INTRODUCING PROCESS CONTROL CONCEPTS TO SENIOR STUDENTS

Using Numerical Simulation

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Among all the courses in the chemical engineering curriculum, students generally find process control the most challenging. Perhaps one reason is that it is one of the final courses of their undergraduate curriculum. Our observation, confirmed by another source,[1] was that students oftentimes characterize the course as an abstract study with extensive mathematical derivations that bear little or no relevance to the practice of chemical engineering. This has prompted a re-examination of process control instruction at Howard University, with interest focused on how knowledgeable the graduating students are with respect to being able to apply their process-control knowledge when they leave for industry.

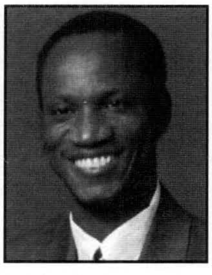
Although this re-examination is still proceeding, we want to share some of our experiences with a learning module that was introduced for the purpose of helping students rethink their views about process control. Understanding how the subject of process control was viewed, we felt there was a need to stimulate interest in the course by adapting the course materials in a manner that makes learning exciting. We have done this through an assignment involving modeling and simulation using the Mathcad software package.

The typical tasks covered in the assignment range from routine material, component, and energy balances to numerical simulation of uncontrolled and controlled systems. The assignment thus formulated substantially covers most of the major topics in the undergraduate process control curriculum. The only set of new material that is needed to complement the students' knowledge in order for them to be able to do the assignment is the control law, under which a brief explanation of the effects of proportional, integral, and derivative control modes are explained. As for modeling and simulation, the knowledge the students have gained from prior courses in chemical engineering calculations,[2] kinetics,[3] heat transfer,[4] and advanced calculus are more than enough to get them through the assignment. The instructors' responsibility lies solely in guiding the students so that they will be able to synthesize ideas based on what they have already learned in these prior courses. With proper guidance, a successful modeling and simulation of the system was found to be beneficial to the students in introducing various aspects of process control, such as the concept of a closed feedback control loop.[5]

PROBLEM STATEMENT

The simulation assignment was taken from established sources[6,7] with slight modification. Given was a CSTR equipped with a cooling jacket in which a first-order exothermic reaction of decomposition of hydrogen peroxide into water and oxygen occurred in the presence of excess sodium hydroxide, which acted as a catalyst.

$$H_2O_2 + (NaOH) \rightarrow H_2O + \frac{1}{2}O_2 + (NaOH)$$



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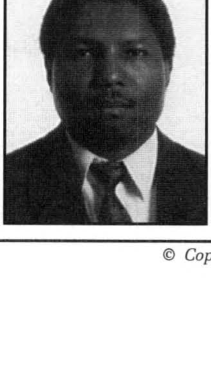

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The reacting mixture flowed in through a linear valve while the product was discharged through a square root valve. We wanted to investigate the uncontrolled and the controlled dynamic behavior of the concentration of H_2O_2 and the temperature of the reactor from time t = 0 to some time after first filling (starting with an empty reactor), following which control was initiated. The need to formulate the relevant mass, component, and energy balances in a manner that was fairly general and capable of accepting different parameter values such as inlet concentration, temperature, reactor volume, and others was emphasized. The parameters of the system are presented in Table 1. The mean temperature difference between the reacting mixture and the coolant was expressed as a function of difference in temperature of the reacting mixture and the inlet temperature of the coolant as

$$T - T_C = \frac{T - T_{Cin}}{\left(1 + \frac{1}{F_C}\right)} \qquad \text{where} \qquad F_C = \frac{2\,Q_C Cp}{UA_C}$$

The students were asked to show all steps of the formulation, including the system diagram (Figure 1), and to state all assumptions clearly. We pointed out that the units of the data provided were all mixed up, which meant that conversion to a uniform system of unit was required before simulation. The problem assignment was to culminate in showing the reactor's liquid height, concentration, and temperature profiles as a function of time with a short comment on the stability of the system.

TABLE 1
Values of Parameters Used in Simulation*

V	16.2 liters
k_o	5.04×10^{10} 1/sec
E	18.620 cal/mol
Cp	0.865 cal/g °C
C_1	62.5 BTU/(hr ft^2°F)/(lb/min)$^{1/3}$
U	$C_1 Q_c^{1/3}$
T_i	22°C
T_{cin}	10°C
T_{set}	14°C
C_{AO}	11.5 mol/liter
F_i	0.5 liter/min
ρ	1.1081 g/cm^3
ΔH	-22.6 kcal/mol
Q_c	900-3600 lb/min
Kv	0.9 cm$^{2.5}$/min
Kp	3 liter/min K
D	25.2 cm
A_c	3.18 ft^2

*Symbol names are stated in the nomenclature

CLASS ORGANIZATION

The class was organized into teams averaging four to five students for the assignment and met three times a week (usually before noon on Monday, Wednesday, and Friday) for one-hour lectures, which was in addition to a 3-hour laboratory period per week, scheduled on Monday afternoon.

