condition in a continuous flow stirred-tank reactor (CFSTR). Using this simulation exercise will enable both process operators and engineers to monitor the progress of a reaction during startup operation. Two methods of dynamic (analytical and numerical) response were developed, and the Excel spreadsheet program was used to compare their results.

Problem statement. The CFSTR is widely used in the organic chemical industry for many chemical reactions (e.g., gas-phase decomposition of sulfuryl chloride, hydrolysis of methyl chloride, isomerization of cyclopropane to propenes and decomposition of dimethyl ether). The advantage for reactor type is superior temperature control. The disadvantage is the low conversion of reactant per reactor volume. Thus, several CFSTR in series are required to gain the desired conversion levels. Fig. 1 illustrates a plant-wide control system for the CFSTR.

Analysis of a CFSTR during normal, i.e., steady-state operation assumes that its contents are perfectly mixed and at constant density. No accumulation occurs within the system. The exit concentration is identical to the system. However, accumulation does occur during startup or shutdown (i.e., unsteady) operation. Our objective is to model the system during such transient operation.

Mathematical model of the system. Consider the dynamic response of component A in a CSTR undergoing a first-order reaction represented by:[10]

$$(-r_A) = kC_A \left(\frac{\text{mol}}{\text{dm}^3\,\text{min}}\right) \tag{1}$$

The rate constant decay is:

$$k = k_o - at^2 \quad (\text{min}^{-1}) \tag{2}$$

The material balance in the system is expressed as:

Input by flow = output by flow + (disappearance by reaction) + accumulation.

This is expressed mathematically as:

$$uC_{AO} = uC_A + (-r_A)V_R + V_R\frac{dC_A}{dt} \tag{3}$$

where:

$$(-r_A) = (k_o - at^2)C_A \tag{4}$$

Substituting Eq. 4 into Eq. 3 gives:

$$uC_{AO} = uC_A + (k_o - at^2)C_A V_R + V_R\frac{dC_A}{dt} \tag{5}$$

Eq. 5 is a first-order differential equation shown as:

$$\frac{dy}{dx} + Py = Q \tag{6}$$

Rearranging Eq. 5 in the form of Eq. 6 gives:

$$\frac{dC_A}{dt} + \left(\frac{u}{V_R} + k_o - at^2\right)C_A = \frac{u}{V_R}C_{AO} \tag{7}$$

An analytical method of determining the concentration of A with time during the transient conditions (e.g., startup/shutdown) can be used:

$$\log_e \text{IF} = \int P dx = \int\left(\frac{u}{V_R} + k_o - at^2\right)dt$$

$$\log_e \text{IF} = \frac{ut}{V_r} + k_o t - \frac{at^3}{3}$$

or

$$IF = e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \tag{8}$$

IF is the integrating factor. Multiplying Eq. 7 by the IF gives:

$$e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \times \frac{dC_A}{dt} + e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \times \left(\frac{u}{V_R} + k_o - at^2\right)C_A = \frac{u}{V_R}C_{AO} \times e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \tag{9}$$

Eq. 9 can be expressed as:

$$\frac{d}{dt}\left[e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \times C_A\right] = \frac{u}{V_R}C_{AO} \times e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \tag{10}$$

or

$$\left[e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \times dC_A\right] = \frac{u}{V_R}C_{AO}\int e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t}dt + \text{Const.} \tag{11}$$

Integrating Eq. 11 and rearranging give:

$$e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \times C_A(t) = \frac{u}{V_R}C_{AO}\left[\frac{e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t}}{\frac{u}{V_R} + k_o - at^2}\right] + \text{Const.} \tag{12}$$

The concentration of A with time can be expressed by:

$$C_A(t) = \frac{u}{V_R}\frac{C_{AO}}{\left(\frac{u}{V_R} + k_o - at^2\right)} + \text{Const.} \times e^{\left(\frac{u}{V_R} + k_o - \frac{at^2}{3}\right)t} \tag{13}$$

At time $t = 0$, $C_A(t) = C_{AO}$, and substituting this in Eq. 13 gives:

$$C_{AO} = \frac{u}{V_R}\frac{C_{AO}}{\left(\frac{u}{V_R} + k_o\right)} + \text{Const.}$$

Const. is:

$$\text{Const.} = C_{AO} - \frac{uC_{AO}}{V_R\left(\frac{u}{V_R} + k_o\right)} \tag{14}$$