The object of this column is to enhance our readers' collections of interesting and novel problems in chemical engineering. Problems of the type that can be used to motivate the student by presenting a particular principle in class, or in a new light, or that can be assigned as a novel home problem, are requested, as well as those that are more traditional in nature and that elucidate difficult concepts. Manuscripts should not exceed ten double-spaced pages if possible and should be accompanied by the originals of any figures or photographs. Please submit them to Professor James O. Wilkes (e-mail: wilkes@engin.umich.edu), Chemical Engineering Department, University of Michigan, Ann Arbor, MI 48109-2136.

TUNING AND ACTIVATION OF A PI CONTROLLER DURING STARTUP OF A NON-ISOTHERMAL CSTR

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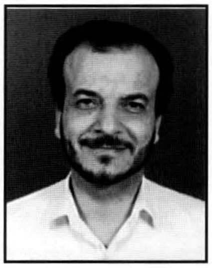
Continuous processes show dynamic behavior during start-up, shutdown, and when upsets occur during steady-state operation. Mathematical modeling, simulation, and control of these processes is relatively difficult because of the nonlinear nature of these processes and the activation and tuning difficulties of the controllers.

This paper applies proportional plus integral (PI) control to start up a non-isothermal CSTR. PI eliminates offsets and maintains an acceptable speed of response. Simple and straightforward schemes of activation are tried to start up the CSTR smoothly and to get the maximum attainable conversion. The importance of this control problem lies in the difficulty of triggering the controller and the retuning of the PI settings.

PROBLEM STATEMENT

We will consider the start-up of a non-isothermal CSTR, which has been studied in detail.[1,2] A reaction of the form $A + B \rightarrow C + D$ and of known kinetics has been considered. The CSTR has an overflow and two feed streams, one for pure A and the other for pure B. Mathematical models along with analytical and numerical solutions have been developed. Various types of start-up have been modeled and simulated, each type being represented by a different model. The models treated A and B as if they were in a total feed flow. In the present study, however, the models are modified to account for separate feed flows, because each feed flow is used here as a manipulated variable. Also, instead of using different models, the equations are grouped here in one general form:

$$\frac{dV}{dt} = F_1 + F_2 \text{ for } V < V_r, \quad \text{otherwise } \frac{dV}{dt} = 0 \qquad (1)$$



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$$\frac{dVC_A}{dt} = F_1C_{Af} - rV \qquad (2)$$

$$\frac{dVC_B}{dt} = F_2C_{Bf} - rV \qquad (3)$$

$$\frac{dVC_C}{dt} = (F_1 + F_2)(C_{Cf}) + rV \qquad (4)$$

$$\frac{dVC_D}{dt} = (F_1 + F_2)(C_{Df}) + rV \qquad (5)$$

$$V\left(\sum_{i=1}^{4} C_iC_{pi}\right)\frac{dT}{dt} = F_1C_{Af}C_{pA}(T_f - T) + F_2C_{Bf}C_{pB}(T_f - T) - rV\Delta H - Q \qquad (6)$$

where

$$r = kC_AC_B \quad k = 10^{9.31}\exp\left(\frac{-48.32}{RT}\right) \quad Q = \frac{4V_r}{D}h_{air}(T - T_{amb})$$

The values of the parameters and the initial conditions are listed in Tables 1 and 2, respectively.

Required

1. Operating conditions during start-up have been found to affect the product quality. For example, changes in pressure drop in the head tanks produce changes in feed flows. Perform an open-loop simulation of the model and find the effect of changing the flow rate on the yield.

2. Operate the system starting from an empty tank with no inlet flows up to a fully filled tank with the maximum product concentration. Perform start-up once without disturbances and then with disturbances in the feed flows and in the input reactant concentration. Use a standard feedback PI control system, with the controlled variable being the concentration of product C.

3. To perform start-up successfully, we need to tune and activate the controller. Use the modified Ziegler-Nichols[3] (Z-N) tuning method to find out the best settings, and then suggest different schemes to activate the controller.

