Theoritical Models and Parameter Estimation

Keywords: Theoretical Models, Lumped Parameter, Parameter Estimation

Procedure for theoretical Process model development

Stage 1: Problem definition

There are several factor that made it very important to have defined very clearly the scope of the problem we wish to solve.

It is impossible to represent all aspects of physical process, we can only hope to capture those aspects that are most relevant to the problem at hard.

the behavior of a dynamic process can be interpreted mathematically in several different ways, the various phenonmenon explained to varying degrees of detail. The result is that several different madels are possible for any given process but from various angles and to varying degrees of complexity

a process model is as useful as the tool available for obtaining solutions to its equation.

As a result before development of a mathematical model for a physical process several questions come in to mind

- What do we intend to use the model for?
- How simple or complex will the model have to be?
- what aspects of the process do we consider the most relevant and therefore should be continued in such a process model?
- to what extent are the fundamental principles underlying the operation of this aspect of the process known?
- how can we test the adequous of the model?
- how much time do we have for model estimation?

The answer of these questions will enable us to decide whether to use the theoretical approach as the alternative approach.

Stage 2: Model formulation

Model formulation is done based on the physics of the problem it involved basic laws of conservation of mass, energy and momentum.

Stage 3: Parameter estimation

In developing a model for a physical process (whether by theoretical or empirical means) certain parameters appear whose values must be specified before the model can be used to predict process behavior. For example the theoretical model obtained for the non iso thermal CSTR

$$\frac{dC_A}{dt} = -\frac{1}{\theta}C_A - k_0 e^{-E/RT} C_A + \frac{1}{\theta}C_{Af} \quad 4.1$$

$$\frac{dT}{dt} = -\frac{1}{\theta}T + \beta\, k_0 e^{-E/RT} C_A + \frac{1}{\theta}T_f - x \quad 4.2$$

contains the following parameters

$$\theta = the\ reactor\ residence\ time$$

$$k = k_0 e^{-E/RT}$$

$$\beta = \frac{-\Delta H}{\rho C_p}$$

Step 4: Model Validation.

The model developed based on theoretical or regression analysis is validated against the experimental data or existing model in the literature.

PARAMETER ESTIMATION IN MODELS

Lumped Parameter Systems

In the lumped parameter systems, variables are essentially uniform throughout the entire system. The stirred heating tank system and the non-isothermal CSTR are typical examples. Consider the non-isothermal CSTR in which the exothermic reaction A→B is taking place

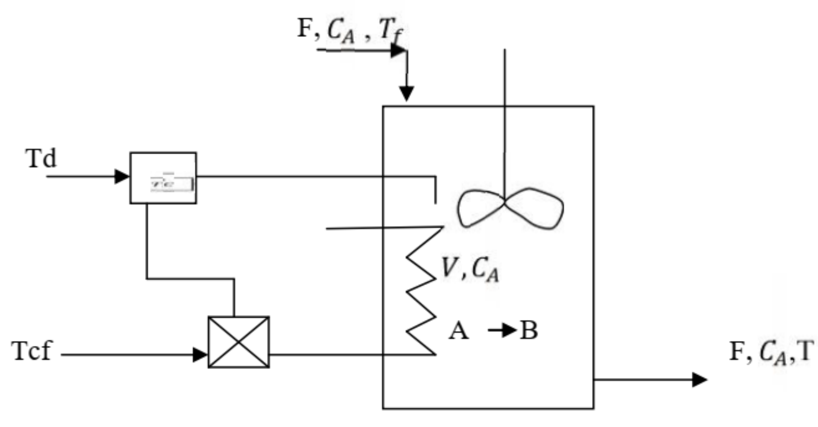

Fig. 4.1: Non-isothermal CSTR

Component mass balance on A

Rate of accumulation of a within the reactor = $\frac{dVC_A}{dt}$

Rate of A input to the reactor = FC_{Af}

Rate of A output from the reactor = FC_A

Rate of consumption of A by chemical reaction = kVC_A

$$\frac{dVC_A}{dt} = FC_{Af} - FC_A - kVC_A \quad 4.1$$

Assuming constant reactor volume and solving we have,

$$\frac{dC_A}{dt} = -\left(k + \frac{1}{\theta}\right)C_A + \frac{1}{\theta}C_{Af} \quad 4.2$$

