CHAPTER V

PARAMETER AND STATE ESTIMATION

Process control by model predictive, controller calculates proper manipulated variable data set by using process model in which composed of measurable and unmeasurable variables. The unmeasured variable can be estimated from some measured variables e.g. effluent sulphur content from the reactor. In order to control suphur content remain from the reactor, there is a need to estimate. Jutan and Uppal (1984) used Newton Rophson filter to estimate the heat release from an exothermic batch reactor. Cott and Macchato (1989) used exponential filter. Later, Kershenbaum and Kittisupakorn (1994) used extended Kalman filter. In this thesis, will be using Kalman filter.

5.1 Parameter Estimation by Kalman Algorithm

Kalman filter parameter estimation was proposed by R. E. Kalman (1960), Kalman and Bucy (1961) which explain discrete linear filter by using least square method and minimum variance method. In the book of Astrom and Wintenmak (1990) and the research of Ricker (1990) had mentioned about continuous linear Kalman filter algorithm from linear state space model. Kalman filter technique estimates a variable by using process model to find a matrix gain for estimating a variable closes to real measured value by using minimum variance estimation technique. The used variance is a covariance function between process model estimation variable and uncertainty process model estimation variable. The state covariance constant, Q, and measured variable covariance, R, has to be defined as constants. We called this observer that steady state Kalman filter.

5.1.1 Estimation Technique

The estimation is based on the process model which model could be constructed by plant test data. This is method called plant identification. Another method, model could be constructed by deriving principle model. The equations could be both linear or nonlinear. In this thesis, the equations will be written in state space form as:

$$\begin{aligned} \hat{x}_{k+1} &= G\hat{x}_k + Hu_k \\ \hat{y}_k &= C\hat{x}_k \end{aligned} \tag{5.1}$$

The new state value will be compared with real measured value y by least square method. The difference between the square of the state estimation error and the square of the measurement estimation error will be combined and written in a performace index form. The relation of both error is as below:

$$S = (\hat{x}_{k+1} - \hat{x}_0)^T a(\hat{x}_{k+1} - \hat{x}_0) + (\hat{y} - \hat{y}_k)^T b(\hat{y} - \hat{y}_k) \tag{5.2}$$

where a, b estimation constant

$\hat{x}_0$ estimated state variable

Take differentiation and made it equal to zero, we got $\hat{x}_{k+1}$ which gave minimum S. Therefore, the estimation equation can be written in the form:

$$\hat{x}_{k+1} = \hat{x}_k + K(y - C\hat{x}_k) \tag{5.3}$$

where K estimation gain

In order to be able to estimate the unmeasured variable, the estimation error could be from process uncertainty. As a result estimation could not be correct. The minimum variance method was introduced to help in estimation by using uncertainty equation (Stochastic) of the process. The equations can be written as below:

$$\begin{aligned} \hat{x}_{k+1} &= G\hat{x}_k + Hu_k + v_k \\ \hat{y}_k &= C\hat{x}_k + w_k \end{aligned} \qquad (5.4)$$

When compare the state variable from process model in equation (5.1) and process uncertainty equation in equation (5.4), we got:

$$(x_{k+1} - \hat{x}_{k+1}) = G(x_k - \hat{x}_k) + KC(x_k - \hat{x}_k) - Kw_k + v_k \qquad (5.5)$$

In order to make sure that the difference of the estimation and the true value has lower variance, Kalman (1960) had used covarience function of process model parameter estimation which had uncertainty and process model in equation (5.1) $\left(P_k = E[(x_k - \hat{x}_k)(x_k - \hat{x}_k)]^T\right)$ to find proper gain. This gain was adjusted every estimation cycle for varience reduction.

