, e(t) is equation error, n denotes the order of the process, d represents the process dead time as an integer number of samples and F(.) is an unknown nonlinear function to be identified. However to be applied in simplify optimization, Linear ARX will be used and the equation is

$$y(k) = F(y(k-1), u(k-1)) + e(k) \quad (3)$$

Where the order n is zero, no deadtime d.

One of the methods to model nonlinear and linear process which is not simple task is neuro-fuzzy method. The main advantage of the neural network is its learning capability from numerical input-output data. However, neural network architecture is rather complicated and difficult to be understood by human. On the other hand, the fuzzy system describes a system with linguistics information which is human understandable, but the learning capabilities of fuzzy system is not as good as neural network. It is then natural to try to integrate the strength of both methodologies in order to achieve learning and adaptation capabilities and knowledge representation via fuzzy if-then rules, producing so-called neuro-fuzzy systems. Using neuro-fuzzy architecture, the fuzzy inference system can be tuned with a neural network algorithm based on some collection of input-output data, which then allow the fuzzy system to learn. An architecture of so-called adaptive neuro-fuzzy inference system/ANFIS [2] will be furthered explored and is described in Figure 1.

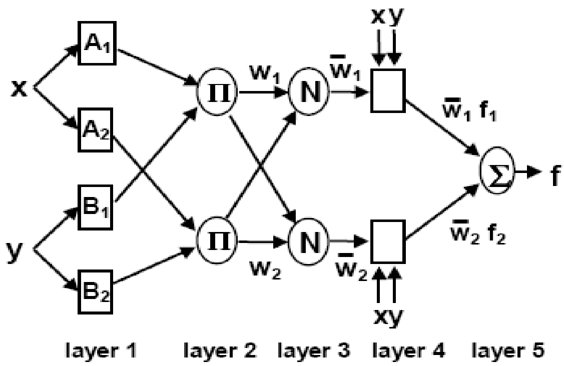

Figure 1 Adaptive neuro-fuzzy inference system architecture

The architecture employs an adaptive network, i.e. a network consists of some adaptive nodes which outputs depend on parameters pertaining to these nodes, and a learning rule, which describes how the above parameters should be change to minimize a prescribed error measure. The basic learning rules deals with how to recursively obtain a gradient vector in which each element is defined as the derivative of an error measures with respect to parameters. A solution called a hybrid learning rule which combines gradient method and the least square estimator is applied to avoid a slow convergence and possibility to be trapped to local minima as experienced by the conventional back-propagation learning rule.

A fuzzy inference system of Takagi-Sugeno of the first order which has two inputs and one output can be described by the following rule base

Rule i-th : If x is A_i and y is B_i Then $f_i = p_i x + q_i y + r_i$

$i = 1,2,\ldots,m$

Where m denotes the number of rules. Figure 1 describes a neuro-fuzzy structure which is equivalent to 2 rules. The architecture consists of 5 layers with different functions in every layer. The description and its function in every layer can be summarized as shown in Table 1 [2].

In the above structure, the adaptive network is manifested only by layer 1 and 4. The parameters in layer 1 and 4 are referred to as *premise parameters* and as *consequent parameters* respectively. In the 1st layer, the adaptive parameter is the parameter of the membership function of input fuzzy set, which is nonlinear function of the system output. The parameters in the 4th layer are the linear function of the system output, assuming that the parameter of the membership function is fixed. In general, the structure has nonlinear adaptive parameter in the 1st layer and linear adaptive parameter in the 4th layer. Due to the linear relationship with regard to the output parameters, then a least-square estimator (LSE) can be applied for the learning process. Suppose that S_1 is a set of nonlinear parameters and S_2 is a set of linear parameters in the architecture. The learning process applies the gradient descend and the least-square algorithm (Jang, *et.al.*, 1997) to update the parameters in S_1 and S_2 respectively.

Table 1 The description and its function in every layer

Layer	Description
1	Adaptive node with node function : $O_{1,i} = \mu_{A_i}(x)$ and $O_{1,i} = \mu_{B_i}(y)$
2	Fixed node with firing strength of a rule : $O_{2,i} = w_i = \mu_{A_i}(x)\mu_{B_i}(y)\,, i = 1{,}2$
3	Fixed node with normalized firing strength: $O_{3,i} = \overline{w}_i = \dfrac{w_i}{w_1 + w_2}\,, i = 1{,}2$
4	Adaptive node with node function : $O_{4,i} = \overline{w}_i f_i = \overline{w}_i(p_i x + q_i y + r_i)$
5	Fixed node which computes the summation of signals : $O_{5,i} = \overline{w}_1 f_1 + \overline{w}_2 f_2$