SOLUTION

Simulation of the model equations (Eqs. 1-6) was performed using the package DASSL. This is a differential/algebraic system solver that uses the backward differentiation formulas of orders one through five. Figure 1 shows an open-loop simulation of the models for two different values of F_1 and F_2. As shown, a lower yield is obtained at a higher flow rate. Thus, the CSTR needs to be operated at lower flow rates. Specifically, $F_1 = F_2 = 0.1$ l/min, which produces $C_C = C_D = 0.0327$ mole/l, is considered as the desired operating condition (set point) in this work.

The manipulated variables are the positions of the valves, where the feedback control law[4] is given by

$$v_1(t) = v_{1o} + k_{c1}\left[C_C^{sp} - C_C(t)\right] + \frac{k_{c1}}{\tau_{11}}\int_0^t \left[C_C^{sp} - C_C(t)\right]dt \qquad (7)$$

$$v_2(t) = v_{2o} + k_{c2}\left[C_C^{sp} - C_C(t)\right] + \frac{k_{c2}}{\tau_{12}}\int_0^t \left[C_C^{sp} - C_C(t)\right]dt \qquad (8)$$

These laws will be implemented in a discrete time fashion with sampling time of 1 min. Note that these control loops form a split-range control scheme, because there are two manipulated variables to control one variable, with the control signal being split into equal parts, each affecting one valve. Although this is not the common split-range configuration, it simplifies the problem. Alternatively, v_2 can be driven by the error signal of C_D, which will result in the same

TABLE 1
Process Parameters

Parameter	*Value*	*Parameter*	*Value*
Tf	24°C	Cp_A	75.25 J/mol°C
T_{amb}	29°C	Cp_B	175.3 J/mol°C
Vr	2.8 l	Cp_C	78.2 J/mol°C
h_{air}	2.5 J/m²°C min	Cp_D	103.8 J/mol°C
ΔH	-1.5 kJ/mol	C_{Af}	0.1 mol/l
D	15 cm	C_{Bf}	0.1 mol/l
T_{ref}	24°C	C_{Cf}	0.0 mol/l
		C_{Df}	0.0 mol/l

TABLE 2
Initial and Starting Conditions

F_1	F_2	C_A	C_B	C_C	C_D	V	T
0.0 l/min	0.0 l/min	0.1 mol/l	0.1 mol/l	0.0 mol/l	0.0 mol/l	0.0 l	24°C

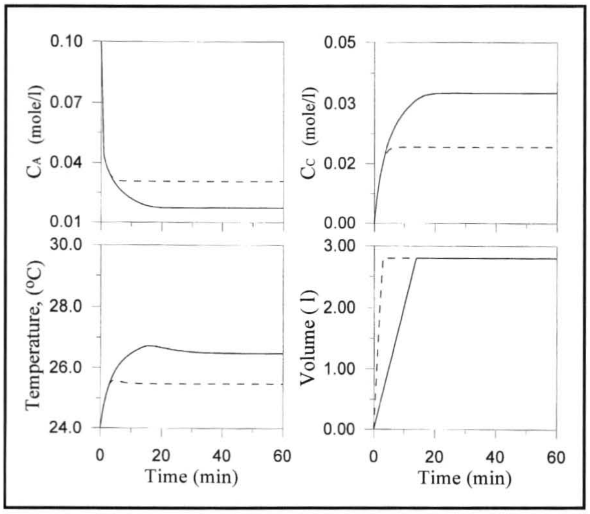

***Figure 1.** Open-loop simulation: solid lines, $F_1 = F_2 = 0.1$ l/min; dashed lines, $F_1 = F_2 = 0.5$ l/min.*

control performance because the reaction has a constant stoichiometric ratio of one and identical valve dynamics. Note that feed flows are taken as linearly proportional to the valve positions of

$$F_1 = C_{v1} v_1 \tag{9}$$

$$F_2 = C_{v2} v_2 \tag{10}$$

Here, $C_{v1} = C_{v2} = 1.0$ mole/min.

