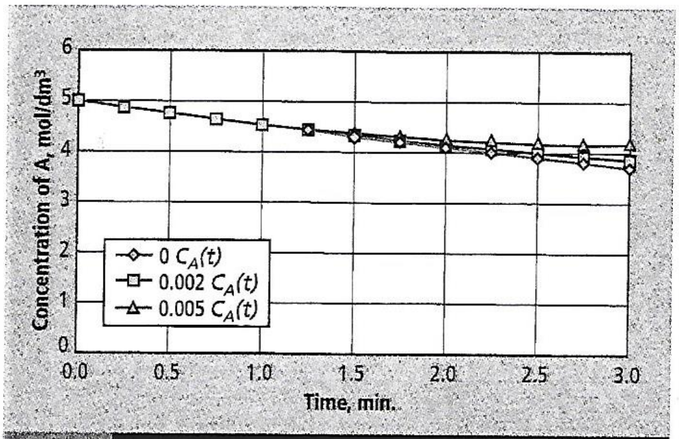

FIG. 3 Dynamic response of component A at varying decay parameter in a CFSTR.

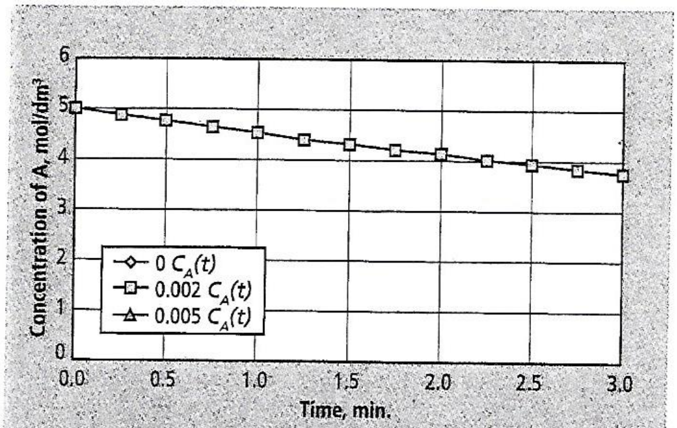

FIG. 4 Dynamic response of component A at varying decay parameter in a CFSTR.

to develop appropriate controller settings. This may be via the Excel program or by direct analysis of the dynamic model. Before startup of a new process, it is advantageous to have reasonable estimates of the controller settings. Furthermore, it may not be feasible to perform experiments to obtain better controller settings for some operating processes.

- *Optimize process-operating conditions.* There are incentives to adjust operating conditions to minimize costs and wastes generation.
- *To design the control strategy:* The developed model allows alternative control strategies to be determined, involving the selection of the measured (controlled) and manipulated variables.

Plantwide control system configuration. During an incomplete reaction, unreacted material is separated from product and recycled to the reactor. A flash vessel is used to separate the raw material from product when raw material is more volatile (Fig. 1). Designing a control system is guided by maximizing profits by converting raw materials into desired products, while satisfying safety, operational constraints, product specifications and environmental regulations.[12]

Newall and Lee have suggested qualitative criteria to guide when selecting controlled and manipulated variables, adequate for an initial analysis in the design of a plantwide control system.[13] For example, a jacketed CFSTR involves a first-order reaction ($A \xrightarrow{k} B$) with an exothermic reaction. The system can be described by 10 variables (Fig. 6) and include: C_A, C_{Ai}, h, T, T_C, T_{CO}, T_i, u_C, u_i, u_O. The variables C_{Ai}, T_i, and T_{CO} are externally specified. At constant density, the CFSTR model involves four equations as:

Overall mass balance:

$$u_i - u_o = A\frac{dh}{dt} \qquad (19)$$

Mass balance on component A:

$$u_i C_{Ai} - u_o C_{AO} - Ah\left(-r_A\right)\left\{C_A, T\right\} = A\frac{d}{dt}\left(hC_A\right) \qquad (20)$$

Energy balance on the reacting mixture:

$$u_i \rho C_p T_i - u_O \rho C_p T + Ah\left(-r_A\right)\left\{C_A, T\right\}\left(\frac{-\Delta H_R}{a}\right) - UA_s\left(T - T_c\right) = A\rho C_p \frac{d}{dt}\left(hT\right) \qquad (21)$$

Energy balance on the jacket coolant (assuming perfect mixing of the coolant in the jacket):

$$u_C \rho_C C_{PC} T_{CO} - u_C \rho_C C_{PC} T_C + UA_s\left(T - T_C\right) = \rho_c V_C C_{Pc} \frac{dT_c}{dt} \qquad (22)$$

The number of variables that can be manipulated independently is defined as:

$$N_{manipulated} = N_{variables} - N_{externally\ defined} - N_{equations} = 10 - 3 - 4 = 3 \qquad (23)$$

In the operation of the CFSTR, two main selections are used for the control system—controlled and manipulated variables. Variables C_A, h and T should be selected as controlled variables. C_A affects the product quality; T must be properly regulated to avoid hazardous problems, production rate, yield and reactor performance, and because it interacts with C_A. In addition, h is selected because it is non-self regulating (i.e., it does not regulate itself to a new steady-state or operating condition. Its transfer function contains an isolated s term in the denominator and is referred to as an integrating system).

Manipulated variables are u_c, u_i and u_o, since u_c controls the reactor temperature T, u_i directly and rapidly affects the conversion, and u_o controls h. Controllability is crucial in the design of chemical reactors for exothermic reactions. These reactors must have enough cooling capacity to avoid runaway reactions; otherwise, the temperature increases can exceed the maximum safe temperature limit for which the reactor is designed.[14] This often results in an explosion or a meltdown.

To prevent this unsafe operation, a safety mechanism should be triggered to stop the process, and the construction material of the reactor must sustain high temperatures for safe operation. However, other non-safe operations may sometimes develop before a high temperature is attained. For example, a new reaction starts to produce a toxic chemical compound beyond a certain temperature.