Note : parameters in layer 1 are referred to as *premise parameters* and parameters in layer 4 are referred to as *consequent parameters*

The Learning Process for the Linear Parameter:

If the parameters in S_1 figure 1 are fixed, then the output of the system can be written as

$$f = \overline{w}_1 f_1 + \overline{w}_2 f_2 = (\overline{w}_1 x)p_1 + (\overline{w}_1 y)q_1 + (\overline{w}_1)r_1 + (\overline{w}_1 x)p_1 + (\overline{w}_1 y)q_1 + (\overline{w}_1)r_1 \quad (4)$$

From the above equation, it can be seen that the consequent parameters are linear parameters with respect to the systems output. If P learning data is applied to the equation (1), it can be shown that it can be represented by $A\theta = y$, where θ is an unknown vector whose elements are parameters in S_2 and y is the output vector whose elements are P learning data. Using the Least-square estimator, the best solution of this equation will be given by

$$\theta_{i+1} = \theta_i + P_{i+1}\alpha_{i+1}\left(y_{i+1}^T - \alpha_{i+1}^T \theta_i\right) \quad (5.a)$$

$$P_{i+1} = P_i - \frac{P_i \alpha_{i+1} \alpha_{i+1}^T P_i}{1 + \alpha_{i+1}^T P_i \alpha_{i+1}} \quad (5.b)$$

with α_i^T is row vector of matrix A , y_i is the i-th eleventh of y, and P_i is the covariance matrix.

The learning process employs the simple steepest descent method, where each parameters are updated using the relation $\alpha_{next} = \alpha_{now} - \eta\,(\partial^+ E / \partial\alpha)$,causing $E(\alpha_{next}) < E(\alpha_{now})$, where α is the node parameter and η is the learning constant and $\partial^+ E / \partial\alpha$ denotes the ordered derivative of the error signals $E(\theta) = (y_d - y)^2$ (i.e. the difference between an actual trajectory and a given desired trajectory) with respect to the node parameter α .

3 Neuro Fuzzy (ANFIS) Based Modelling

To quantify the "best solution", first we need an *objective function* that serves as a quantitative indicator of "goodness" for a particular solution. Objective in this case is minimization the output of methane gas to produce highest hydrogen. The values of the objective function are determined by manipulation of the *problem variables*. These variables can physically represent operating conditions (e.g. pressure, temperature, and flowrate). Finally, the limit of process operation, validity of model, and relationship among the problem variables need to be considered as constraints in the process. [4]

In many cases, the task of finding an improved flowsheet through manipulation of the decision variables is carried out by trial and error. Instead, with optimization methods we are interested in a *systematic* approach to find the best flowsheet and this approach must be as efficient as possible. Related areas that describe the theory and concepts of optimization is called as *mathematical programming*, and a large body of research is associated with this areas. Optimization problems that have nonlinear objective and/or constraints functions of the problem variables are referred to as *nonlinear programs*, and analysis and solution of this optimization problem is referred to as *nonlinear programming (NLP)*.

We consider the constrained nonlinear programming problem for optimization (Bazaraa and Shetty, 1979; Minoux, 1986), given in general form as :

$$\begin{aligned} &Min \quad z = f(x) \\ &Subject\ to \quad h(x) = 0 \\ &\qquad\qquad\qquad g(x) \le 0 \\ &\qquad\qquad\qquad x \in R^n \end{aligned} \tag{6}$$

Where $z = f(x)$ is objective function , $h(x) = 0$ is the set of m equations in n variables x, and $g(x) \le 0$ is the set of equations m, and the difference (n-m) is commonly denoted as the number of degree of freedom of the optimization problem. Any optimization problem can be represented in the above form. For example, if we want to maximize a function, this is equivalent to minimizing the negative of that function. Also, if we have inequalities that are greater or equal to zero, we can reformulate them as inequalities that are less or equal than zero multiplying the two terms of the inequality by -1, and reversing the sign of the inequality.

