Parameter Estimation in Different Equation Models: Numerical Methods

Keywords: Models, Numerical Methods, Steady State Approach, Unsteady State Approach

The mathematical models for many realistic systems contain enough complexity that they are amenable only to numerical methods of solution. For such systems the following typical procedure for estimating the set of unknown parameters contained in the model. We start by assuming that the model is of the form:

$$\frac{d\eta}{dt} = f(\eta, z, \theta, t) \qquad \ldots 1$$

Where $f(*)$ is some nonlinear function of the indicated arguments, and, as usual θ represents the set of unknown parameters to be estimated.

It is also assumed that experiments have been performed on the physical process which have yielded N independent measurement of the vector of process output η, for various settings of the input variables z and time. There measurement are represented as $y_k, k = 1, 2, \text{---}$ N.

General Algorithm for Numerical Parameter Estimation

- Start with an initial guess for the value of the vector of parameters, denote this as $\theta^{(0)}$.
- For the same conditions under which the experiments were performed, integrate the process model (numerically) to produce predicted model output η_k, given that the value of the unknown parameter vector is $\theta^{(0)}$.

- Evaluate the sum of squares function by subtracting the model prediction. η_k from y_k (the actual data it is supposed to predict) and finding the norm of the resulting discrepancy vector i.e.

$$S_j = S\left(\theta^{(j)}\right) = \sum_{k=1}^{N}\left[y_k - \eta_k\left(\theta^{(j)}\right)\right]^T\left[y_k - \eta_k\left(\theta^{(j)}\right)\right] \qquad \ldots 2$$

- Update the estimate $\theta^{(j)}$, this is where specific methods for nonlinear parameter estimation in nonlinear process models differ. We will later discuss some of the more popular methods for carrying out this step. Let the updated estimate be $\theta^{(j+1)}$.
- Return to step-2 and iterate, obtain S_{j+1} using the updated estimate.
- Continue until $\left|S_{j+1} - S_j\right|$ is less than some predetermined tolerance. The final updated estimate is the required least squares estimate, $\hat{\theta}$.

Procedure of Step-4

Gradient Methods

The general parameter updating expression for a host of methods known by this name is

$$\theta^{(j+1)} = \theta^{(j)} - \lambda \Omega g \qquad \ldots 3$$

Where; λ = some scalar

Ω = matrix

g = gradient vector of the sum of squares surface S

$$g_i = \frac{\partial s}{\partial \theta_i} \qquad \ldots 4$$

There are several methods that operate according to Eq. 3, and they acquired their collective name because they require the computation of the indicated gradient. The choice of matrix Ω, and scalar λ is what differentiate one gradient method form the other.

- For Ω=1, we have the method of steepest descent, it converges too slowly in most practical problems.
- The N-R method used for Ω, the inverse of the Hessian matrix H, defined as.

$$H = \left[\frac{\partial^2 S}{\partial \theta_i \partial \theta_j}\right]$$

i.e. $\Omega = H^{-1}$ $\qquad \ldots 5$

It works well close to the minimum but in general does not guarantee the at each step $S\left(\theta^{(j+1)}\right) < S\left(\theta^{(j)}\right)$; besides, its requirement of the computation of second derivatives can prove very tedious.

- The Levenberg- Marquardt method uses

$$\Omega = (H + KI)^{-1} \quad \ldots 6$$

Its is usually more efficient than the N-R method.

For all these methods the value of λ is set at 1, but with the Levenberg- Marquardt method, the value of the scalar K can be attend during the course of computation, depending on certain circumstances.

Non-Isothermal CSTR

The heat balance and mass balance of a non-isothermal CSTR are as follows:

$$\frac{dc_A}{dt} = \frac{1}{\theta}\left(C_{A_f} - C_A\right) - k_0 e^{-E/RT}.C_A$$

$$\frac{dT}{dt} = \frac{1}{\theta}\left(T_f - T\right) + \beta k_0 e^{-E/RT}.C_A - Uq_c\left(1 - e^{-\alpha/q_c}\right)(T - T_{C_f})$$

These contain three unknown parameters k_0, E, α which must be estimated. The first two are kinetic parameters, while the third is a neat transfer parameter. There are two distinct philosophies of approaches to this problem of estimating these unknown parameters.

- The parameters could be estimated in classical fashion using data from a set of steady state experiments specially designed for independent determination of reactor parameters, this usually involves the use of process knowledge.
- They could be estimated one or more dynamic experiments: by solving the differential equation model and simply choosing the parameters to match the model prediction to the data collected in time.

Steady State Approach

Two types of steady- state experiments.

- One for estimating the kinetic parameters
- Second for estimating the heat transfer parameters

Kinetic Parameter

Steady state experiments at there different temperatures T_1, T_2, T_3 to be performed to determined the kinetic parameters k_0 & E.