Energy Balance:

Rate of energy accumulation in the reactor = $\frac{d\{\rho VC_p(T-T^*)\}}{dt}$

Rate of energy input to the reactor = $F\rho C_p(T_f - T^*)$

Rate of Heat Transfer to the coil =Q_C

Rate of heat generation by chemical reaction = $(-\Delta H)kVC_A$

Assumptions; $\rho, C_p$of the reacting material to be const., $T^*$is the reference temperature, $-\Delta H$is the heat of reaction with the convention that it is positive for exothermic reaction and negative for endothermic reaction.

Thus the energy balance equation becomes,

$$\rho VC_p\frac{d\{(T-T^*)\}}{dt} = \rho FC_p(T_f - T^*) - \rho FC_p(T - T^*) + (-\Delta H)kVC_A - Q_C \quad 4.3$$

$$\frac{dT}{dt} = -\frac{1}{\theta}T + \beta kC_A + \frac{1}{\theta}T_f - x \quad 4.4$$

If the rate const. is expressed as $k = k_0exp\left[-{}^{E}/_{RT}\right]$ the eq. 2 and 4 becomes,

$$\frac{dC_A}{dt} = -\frac{1}{\theta}C_A - k_0e^{-E/RT}C_A + \frac{1}{\theta}C_{Af} \quad 4.5$$

$$\frac{dT}{dt} = -\frac{1}{\theta}T + \beta k_0e^{-E/RT}C_A + \frac{1}{\theta}T_f - x \quad 4.6$$

$$x = \frac{Q_C}{\rho C_p V} = \frac{hA}{\rho C_p V}\,(T - \overline{T}_c) \qquad 4.7$$

Where h is the coil heat transfer coefficient; A is the total coil heat transfer area and

$$\overline{T}_c = \frac{1}{L}\int_0^L T_C(z)dz \qquad 4.8$$

The average temperature along the length of the coil is 0<Z<L. It is known that x depends nonlinearly on the coolant flowrate q_c according to Aris Model following equation is used:

$$x = Uq_C\left(1 - e^{-\alpha/q_c}\right)\left(T - T_{cf}\right) \qquad 4.9$$

Where T_{cf} = coolant inlet temperature

$\rho_C C_{pc}$ = volumetric heat capacity of the coolant

$$U = \frac{\rho_C C_{pc}}{\rho C_p V} \qquad 4.10$$

$$\alpha = \frac{hA}{\rho_C C_{pc}} \qquad 4.11$$

Observe that our model has five parameters β, U, E, α, k_0. Two of these, $\beta\ and\ U$ are typically available in the literature, and the other to be determined. In addition there are five variables $C_{Af}, \theta, T_f, T_{cf}, q_c$ determined by the reactor operating conditions.

Parameter Estimation in Theoritical Models

Keywords: Theoretical Models, Parameter Estimation & basic Principles

There are three ways by which the value of unknown parameters in a process model may be determined as;

1. Extracting needed parameters from the published literature.
2. Conveying out independent experiments to determine fundamental model parameters; for example lab experiments for determining kinetic rate constants, to be used in a model for a full scale industrial reactor.
3. Performing experiments on the particular physical systems of interest and determine the unknown parameter values that produce model predictions that are closest fit to the experimentally observed data.

When the required parameters are unavailable in the literature, the only other alternative is to estimate them from experimental data.

BASIC PRINCIPLE OF PARAMETER ESTIMATION

For parameter estimation purposes, the theoretical model for any process can be represented in the following form;

$$\eta = f(Z, \Theta) \qquad 5.1$$

where;

η= an n-dimensional vector of actual process output that can be measured in an experiment.

Z= an m-dimensional vector of independent variables that can be specified arbitrarily for each experiment, or variables that, for each experimental observation are known precisely.

