Theoritical Models and Parameter Estimation

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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

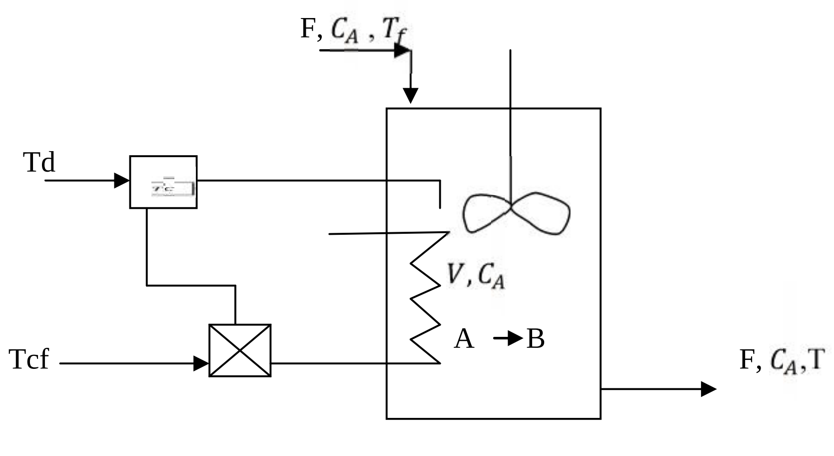

Fig. 4.1: Non-isothermal CSTR

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

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

Assuming constant reactor volume and solving we have,

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

Energy Balance:

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

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

Rate of Heat Transfer to the coil =Q_C

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

Assumptions; ρ, 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,

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

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

If the rate const. is expressed as $k = k_0 exp\left[-{}^{E}/_{RT}\right]$ the eq. 2 and 4 becomes,

$$\frac{dC_A}{dt} = -\frac{1}{\theta}C_A - k_0 e^{-E/_{RT}}C_A + \frac{1}{\theta}C_{Af} \qquad 4.5$$

$$\frac{dT}{dt} = -\frac{1}{\theta}T + \beta k_0 e^{-E/_{RT}}C_A + \frac{1}{\theta}T_f - x \qquad 4.6$$

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

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, β 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.

Source:
http://nptel.ac.in/courses/103107096/4