From using covarience function to solve the equation for finding varience matrix of state parameter $x_{k+1} - \hat{x}_{k+1}$, matrix P is used for adjusting the gap of both process parameter estimation uncertianty and process model parameter uncertianty. In this thesis, we use Ricatti's equation for finding proper P in order to find Kalman matrix gain K as follow:

$$P_{k+1} = Q + GP_kG - GPC^T\left(R + CPC^T\right)^{-1}CPG^T \qquad (5.6)$$

$$K = GP_kC^T\left(R + CP_kC^T\right)^{-1} \qquad (5.7)$$

where $P_k = E\{\tilde{x}_k\tilde{x}_k^T\}$, $Q_k = E\{v_k v_k^T\}$, $R = E\{w_k w_k^T\}$, $E\{v_k\} = 0$, $E\{w_k\} = 0$

$R + CP_kC^T > 0 \qquad P_k > 0$

In order to be able to estimate the parameter could be obtained only if the relation between the measurable and unmeasurable variables have observability.

5.1.2 Kalman Algorithm

For this study, Kalman filter algorithm can be written in steps for decreasing covariance in order to be able to calculate a gain matrix and estimate the state variable for feeding to the control system as follow:

1) Measure the control variable at previous cycle.

2) Calculate constant matrix G and H of the process at the estimating time.

3) Calculate state variable at current time from state model

4) Measure the measurable variables y

5) Use constant matrix G and C to calculate covarience matrix P_k from Richatti's equation until matrix P_k equal to a constant.

$$P_{k+1} = Q + GP_kG - GPC^T\left(R + CPC^T\right)^{-1}CPG^T$$

6) Use the calculated matrix P_k to calculate estimation gain matrix as follow:

$$K = GP_kC^T\left(R + CP_kC^T\right)^{-1}$$

7) Calculate state variable of the process at current time.

$$\hat{x}_{k+1} = \hat{x}_k + K\left(y - C\hat{x}_k\right)$$

8) Use the calculated state variable for feeding to the control system for calculating the manipulated variable data set and repeat step 1) again.

5.2 Sulphur Content in Product Prediction with Lab Update

As the on-line sulphur analyzer is not available and the model is derived based on the assumption that the feed content has no other compound beside sulphur. Furthermore, the heat released was calculated based on sulphur reaction only. In fact, the process has other parameters and reactions. To be able to have correct sulphur content prediction, the model needs to be updated periodically from time to time by a known sulphur content in product value from the laboratory. A smart method for updating the model is using Kalman filter.

From the rate of sulphur content change from eqaution 4.9 in Chapter IV, if we write a steady state model (for lab update, we are interested only at steady state), we rewrite the equation 4.9 as:

$$0 = \frac{WHSV}{\rho}\left(S_f - S_p\right) - \alpha k_0 e^{-E/R \cdot WABT} S_p^{\,2} \qquad (5.8)$$

In order to make the calculation easier, we will simplify the rate of reaction as:

$$r_S = C \cdot WABT \cdot S_p \qquad (5.9)$$

Therefore the eqaution 5.8 can be written as:

$$S_p = \frac{WHSV}{\rho} S_f \left(\frac{1}{\frac{WHSV}{\rho} + C \cdot WABT} \right) \qquad (5.10)$$

We can see that sulphur content in product at steady state is a function of 3 indepent measurable variables i.e. space velocity $\left(\frac{W}{V_r}\right)$, sulphur content in feed (S_f), weight average bed temperature $\left(\frac{1}{3}T_{ri}+\frac{2}{3}T_{ro}\right)$.

$$S_p = f(WHSV, S_f, WABT) \quad (5.11)$$

To simplify the form for being applied Kalman filter lap update mechanism, we linearised the equation 5.10 around a steady state condition. The steady state sulphur estimation can be written in the form below:

$$S_p = a_1 \cdot WHSV + a_2 \cdot S_f + a_3 \cdot WABT + b \quad (5.12)$$

where a_1, a_2, a_3, b are steady state constants

In this thesis, it is assumed that the rate of feed intake and properties are constants. The sulphur content in product only relates to the reaction temperature which is WABT. Therefore the simple model can be written in the form:

