The final transient concentration of A during startup or shutdown is given as:

$$C_A(t) = \frac{u}{V_R}\frac{C_{AO}}{\left(\frac{u}{V_R}+k_o-at^2\right)} + \left[C_{AO} - \frac{(u/V_R)C_{AO}}{\left(\frac{u}{V_R}+k_o\right)}\right] e^{-\left(\frac{u}{V_R}+k_o-\frac{at^3}{3}\right)t} \qquad (15)$$

where $\bar{t} = \frac{V_R}{u}$ = mean residence time

Rearranging Eq. 7 to a first-order differential equation gives:

$$\frac{dC_A}{dt} = \frac{u}{V_R}C_{AO} - \left(\frac{u}{V_R}+k_o-at^2\right)C_A \qquad (16)$$

Both Eqs. 15 and 16 provide the dynamic response of component A undergoing a first-order reaction in a CFSTR. Their limitation is that the rate constant, k, defined by Eq. 2, must be positive. This constraint should be introduced in the model; otherwise, the concentration response will be invalid. Table 1 shows the data used in the Excel spreadsheet.

Spreadsheet programming. The Excel program is used to create both analytical and numerical solutions. The latter method uses the fourth-order Runge-Kutta method for solving the first-order differential Eq. 16 with the Excel spreadsheet. In applying the fourth-order Runge-Kutta numerical method using the Excel spreadsheet program, Eq. 16 can be rearranged to yield:

$$\Delta C_A = C_A - C_{AO} = \left[\frac{uC_{AO}}{V_R} - \left(\frac{u}{V_R}+k_o-at^2\right)C_A\right]\Delta t \qquad (17)$$

The transient response concentration, C_A, is:

$$C_A = C_{AO} + \left[\frac{uC_{AO}}{V_R} - \left(\frac{u}{V_R}+k_o-at^2\right)C_A\right]\Delta t \qquad (18)$$

The fourth-order Runge-Kutta numerical method is used in Eq. 18 at varying decay parameter. This alternative method is used to reduce over-confidence of the earlier analytical method, and as a self-check.[11]

Results. Fig. 2 shows the worksheets of both methods and the computer results for comparison. Figs. 3–5 show the results of component A with time during transient state condition. Fig. 3 illustrates the results of the Excel spreadsheet program using the analytical method. Figs. 4 and 5 respectively show the results of the Excel spreadsheet and Fortran programs using the fourth-order Runge-Kutta numerical method.

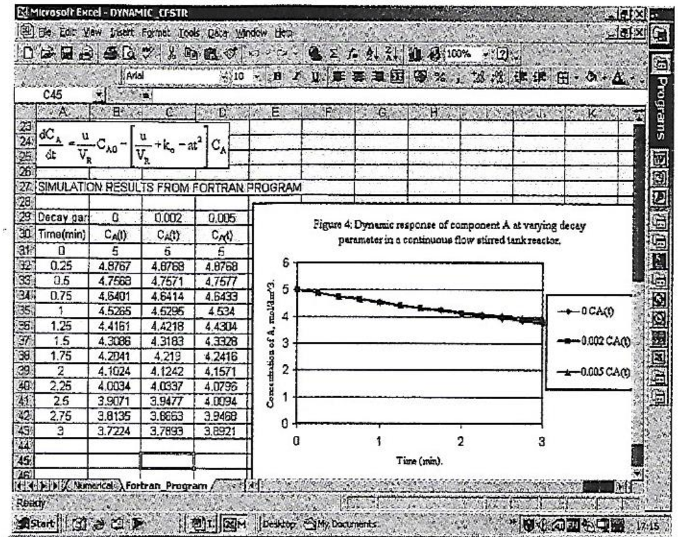

FIG. 2 Simulation for CFSTR reaction with the Excel model.

Table 1. Parameters for the dynamic response of a CFSTR.

Decay parameter a, min^{-3}	0.0
Decay parameter a, min^{-3}	0.002
Decay parameter a, min^{-3}	0.005
Volumetric feed u, dm^3/min	10
Volume of the reactor, V_R, dm^3	1,000
Initial concentration of A, C_{AO}, mol/dm^3	5
Rate constant, k, min^{-1}	0.1

The simulation was done at varying decay parameter (*a*). These figures demonstrate good agreement between the methods in determining the unsteady-state condition of the system. Analysis of the results also shows how the dynamic response is slowed as the decay parameter (*a*) increases. The Excel spreadsheet program allows both the results and the dynamic response of the model to be displayed simultaneously. Using the Excel spreadsheet program shows that the dynamic profiles involving these methods are in good agreement and can thus be employed to simulate the various measured variables.

Model of the process plant. This mathematical model can be helpful for process analysis and control in several ways:

- *Improve the understanding of the reaction mechanism.* The Excel spreadsheet program can be used to investigate the transient response without the cost and potential hazard of operating the real process. This approach may be justified when it is not feasible to perform dynamic experiments in the plant or before it has been constructed.
- *Train plant-operating personnel.* Plant operators can be trained to operate a complex process, if the program is interfaced to standard process control instrumentation. A realistic environment can be created for operator training without the cost or possible exposure to hazardous conditions that might exist in a real plant situation.
- *Select controller settings.* The transient model may be used