Controller Tuning

Tuning determines the best settings for the adjustable parameters of a feedback controller. Closed-loop testing that produces constant output cycling is used in selecting these values. The desired values for k_{ci} and τ_I are determined based on the modified Z-N tuning criterion. The original Z-N[5] method is based on the quarter decay ratio, which might result in oscillatory feedback response. The modified Z-N method gives more conservative settings. The purpose of the controller tuning is to obtain an initial value for the PI settings, which will be adapted on-line in a gain-scheduling formulation.

Tuning of the feedback control using an ultimate gain methods, *i.e.,* Z-N, is based on continuous incrementation of k_{ci} and observation of the resulting closed-loop response. The proportional gain that produces sustained oscillation is known as the ultimate gain from which the PI settings can be inferred.[6] Since the zero steady state is an unstable one, this method cannot be applied at this operating point. Thus, the PI settings are obtained by applying the Z-N as

$$k_{c1} = k_{c2} = -76.0$$

$$\tau_{I1} = \tau_{I2} = 1.0 \text{ min}$$

The negative controller gain is an indication of the reverse action mode, because the process has a negative static gain, k_p (see Figure 1).

Controller Activation

Consider Eqs. (7) and (8). In order to start up the reactor at t=0, the following condition must be satisfied:

$$v_i(0) = v_{io} + k_{ci}\left[C_C^{sp} - C(0)\right] > 0 \tag{11}$$

Obviously, this cannot be satisfied for a negative controller gain and a zero value of initial valve position. In order to overcome this problem, we examine four strategies of start-up:

Strategy I Perturb the inflows manually and trigger the PI algorithm simultaneously.

Strategy II Perturb the inflows manually and trigger the PI algorithm after a specific time interval.

Strategy III Trigger the PI algorithm with gain-scheduling according to $k_{ci}k_p$ = constant.

Strategy IV Trigger the PI algorithm with gain-scheduling using the IMC-type controller, $k_{ci}k_p = \tau / \lambda$

Notice that for Strategy 1, a large value of k_{ci} might cause v_i to remain zero for any value of v_{io} in its allowable range of [0,1]. The maximum allowable magnitude of k_{ci} in this case is $|k_{ci}| < v_{io} / C_C^{sp}$. Thus, a value of 0.1 for v_{io} and -2.0 for k_{ci} are used in Strategy I. As for Strategy II, the larger value of k_{ci} obtained by the Z-N method can be used with v_{io}=0.1 and the controller can be triggered one sampling time later.

In Strategy III, the controller gain will be adapted on-line according to $k_{ci}(t) = k_{co}k_{po}/k_p(t)$, where k_{co} and k_{po} are constant reference values. In this investigation, k_{co} is taken equal to -76, which is found by the Z-N method, and k_{po} as the static gain corresponding to $F_1 = F_2 = 0.1$ l/min. Values of $k_p(t)$ can be estimated from Table 3, which lists different values for the static gain at various operating conditions. Values of k_p for $F_1>0$ were computed using the exact linearization of the process model and using the reaction-curve method. Both methods gave almost identical results. Initially, with $F_1=0$, the operation behaves like an integrator process; hence $k_p(0)$ was found by the pulse testing.[7]

For Strategy IV, the controller gain will also be adapted on-line with a changing process gain (k_p) and time constant (λ) according to $k_{ci} = \tau(t)/\left[\lambda k_p(t)\right]$ where λ is the IMC filter parameter or closed-loop time constant used to adjust the speed of the closed-loop response. Usually, an IMC-type tuning is used to determine fixed PI settings using identified process parameters. In addition, robustly tuned PI settings can be obtained by conducting an adequate robustness analysis.[8] Here, we allow the IMC-type controller gain to vary in order to adapt to the process changing gain.