The solution of the NLP problem (3),satisfies the following first order Kuhn Tucker conditions. These conditions are necessary for optimality :

1. Linear Dependence of Gradients :

$$\nabla f(x)+\sum_{j=1}^{m}\lambda_j \nabla h_j(x)+\sum_{j=1}^{r}\mu_j \nabla g_j(x)=0 \quad (7.1)$$

2. Constraint Feasibility

$$h_j(x)=0 \;\; j=1,2,\ldots,m \quad g_j(x)\le 0 \;\; j=1,2,\ldots,r \quad (7.2)$$

3. Complementarity Conditions

$$\mu_j g_j(x) \;\; \mu_j \ge 0 \;\; j=1,2,\ldots,r \quad (7.3)$$

where μ_j are the Kuhn Tucker multipliers corresponding to the inequalities, which are restricted to be non-negative, and these are given by $\mu_j = -\left(\frac{\partial f}{\partial g_j}\right)_{\partial g_i = 0, i \neq j}$

4 Primary Reformer Modelling

Steam reforming of hydrocarbons has been used as the principal process for generation of hydrogens and synthesis of gases needed in the Ammonia and Urea production. In Primary Reformer, natural gas (assumed to be pure methane in this study) is mixed with appropriate quantity of steam and recycled hydrogen before entering the reformer furnace. The following important catalytic reaction is taking place :

$$CH_4 + H_2O \Leftrightarrow CO + 3H_2,\ \Delta H_R(298) = -2.061 \times 10^5 \text{ kJ/mol} \quad (8)$$

Optimal operation of existing steam reformer is crucial from the point of view of high energy consumption and large value addition involved in the process. The economic objective of the process is determined by the cost of gas (Methane), additional fuel and the cost of steam. An optimum steam to gas ratio is expected from an optimum process control. This ratio will be applied on ratio control parameter for natural gas feed.

Ratio control is used to ensure that steam and gas flows are kept at the same optimum ratio even if the flows are changing. The optimum steam to gas ratio for Primary Reformer must be obtained before being used in ratio control parameter. Figure 2. is the Process Diagram before Ratio control is applied.

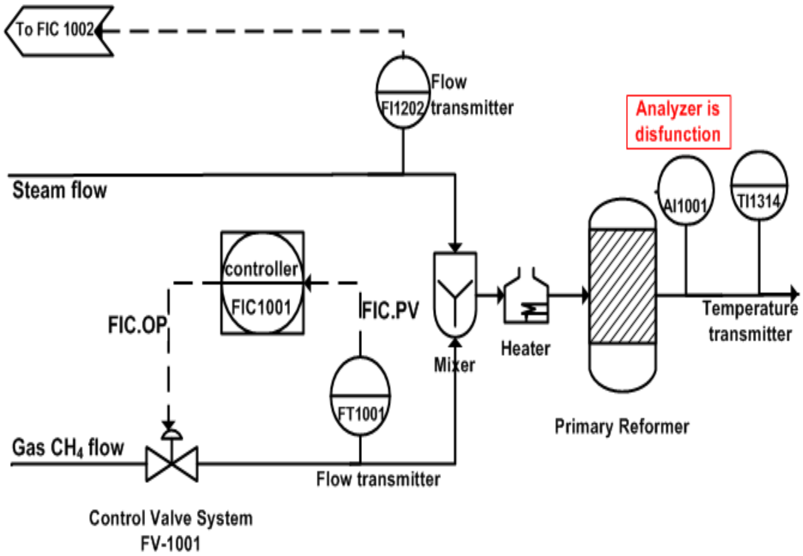

Figure 2 Process diagram before ratio control applied

The first step to get process optimization in design ratio control is modelling process Primary Reformer by identification. The first process model is represented in a NARX model form a state in equation (2). For the first order process without time delay *(d=0)*, this model become $y(k) = F(y(k-1), u(k-1)) + e(k)$, same as equation (3). The configuration of neuro-fuzzy system being used in this investigation is as follows:

Sistem Fuzzy = TSK orde 1

1. Number of *epoch* = 10
2. Inputs : $x_1(k\text{-}1), x_2(k\text{-}1), y(k\text{-}1)$
3. Output : $y(k)$
4. Step size = 0,01

Number of rules : 6

With number of data training = 13 48 and number of data validation = 1400.

After 10 epochs in learning step, the premis and consequent parameters :

Table 2 ANFIS parameters

Parameter premis		
0.265	-2.48	1.006
0.242	2.453	1.006
1.003	0.989	1
0.534	2.005	1.016
1	0.999	1
1	1.001	1

Parameter konsekuen			
1.021	0.287	0.866	6.81
-1.03	-0.83	1.137	6.587
0.105	-0.34	1.035	5.841
-0.07	-0.24	0.964	5.645
0.059	-0.08	1.029	7.135
-0.06	-0.03	0.954	6.887
0.047	-1.01	0.928	2.293
0.071	-0.92	1.123	2.241

These parameter is used for validation with different amounts of data. The results is shown in Figure 3.