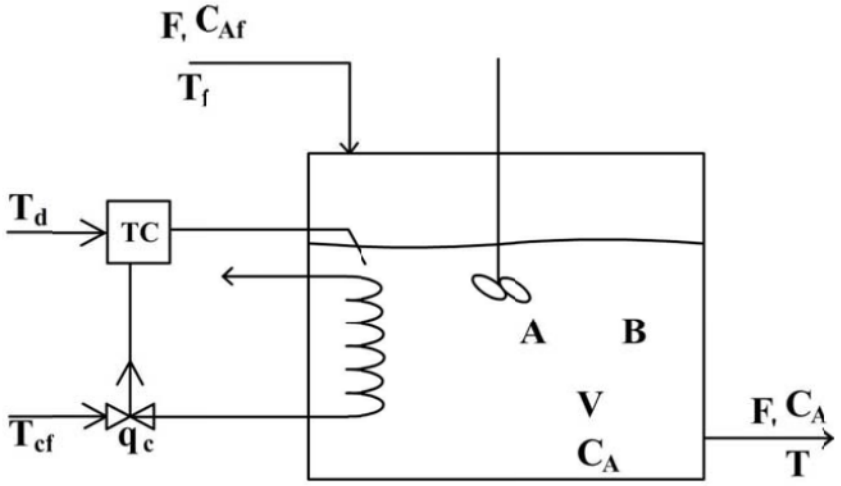

Fig. 6.1

The feedback controller shown is figure will be used to hold the reactor temp. Constant at these steady states. Note that the specific values of these temperatures T_1, T_2, T_3 is not important, they need only be sufficiently different to allow the activation energy E to be determined. By feed back controller, the energy balance equation is removed from consideration, and we need only consider the steady state material balance on A at each temp.

$$\frac{dc_A}{dt} = \frac{1}{\theta}\left(C_{A_f} - C_A\right) - k_0 e^{-E/RT}$$

$$\frac{1}{\theta}\left(C_{A_f} - C_A\right) = k_0 e^{-E/RT} = k$$

$$C_{A_f} - C_A = k\theta$$

$$Y = \frac{C_{A_f}}{C_{A_S}} - 1 = k\theta + \varepsilon$$

Where, C_{AS} = steady state concentration of C_A

ε = experimental error

This is linear equation in the parameter k, but k is $k = k_0 e^{-E/RT}$

By running several steady state experiments at different values of mean residence time θ, good estimates of the rate constant k are first obtained for the above equation. When this is done at all three temperatures, T_1, T_2, T_3 the resulting three values, $k(T_1), k(T_2)$ & $k(T_3)$ can be used to estimate the parameter k_0 & E using the following equation.

$$\ln k(T_i) = \ln k_0 - \frac{E}{RT_i},\ i = 1, 2, 3$$

$Y = \frac{C_{A\delta}}{C_{AS}} - 1$	$\theta(h)$	$T, ^0C$	k
0.445	1	40	0.445
0.910	2	40	0.455
1.340	3	40	0.447
0.490	0.5	60	0.98
0.960	1.0	60	0.96
1.92	2.0	60	0.96
0.490	0.25	80	1.96
0.950	0.50	80	1.90
2.860	1.50	80	1.91

T^oc	k (h^{-1})
40	0.45
60	0.96
80	1.91

The least squares estimates are:

$k_0 = 158300\ \left(h^{-1}\right)$

E=7996 (cal/gm mole)

Heat Transfer Parameter

α is composed of four parameter that are all unknown except of the heat transfer coefficient h. Thus we need to design experiments to estimate h. One approach is to use steady state experiments without reaction with a liquid for which the values of ρ, C_p , μ etc match those of the reaction medium. In this case, the steady state energy balance becomes

$$T_S = \frac{T_f + \theta U q_c (1 - e^{-\alpha/qc}) T_{Cf}}{1 + \theta U q_c \left(1 - e^{-\alpha/q_c}\right)} + C$$

And can be used with steady state data in which T_S varies wish parameter q_c, T_f, T_{Cf}, θ to estimate the parameter α using nonlinear estimation. Alternatively, the steady state equation could be transformed to become linear in the parameter α

$$Y = \ell n\left[1 + \frac{1}{\theta U q_C}\left(\frac{T_S - T_f}{T_S - T_{Cf}}\right)\right] = -\frac{\alpha}{q_C} + \varepsilon$$

Thus experiments in which q_C & T_f vary independently would allow estimation of α by linear regression.

$\theta = 0.5,\ T_{cf} = 30^o c,\ U = 0.5$

$q_C\left(m^3/h\right)$	$\left[1 + \frac{1}{\theta U q_C}\left(\frac{T_S - T_f}{T_S - T_{Cf}}\right)\right]$	$T_f\ ^0C$	T_S^0C
1	0.37	85	77.5
3	0.70	85	75.3
5	0.81	85	74.8
1	0.36	100	90.4
3	0.71	100	87.7
5	0.82	100	87.0

$\alpha = 1.0\left(m^3\ /\ h\right)$

Dynamic Approach

To estimate the kinetic parameter k_0 & E, we could conduct dynamic step test experiments where the reactant feed concentration C_{A_f}, is increased by ΔC_{A_f} at t = 0. If we employ a temp. controller to keep the reactor at a fixed temperature during the step, test, then the material balance equation can be solved and analytically.

$$y = \frac{C_A - C_{A_S}}{C_{A_S}} = \left(\frac{\Delta C_{A_f}}{C_{A_S}} \right) \frac{1}{1 + k\theta} \left[1 - e^{-\frac{(1+k\theta)t}{\theta}} \right] + C$$