A substantial portion of this open-ended assignment was treated within the framework of the laboratory. The importance of teamwork was stressed, with an emphasis on including the workload distribution in the final report as a requirement. The team members were also asked to exclude the names of any inactive participant in the report (the student in question would receive a failing grade). One of the items in the list of topics to be discussed each week was how well the team members interacted and whether there was a need to either exclude or split any team into small number of students. Usually, the students refrained from creating conditions that would precipitate splitting their team since it would amount to a heavier workload per student left on the team. Perhaps as a result of these prior arrangements, no team was split.

THE MODELING

The model of the CSTR system was expressed in dimensionless state-space form, in terms of liquid height (equivalent to liquid volume for the reactor vessels that were not uniform in cross-sectional area), concentration, and temperature. Equations (1) and (2) (see Table 2, next page), respectively, designated the dimensionless state space of the system under uncontrolled and controlled conditions, with applicable initial conditions and Jacobian defined by Eqs. (3) and (4), respectively. These systems characterize the time variations of the state space, which belong to a class of nonlinear autonomous equations in which there was no time variable involved in the definition.

Large nonlinear systems occur in many important applications such as the simulation and control of chemically reacting systems

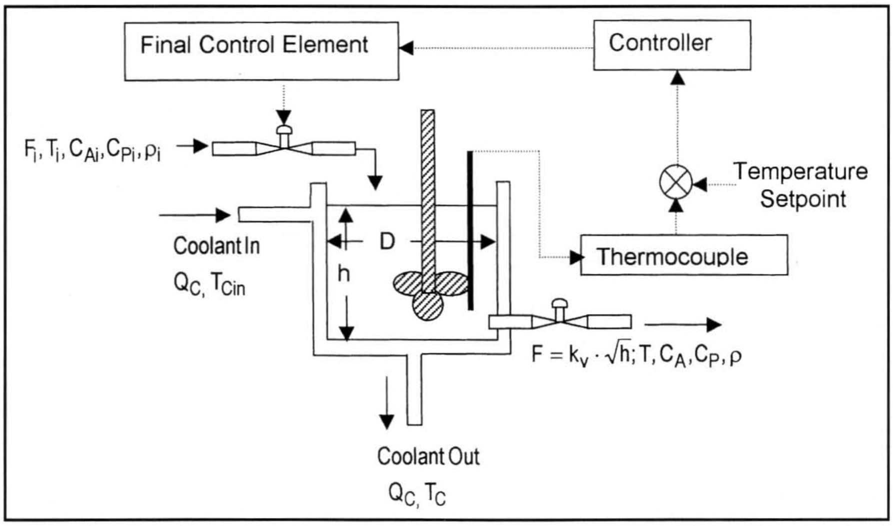

__Figure 1.__ A closed feedback control loop of the modeled CSTR showing the essential components and parameters.

whose solutions sometimes precipitate what is known as "still problems." The still problems usually arise from mixing of terms of fast and slow dynamics with the consequence that the use of Runge-Kutta's fixed-step technique will yield unsatisfactory results. Students were therefore reminded that stiff problems are more competently resolved by employing varying-step methods such as the modified-adaptive step, Brulisch-Stoer or Rosenbrock techniques, all of which are built into the Mathcad software package (see Table 3).

Most students were already familiar with Mathcad and the decision to use it for the problem assignment enabled a focused attention on the problem solution rather than being worried with writing a correct high-level programming language. Additionally, it enabled a different understanding of other process control simulation modules, such as the use of Process Identification and Control Loop

TABLE 2

$$\frac{d}{d\theta}\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{bmatrix} F_{ino} - a\sqrt{X_1} \\ \dfrac{F_{ino}(X_{2in} - X_2)}{X_1} - b\exp\left(\dfrac{\gamma}{X_3}\right)X_2 \\ \dfrac{F_{ino}(X_{3in} - X_3)}{X_1} + P_1\exp\left(\dfrac{\gamma}{X_3}\right)X_2 - \dfrac{P_2(X_3 - X_{Cin})}{X_1} \end{bmatrix} \tag{1}$$

$$\frac{d}{d\theta}\begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{bmatrix} F_{ino} - a\sqrt{X_1} \\ \dfrac{F_{ino}(X_{2in} - X_2)}{X_1} - b\exp\left(\dfrac{\gamma}{X_3}\right)X_2 \\ \dfrac{c(X_3 - X_{set})(X_{3in} - X_3)}{X_1} + P_1\exp\left(\dfrac{\gamma}{X_3}\right)X_2 - \dfrac{d(X_3 - X_{Cin})}{X_1} \end{bmatrix} \tag{2}$$

$$X = \begin{bmatrix} X_1(\theta) \\ X_2(\theta) \\ X_3(\theta) \end{bmatrix} \tag{3}$$

$$J = \begin{bmatrix} \dfrac{df_1}{d\theta} & \dfrac{df_1}{dX_1} & \dfrac{df_1}{dX_2} & \dfrac{df_1}{dX_3} \\ \dfrac{df_2}{d\theta} & \dfrac{df_2}{dX_1} & \dfrac{df_2}{dX_2} & \dfrac{df_2}{dX_3} \\ \dfrac{df_3}{d\theta} & \dfrac{df_3}{dX_1} & \dfrac{df_3}{dX_2} & \dfrac{df_3}{dX_3} \end{bmatrix} \tag{4}$$