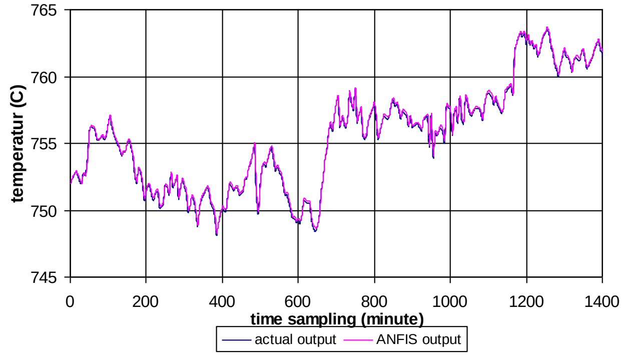

Figure 3 Actual model output and ANFIS model

And the RMSE in validation with 1400 data is 0,234 which error is shown in Figure 4.

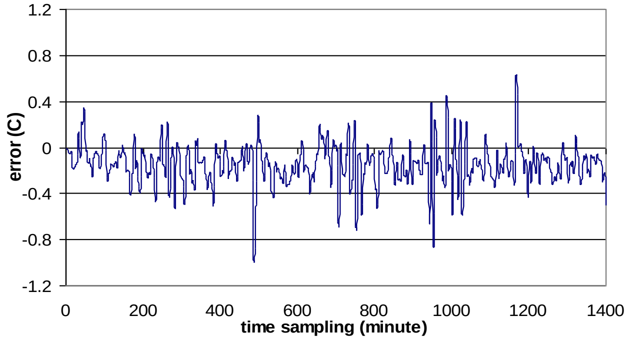

Figure 4 ANFIS error estimation

Because the graphics above and RMSE show a good performance of this modelling, now we can use this parameters for nonlinear model.

To get one of optimization function, we need parameters of a linear ARX model for simplicity. These parameters obtained in ANFIS method from layer 4. this equation in 10 epochs :

$$y(k) = 0{,}0155054\, x_1(k-1) - 0{,}262617\, x_2(k-1) + 0{,}998566\, y(k-1) + 6{,}69952 \quad \{9)$$

5 Ratio Optimization

To quantify the "best solution" we first need an *objective function* that serves as a quantitative indicator of "goodness" for a particular solution. Objective in this case is minimization the output of methane gas to produce highest hydrogen. Because the analyzer to measure composition of methane is not functioning, there is no relationship between composition of methane (CH_4) and steam to gas ratio. Because of that, it must be obtained the relationships between composition of gas (CH_4) output and temperature which is temperature as a function of steam and gas flow.

The relationships between %output CH_4 is derived from kinetics model of reactor (in this case : Reformer) :

$$\begin{aligned} \frac{dc_A}{dt} &= \frac{Fi}{V\rho}(c_{Ai} - c_A) - k_0 e^{-E/RT} c_A \\ \frac{dT}{dt} &= \frac{Fi}{V\rho}(Ti - T) + Jk_o e^{-E/RT} c_A - \frac{Q}{\rho c_p V} \end{aligned} \tag{10}$$

Where $J = (-\Delta H_r)/\rho c_p$, J is heat capacity, Q is heat energy, V is volume (m^3), c_A is normalized output composition of CH_4 (%), c_{Ai} is normalized output composition of CH_4 (%), T_i = Temperatur inlet *Primary Reformer* (Kelvin), T = temperatur outlet *Primary reformer* dan F adalah massa flow (kg/s).

Data which is obtained from the plant:

T_i - To = 352 ^{o}C - 759 ^{o}C = - 407

F_i = total flow input of *Primary Reformer* = *steam* flow + gas flow= 85+26 =111 T/hr= 30,833 kg/s

Because ρ, V, k_o, J, Q are unknown, so the relationship between %CH_4 and temperature is derived by available process data. So the composition of %CH_4 is

$$\%CH_4 = \frac{4{,}6996}{30{,}833 - 24{,}1145 e^{\frac{243{,}3078}{(T+273)}}} \tag{11}$$

The equation (11) is objective function of optimization. After that, state function (equality constraint) of $h(x) = 0$ will be defined. In this case is *steady state* model of input-output of *Primary Reformer*. This model is obtained from ARX-ANFIS 1st order. Because model is must be in steady state condition, so it is assumed that $y(k) = y(k-1)$ and also $x(k) = x(k-1)$, so the equation is become to

$$0 = 0{,}0155054\,x_1 - 0{,}262617\,x_1 + (0{,}998566 - 1)y + 6{,}69952 \quad (12)$$

where x_1 is *steam* flow, x_2 is gas flow and y is temperature .