The gain-scheduling approaches (Strategies III and IV) are conducted as follows:

- At t = 0

  set $k_p(0) = k_p(F_1=0)$ and $\tau(0) = \tau_{av}$

- At t > 0

  set $k_p(t) = k_{p,av}$ or interpolate k_p from the various values of k_p in the range $F_1 \in [0.01, 1.0]$

  set $\tau(t) = \tau_{av}$ or interpolate τ from the various values of τ in the range $F_1 \in [0.01, 1.0]$

RESULTS AND DISCUSSION

Start-Up Without Upsets

Closed-loop simulation for C_C^{sp}=0.0327 using the proposed activation strategies is depicted in Figure 2, which shows the time response of the product concentration, C_C, and the inlet flow of pure A, F_1. In all cases the controller was able to bring the product concentration to the desired

TABLE 3
Identified Process Gain and Time Constant at Various Operating Conditions

Step Change in F_1 (1/min)	τ (min)	Operating Condition	k_p
0.01	8	V=0	0.0111
0.05	6.5	V= 2.8, F_1 = 0.01	-0.1382
0.1	5	V = 2.8, F_1 = 0.1	-0.0338
0.2	3.5	V = 2.8, F_1 = 0.2	-0.02
0.4	2.5	V = 2.8, F_1 = 0.4	-0.0108
0.6	2.0	V = 2.8, F_1 = 0.6	-0.0071
0.8	1.5	V = 2.8, F_1 = 0.8	-0.0051
1.0	1.35	V = 2.8, F_1 = 1.0	-0.0039

value. The feed flows varied initially and then settled at their expected values of 0.1 1/min; however, the smooth response for Strategy II was only achieved by de-tuning the PI settings to k_{c1} = k_{c2} = -9.1, whereas the feedback response using the original values of the PI settings was found to be very aggressive.

It is clear from Figure 2 that Strategy I has the slowest response due to a small controller gain. A larger value of k_{ci} and consequently a faster response of Strategy I can be achieved using a larger initial perturbation value. With respect to the responses, Strategy III outperformed other strategies where the closed-loop response using a constant average value and a variable interpolated value of k_p are almost the same. Initially, F_1 varies for a few samples, then settles down to a constant value, giving a constant process gain. For strategy IV, the use of average values for the process parameters gave a smoother closed-loop. A value of λ = 2 produced a less aggressive performance, which took Strategy IV to a slightly slower response than that of Strategy III.

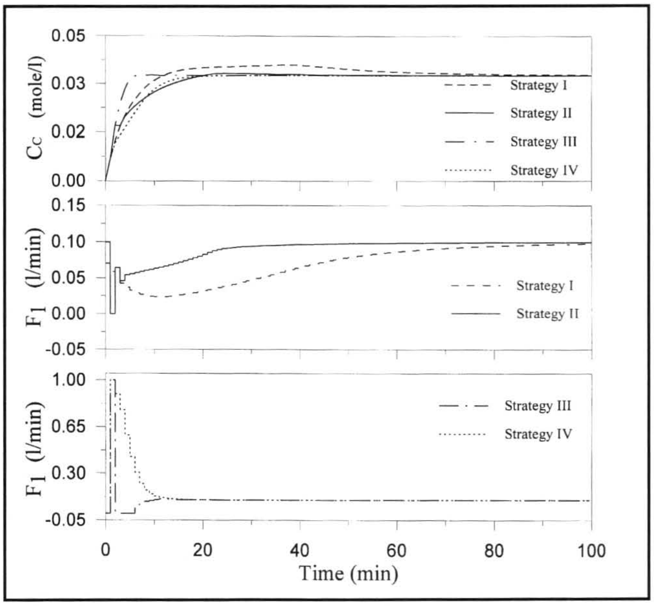

Figure 2. *Closed-loop response for C_C^{sp}=0.0327 mole/l.*

Start-Up with Upset in the Feed Flow

We next examine the change in the set point with a step of -0.05 in the feed flows at t=5 min during start-up (see Figure 3). The associated response of the valve openings is demonstrated in Figure 4. Obviously, the upset in the feed flows has marginal effect on feedback response of the product concentration for all cases except for Strategy I with $v_{io}=0.1$, where a larger overshoot is observed. Unlike the previous case, the valve response differs from that of the feed flow since the disturbance affects the latter only. In this case, the