Θ= is a P-dimensional vector of the unknown parameter.

f= some functional relationship between these above variables, it may be an explicit functional relationship , or an analytical solution to a differential equation model, it may also be an implicit function as in the differential equation itself but the form f takes is unknown.

Example: Explicit functional form for the Model of Isothermal Batch Reactor

A batch reactor is one in which the isothermal 1st order conversion of reactant A to product is taking place and is modeled by;

$$\frac{dC_A}{dt} = -kC_A \qquad 5.2$$

This is linear first order O.D.E whose solution is given as;

$$C_A = C_{A0}e^{-kt} \qquad 5.3$$

Observe that eq. (3) is in the form of eq. (1) with

$$\eta = C_A;\ Z = [C_{A0}, t]; \Theta = k$$

Linear or non linear parameter estimation

The parameter estimation is said to be linear or non linear with regards to the vector of parameters and not with regards to the state variables. IF in eq 1 function t is linear with respect to the vector θ then the model is said to be linear in the parameters estimation when the parameters enter the model in a nonlinear fashion we have a nonlinear parameter estimation.

to check the parameter estimation problem for linearity obtain $\frac{\partial f}{\partial \theta}$, if the result is independent of θ then the problem is linear in θ otherwise it is a nonlinear in that parameter.

Elements of parameter estimation

each single experiment involves measuring all the n output variables η_1 η_2.... η_n for a specified set of values for the independent variables z1 , z2 .... zn. In order to determine the p parameters $\theta 1, \theta 2, \ldots\ldots \theta p$

independently. It is necessary to perform at least p such experiments. The greater the number of experiments performed better our estimates will be.

the result of each individual experiment is a set of vector η and z that may be related to the process model in particular for the k^{th} experiment we have

$$\eta(k) = f(z(k), \theta); k = 1,2....N \qquad 5.4$$

N= no of separate experiments have been performed.

We now note that the experimental measurements of $\eta(k)$ will not be exactly equal to its true value because of measurement error. Hence we differentiate the actual process output $\eta(k)$ from its experimentally observed measurement denoted by y(k)

$$y(k) = f(z(k), \theta) + E(k); k = 1,2....N \qquad 5.5$$

where E(k) is the vector of errors between the model prediction and the actual data.

Parameter estimation is now involved to find a specific set of parameters value θ such that osme scalar function S of the error vector known as objective function and usually represented as $S(\theta)$ since it depends on the θ parameter value is minimized over the entire range of possible value of θ. The smallest value of $S(\theta)$ is given by $S(\bar{\theta})$

Error criterion

Several criteria are used to obtain optimal estimates of unknown model parameters but the most widely used is the least square criterion. In this case the sum of squares of the errors is the function to be minimized

$$S(\theta) = \sum_{k=1}^{N}[E(k)]^T[E(k)] \qquad 5.6$$

$$S(\theta) = \sum_{k=1}^{N}[y(k) - f(z(k), \theta)]^T[y(k) - f(z(k), \theta)] \qquad 5.7$$

where the summation is over all the data points.

Some times it might be necessary to assign more weight to more precise measurements and less less weight to the others. This is accomplished by introducing a weighting matrix as follows:

$$S(\theta) = \sum_{k=1}^{N}[y(k) - f(z(k), \theta)]^T w(k)[y(k) - f(z(k), \theta)] \qquad 5.8$$

where w(k) is the n*n weighting matrix where elements reflect the relative precision of various measurements (weighting least squares)

Parameter estimation in Differential equation models with analytical solution:

When the process model is such that it possess an analytical solution the parameter estimation problem is made such that much easier since an explicit expression of the form gicen in eq 1 is obtained directly from the analytical solution

case I f(z, θ) is linear in θ

case II f(z, θ) is non linear in θ

Linear Estimation:

When the analytical solution of a process model is obtained in the form

$$\eta = f(z, \theta) \qquad 5.9$$

then from Eq(5.9) we see that the experimentally obtained measurements of process output (which we have referred as y(k) obtained for various values of the vector of independent variables, z(k) are related to the process modeled according to

$$\begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ . \\ y(N) \end{bmatrix} = \begin{bmatrix} f(z(1),\theta) \\ f(z(2),\theta) \\ \vdots \\ . \\ f(z(N),\theta) \end{bmatrix} + \begin{bmatrix} E(1) \\ E(2) \\ \vdots \\ . \\ E(N) \end{bmatrix} \qquad 5.10$$

if f(z, θ) is linear in the θ then it can be shown that eq(6) becomes

$$Y = X\theta + E \qquad 5.11$$

where X is the complete matrix of independent variables compiled for each data set, Y is the entire collection of the experimentally obtained data E is the collection of errors

The linear parameter estimation is now to find the vector $\hat{\theta}$ for which the squard direction of data set Y from the model X θ is minimized

$$\hat{\theta} = (X^T X)^{-1} X^T Y \qquad 5.12$$

Example:

The theoretical model for a storage tank

$$\frac{dh}{dt} = K^* \, (F_i - f)$$

Fi = inlet stream flow rate

f = outlet stream flow rate

metered outlet flow rate

the only process parameters is K* is to be estimated from experimental data

show that for the situation in which a unti step increase is made in the inlet flow rate Fi

$$\frac{dh}{dt} = K^*$$

$$(F_i - f) = 1$$

$h = K^* t + c$

$h_o = c$

$h = h_o + K^* t$

$\eta_1 = h - h_o$

$z_1 = t$

$\theta_1 = K^*$

$\eta_1 = z_1 \theta_1$

If the level measurement at times t_1 t_2 …. tn are respectively h_1 h_2 ….. h_N

$y_1 = h_1 - h_o = K^* t_1 + E_1$

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$y_N = h_N - h_o = K^* t_N + E_N$

$$\begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ . \\ y(N) \end{bmatrix} = \begin{bmatrix} t(1) \\ t(2) \\ \vdots \\ . \\ t(N) \end{bmatrix} K^* + \begin{bmatrix} E(1) \\ E(2) \\ \vdots \\ . \\ E(N) \end{bmatrix}$$

$Y = X\,\theta + E$

$$X = \begin{bmatrix} t(1) \\ t(2) \\ \vdots \\ . \\ t(N) \end{bmatrix}$$

$$Y = \begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ . \\ y(N) \end{bmatrix}$$

If we apply Eq(5.12) using these specific vectors we obtain that K* the least square estimates of K*

$$X = \begin{bmatrix} t(1) \\ t(2) \\ \vdots \\ . \\ t(N) \end{bmatrix} \qquad X^T = [t1 \quad t2 \quad . \quad . \quad t_N]$$

$$X^T X = [t1 \quad t2 \quad . \quad . \quad t_N] \begin{bmatrix} t(1) \\ t(2) \\ : \\ . \\ t(N) \end{bmatrix}$$

$$= \sum_{k=1}^{N} t_k^2$$

$$X^T Y = [t1 \quad t2 \quad . \quad . \quad t_N] \begin{bmatrix} y(1) \\ y(2) \\ : \\ . \\ y(N) \end{bmatrix}$$

$$= \sum_{k=1}^{N} t_k y_k$$

$$\widehat{K^*} = \frac{\sum_{k=1}^{N} t_k y_k}{\sum_{k=1}^{N} t_k^2}$$

Non linear Estimation:

The more common situation with process models for which analytical solutions exist is for the functional form of f(z, θ) to be nonlinear in θ e.g. for any first order system

$$\tau \frac{dy}{dx} + y = Ku(t) \qquad 5.13$$

The general solution to this model for a unit step input in u(t) is

$$y(t) = K\,(1\text{-}e^{-t/}\tau) \qquad 5.14$$

which is linear in K but nonlinear in τ non linear estimation problems are handled in general by numerical techniques

Linearize to model by taking its log in both sides

$$1 - \frac{y(t)}{K} = e^{-t/\tau}$$

$$ln\left\{1 - \frac{y(t)}{K}\right\} = -{}^{t}/_{\tau} \qquad 5.15$$