And from the operational conditions, it is known that inequality constraints for x1, x2 and y are :

$80 \le x1 \le 90$

$20 \le x2 \le 30$

$745 \le y \le 775$

After optimization problem is defined, so optimize *nonlinear programming with constrains* method to get the value of CH_4 optimal composition, temperature, *steam* flow and gas, and *steam*-gas ratio. Optimization results can be seen in Figure 5 with using optimization function *fmincon* in Matlab [19].

```
reformer flow ratio optimization

                              max                  Directional   First-order
 Iter F-count        f(x)   constraint    Step-size   derivative   optimality Procedure
    0      4      14.9655      0.08414                                         Infeasible start point
    1      9      14.8569   1.327e-010            1       -0.108       0.328
    2     14      14.6455   1.678e-011            1       -0.208       0.326
    3     19       11.277    3.32e-010            1        -2.56      0.0718
    4     24       11.277   1.776e-015            1   -3.68e-009    3.99e-011
Optimization terminated: first-order optimality measure less
 than options.TolFun and maximum constraint violation is less
 than options.TolCon.
Active inequalities (to within options.TolCon = 1e-006):
  lower      upper     ineqlin   ineqnonlin
                                      3


xol =

  775.0000
   86.7237
   26.3991



olf =

   11.2770

    T reformer = 775.000, u1 = 86.724, u2 = 26.399, Objective function = 11.277
>> r = 86.724/26.399

r =

    3.2851
```

Figure 5 Iteration of *nonlinear programming* method in *Matlab*

From this iteration, it is resulted that value of optimal ratio is 3,2851 with *steam* flow = 86,724 T/hr, gas = 26,399 T/hr and tempeature is 775 °C that gives minimum objective % CH_4 output is 11,277%.

To validate the value above from Iteration of *Nonlinear Programming* method, it would shown by graphic in Figure 6 and 7 which are obtained from equation of objective function and steady state equation.

From the objective function in Figure 6 shows that higher temperature produce smaller composition of CH_4 which is resulted. It is because *Primary Reformer* has an endothermic reaction that need heat energy. This case, composition is limited by the maximum temperature in 775°C. Objective function in this graphic in temperature 775°C is 11,28 because of the resolution, the value in iteration is 11,277. It is almost same value.

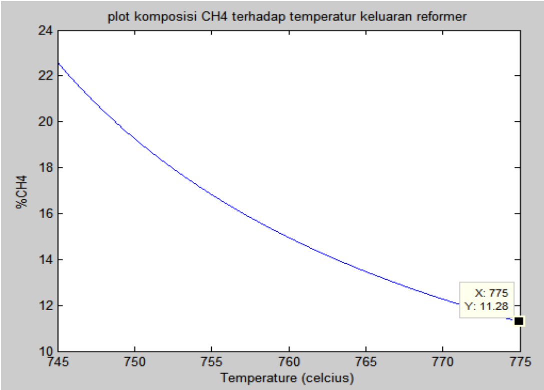

Figure 6 Objective function graphic (% CH_4 vs temperature)

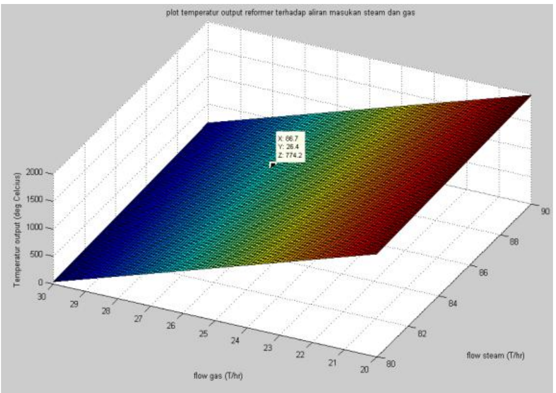

Figure 7 Steady state equation model *primary reformer*

Figure 7 is used to illustrate the relationships between steam flow, gas and temperature. To compare ratio that is obtained in iteration method, it can be seen in *steam* and gas flow in temperature is 775 °C. From the graphic above, the value of *steam* flow is 86,7 T/hr and gas flow is 26.4 T/hr because of the resolution limited. The value in iteration is 86.724 T/hr and gas is 26.399 T/hr .In the graphic can be seen that temperature is 774,2 °C. The value of iteration is almost same with the graphic and it proves the valid method. So, the optimal steam-gas ratio can be applied as ratio controller is 3.2851.

6 Conclusions

An adaptive neuro-fuzzy inference system (ANFIS) method can be used to identify NARX and ARX models. Validation in this model is get with the RMSE is 0.234 and the estimate output can reach the actual output with small error. This ARX model is used to get an optimal product of Hydrogen by getting the optimal value of steam-gas ratio. With constrained nonlinear programming method, the optimal ratio is obtained. The value is 3.2851. This ratio is used to as ratio control parameter in flow input of Primary Steam Reformer.

7 References

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