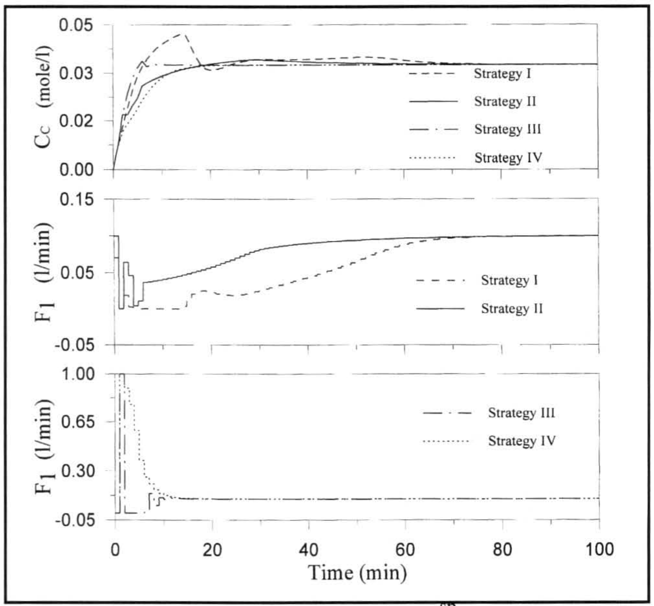

Figure 3. *Closed-loop response for C_C^{sp}=0.0327 mole/l with -0.05 step change in both feeds starting at t=5 min.*

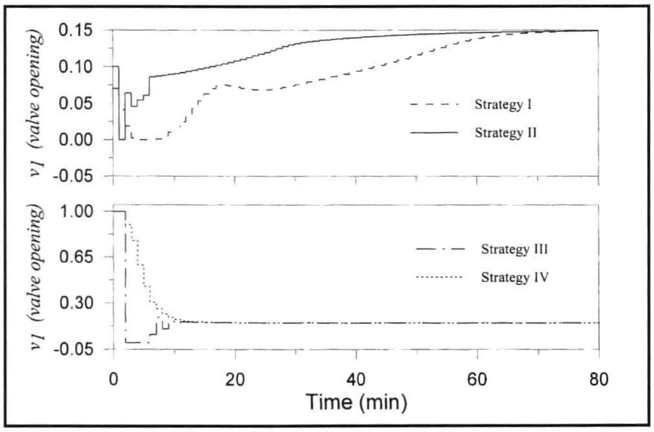

Figure 4. *Time response of valve position for C_C^{sp}=0.0327 mole/l with -0.05 step change in both feeds starting at t=5 min.*

valve position settles at a steady-state point higher than that in Figure 2. This increase in the valve opening was made by the controller to balance reduction in the feed flows produced by the disturbances.

Start-Up with Upset in the Feed Concentration

In order to illustrate the efficiency of the feedback control scheme, all of the control activation strategies were tested for the same set point as above, but with a disturbance in C_{Bf}. A step change of -0.02 mole/1 starting at t=10 min was considered (see Figure 5). Obviously, the proposed feedback schemes maintained the product quality at the desired value despite the sudden reduction in the inlet concentration, C_{Bf}. Ultimately, the inlet flows reached a value lower than that without upsets.

Start-Up with Different Set Point

Another advantage of the feedback scheme is its ability to maintain desired specifications without the knowledge of the optimal operating conditions beforehand. For example, in order to maximize the product yield, a larger set point for the product concentration can be specified for the controller. Figure 6(a,b), for example, illustrates the feedback response of the process for C_C^{sp}=0.04 mole/l. Although simulation indicates that such a yield is achievable, it operates the process at a very low throughput of 0.03 l/min. Similarly, Figure 6(c,d) demonstrates the process dynamic behavior for C_C^{sp} = 0.05 mole/l. Obviously, the reaction can be brought to such a high yield, but this would be at the expense of operating the process in a semi-batch mode as the feed flows approached zero at steady state.