$$S_p = a \cdot WABT + b \quad (5.13)$$

where $$WABT = \frac{1}{3}T_{ri} + \frac{2}{3}T_{ro} \quad (5.14)$$

$a =$ coefficient of WABT

$b =$ bias

In order to find the model, data of WABT and sulphur content in product were generated from the model in Chapter 4. By using simple regression technique. We got the initial model as:

$$S_p = -0.00072639 \cdot WABT + 0.308085 \quad (5.15)$$

To be able to find coefficient a and bias b when there is a lab result available in real time, Kalman filter is used to minimize the varience due to lab result uncertainty. The state model can be written as:

$$\begin{bmatrix} a_{k+1} \\ b_{k+1} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} a_k \\ b_k \end{bmatrix} \quad (5.16)$$

$$[Sp_k] = [WABT \quad 1] \cdot \begin{bmatrix} a_k \\ b_k \end{bmatrix} \quad (5.17)$$

Where $WABT$ is the known value at lab sampling time.

5.3 Kalman Filter for State Variable Estimation

Because the measured variable either from reactor temperatures or sulphur content in prodcut prediction which was defined as item 5.2, the measurement need to be estimated their state for noise rejection before sending to any controllers. For this thesis, we will simplify the model for being able to be fast calculation. Some assumption is made as below:

1) Heat distribution is uniform in within reactor.

2) Constant specific heat

3) Sulphur content is related to 2 temperature parameters i.e. T_{ri} and T_{ro}.

$$r_S = C\left(\frac{1}{3}T_{ri} + \frac{2}{3}T_{ro}\right)$$

4) Measured parameters are true values.

For ease of Kalman filter calculation, we assume the rate of sulphur content change as:

$$\frac{dS_p}{dt} = C\left(\frac{1}{3}T_{ri} + \frac{2}{3}T_{ro}\right) \qquad (5.18)$$

where $C = 0.000122449$

From the relation above, the state space model can be written for Kalman filter algorithm as below:

or
$$\begin{bmatrix} \dot{T}_{ri} \\ \dot{T}_{ro} \\ \dot{S}_p \end{bmatrix}_{3\times1} = [A]_{3\times3} \begin{bmatrix} T_{ri} \\ T_{ro} \\ S_p \end{bmatrix}_{3\times1} + [B]_{3\times1} [T_{risp}]_{1\times1} \qquad (5.19)$$

where

$$[A]_{3\times3} = \begin{bmatrix} a_{11} & 0 & 0 \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & 0 \end{bmatrix}_{3\times3}$$

$$a_{11} = -\frac{1}{\rho V_{tube}}$$

$$a_{21} = \frac{W}{\rho V_r} - \frac{\Delta H \alpha k_0}{\rho V_r C_p} e^{-E / R\left(\frac{1}{3}T_{ri} + \frac{2}{3}T_{ro} + 273.15\right)} \cdot \frac{E}{R} \cdot \left(\frac{1}{3}T_{ri} + \frac{2}{3}T_{ro} + 273.15\right)^{-2} \cdot \frac{1}{3} S_p^2$$

$$a_{22} = \frac{W}{\rho V_r} - \frac{\Delta H \alpha k_0}{\rho V_r C_p} e^{-E / R\left(\frac{1}{3}T_{ri} + \frac{2}{3}T_{ro} + 273.15\right)} \cdot \frac{E}{R} \cdot \left(\frac{1}{3}T_{ri} + \frac{2}{3}T_{ro} + 273.15\right)^{-2} \cdot \frac{2}{3} S_p^2$$

$$a_{23} = -\Delta H \alpha k_0 e^{-E / R\left(\frac{1}{3}T_{ri} + \frac{2}{3}T_{ro} + 273.15\right)} \cdot 2S_p$$

$$a_{31} = \frac{1}{3} C$$

$$a_{32} = \frac{2}{3} C$$

$$[B]_{3\times 2} = \begin{bmatrix} \dfrac{W}{\rho V_{tube}} \\ 0 \\ 0 \\ \end{bmatrix}_{3\times 1}$$

$$[C]_{4\times 1} = [1 \quad 1 \quad 1]_{1\times 3}$$