CONCLUSIONS

Automatic start-up of a non-isothermal CSTR using a conventional PI control algorithm was considered. Four controller activation/adaptation schemes were tested and compared. Overall, Strategy III presented superior performance, full automation, and ease of implementation. Strategy I had the most sluggish response since the maximum allowable controller gain is restricted by the value of the initial valve opening. Strategy II lacks full automation and requires re-tuning for stability. On the other hand, Strategy IV requires proper adjustment of the IMC filter for good performance. Nevertheless, the performance of gain-scheduling approaches (Strategies III and IV) depends on the identified process parameters.

A theoretical model should be developed or identification methods be used along with these approaches. Another practical operation of the process is to maximize the yield and throughput. This issue can be addressed through implementation of optimal control

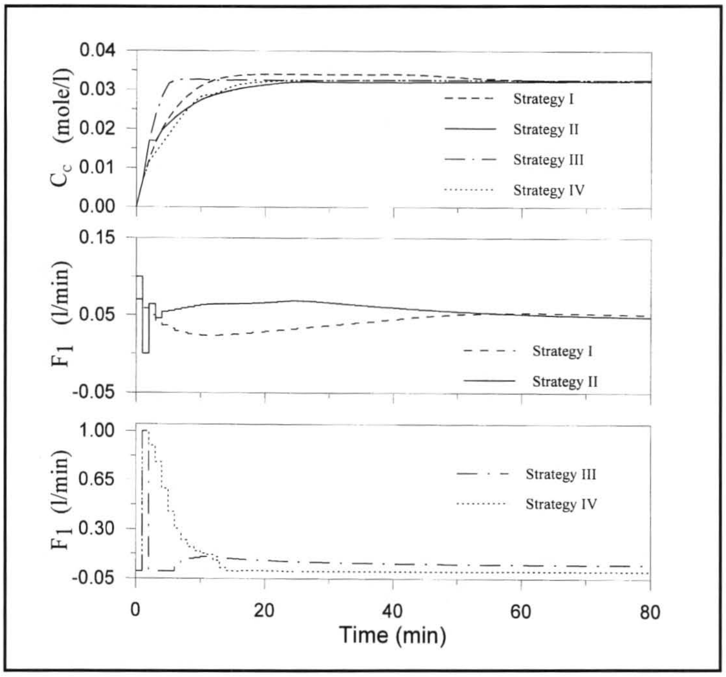

Figure 5. *Closed-loop response for* C_C^{sp} *=0.0327 mole/l with -0.02 step change in* C_{Bf} *starting at t=10 min.*

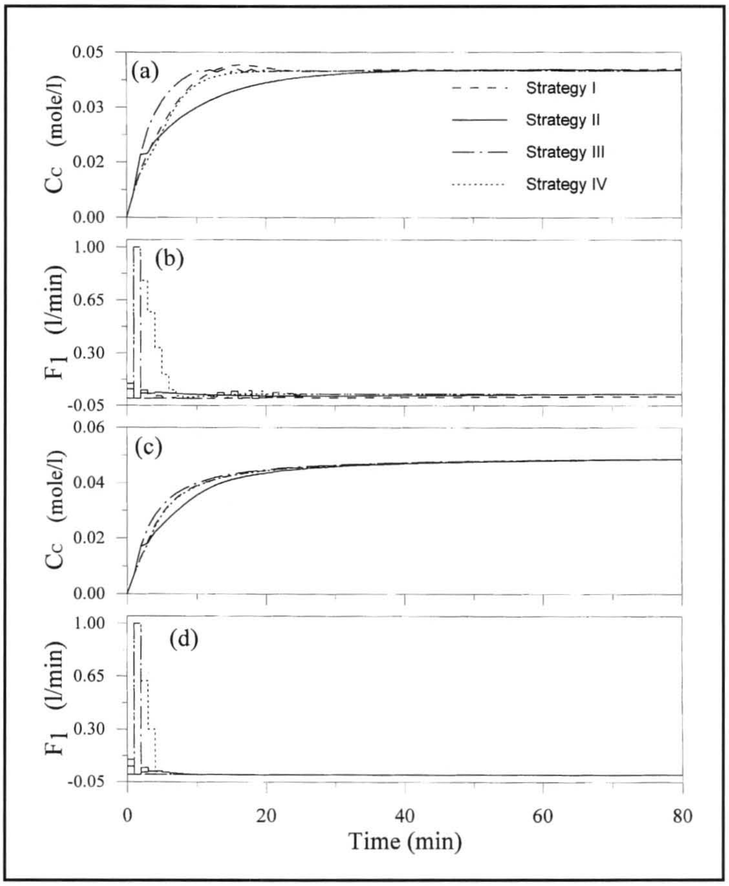

Figure 6. *Closed-loop response for* C_C^{sp} *=0.04 mole/l (a,b) and* C_C^{sp} *= 0.05 mole/l (c,d).*

theory.

Questions for Further Study

- ❑ ***Question #1:*** Derive the model equations considering one mode of start-up, *e.g.,* adding both reactants simultaneously, until the reactor overflows.
- ❑ ***Question #2:*** Consider an emergency shutdown in which the feed flows are suddenly stopped and the reactor is to be drained. Would the equations for this case be different from those representing start-up? How?
- ❑ ***Question #3:*** Repeat the above calculations using a first-order reaction.[9] Is it going to affect the controller settings and activation?
- ❑ ***Question #4:*** What would be the effect of adding a derivative action to the controller (*i.e.,* using a PID) on the start-up of the process?

NOMENCLATURE

C_i	concentration of species i, mole/l
C_{if}	feed concentration of species i, mole/l
C_i^{sp}	concentration set point for species i, mole/l
C_{pi}	heat capacity of species i, J/mole °C
C_{vi}	characteristic constant for valve i
D	reactor diameter, m
F_1	feed flow rate of pure component A, 1/min
F_2	feed flow rate of pure component B, l/min
h_{air}	heat transfer coefficient for air, kJ/m^2°C min
ΔH	standard heat of reaction, kJ/mole
K	reaction rate constant, l/mole min
k_{ci}	controller gain for loop i
k_p	process gain
k_p,av	average process gain
Q	rate of heat loss to the surrounding, kJ/min
r	reaction rate, mole/l min
R	gas constant, 0.008314 kJ/mole K
T	reactor temperature, °C
T_{amb}	ambient temperature, °C
T_f	feed temperature, °C
T_{ref}	reference temperature, °C
t	time, min
V	fluid volume, 1
v_i	valve i position
v_{io}	initial position for valve i
V_r	reactor volume, 1
λ	IMC filter (closed-loop time constant)
τ	process time constant
τ_{av}	average time constant
τ_1	integral time for PI controller

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ChE letter to the editor

To the Editor:

In the Winter 2000 issue of *Chemical Engineering Education* there was an interesting paper by S.H. Munson-McGee[1] that presented a laboratory sequence with the objective of developing abilities in chemical engineering students according to EC 2000 criteria.[2] The author describes a four-course sequence, beginning with the study of the theoretical aspects of experimental design and data analysis and finishing with a unit operations laboratory.

Table 1 of that paper shows a short description of each of the nine experiments that can be carried out by the students with the Process Instrumentation Laboratory course. Unfortunately, the mentioned Table 1 contains a typographical mistake and the simple change of a "d" for a "b" causes a considerable conceptual effect: effectively, the experiment, titled "A*b*sorption by activated carbon. Blue food coloring was a*b*sorbed from aqueous solutions..." is actually an a*d*sorption experiment. (Table 2 refers, correctly, to this experiment as an a*d*sorption process.)

From my point of view, it is important to correct this type of typographical error where two very similar words refer to two very different processes, in order to prevent confusion and conceptual mistakes among students. This is especially important in journals such as *Chemical Engineering Education* because of its content, which is very readable by chemical engineering undergraduates.

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Universidad de Alicante

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2. "Engineering Criteria 2000," Accreditation Board for Engineering and Technology, Inc., 111 Market Place, Suite 1050, Baltimore, MD (1998) ❑