$$\left.\begin{array}{lllll} X_1 = \dfrac{h}{h_o} & X_2 = \dfrac{C}{C_{Ao}} & X_3 = \dfrac{T}{T_o} & X_{2in} = \dfrac{C_{Ai}}{C_o} & X_{3in} = \dfrac{T_i}{T_o} \\ X_{set} = \dfrac{T_{set}}{T_o} & X_{Cin} = \dfrac{T_{Cin}}{T_o} & \theta = \dfrac{V}{F_o} = \dfrac{Ah_o}{F_o} & F_{ino} = \dfrac{F_i}{F_o} & U = \sqrt[3]{Q_C}C_1 \\ a = \dfrac{k_V\theta}{A\sqrt{h_o}} & b = k_o\theta & c = \dfrac{k_C T_o\theta}{Ah_o} & d = \dfrac{UA_C\theta}{\rho CpAh_o\left(1+\dfrac{1}{F_C}\right)} & \gamma = \dfrac{-E}{RT_o} \\ P_1 = \dfrac{(-\Delta H)bC_{Ao}}{\rho CpT_o} & P_2 = \dfrac{UA_C\theta}{\rho CpAh_o} & & & \end{array}\right\} \tag{5}$$

Explorer system, PICLES,[8] and MATLAB/SIMULINK,[9-11] which were introduced later for different process-control problem assignments. Advanced control system[12] is a similar software package that is also available.

CASE STUDIES

The tasks of the problem assignment encompassed simple case studies aimed at determining the dynamics of the

- *Uncontrolled system during fill-up*
- *Uncontrolled system at constant liquid height*
- *P-only controlled system at constant liquid height*
- *P-only controlled system right from start-up*
- *Effects of multiple-fold increase in cooling rate*

Typical simulation conditions associated with each case study are explained in Table 4, with representative graphical results shown in Figures 2 through 4. Prior to simulation, it was instructional for the students to make the equations dimensionless and to prepare a table of variables detailing the input values assigned to each parameter under each case study, as shown in Table 5.

OBSERVATIONS AND CONCLUSIONS

Our observations can be summarized in two categories: the pedagogical value of the approach and the usefulness of simulation as a powerful tool in learning various concepts in process control. From the standpoint of pedagogy, it was

TABLE 3
Various Built-In Solution Tools of Mathcad

Method	*Inputs*	*Outputs*
Varying Step Technique	Z=Rkadapt(X, θ_i θ_f, npoints, D(θ,X))	Z=F(θ,X_1,X_2,X_3)
Rosenbrock Technique	Z=stiffr(X, θ_i θ_f, npoints, D(θ,X),J)	Z=F(θ,X_1,X_2,X_3)
Fixed StepTechnique	Z=rkfixed(X, θ_i θ_f, npoints, D(θ,X))	Z=F(θ,X_1,X_2,X_3)
Burlisch-Stoer Technique	Z=stiffb(X, θ_i θ_f, npoints, D(θ,X),J)	Z=F(θ,X_1,X_2,X_3)

TABLE 4
Various Simulation Case Studies Investigated

	Case Studies	*Conditions*
I	Uncontrolled dynamics during fill-up	(1) X_1=0; X_2=1; X_3=1
II	Uncontrolled dynamics at constant height	(2) F_{ino}=F_{out}; X_1=1; X_2=1; X_3=1
III	P-only controlled system at constant height	(3) F_{ino}=K_C(X_3-X_{set}) and (2)
IV	P-only controlled system at startup	(4) F_{ino}=K_C(X_3-X_{set}) and (1)
V	Effects of multiple-fold increase in cooling rate	(5) n=1,2..N; Qc=nQc_n and (2)

TABLE 5
Input Values Used in the Calculation

Parameter	*Case Studies* *I*	*II*	*III*	*IV*	*V*	*Description*
θ	0/5	0/5	0/5	0/5	0/5	Time (Initial/Final)
a	0	0.01	0.01	0.01	0.01	Coefficient
b	1.63E13	1.63E13	1.63E13	1.63E13	1.63E13	Coefficient
c	-	-	49.17	49.17	49.2 - 245.8	Coefficient
d	-	-	0.907	0.907	0.91 - 1.55	Coefficient
e	-	-	1.5E13	1.5E13	1.5E13	Coefficient
F_{ino}	1	1	1	1	1	Flow rate
P_1	1.5E13	1.5E13	1.5E13	1.5E13	1.5E13	Coefficient
P_2	9.342	9.342	9.342	9.342	9.342 - 14.83	Coefficient
γ	-31.78	-31.78	-31.78	-31.78	-31.78	Arrhenius Number
X_{2in}	1	1	1	1	1	Inlet Concentration
X_{3in}	1	1	1	1	1	Inlet Temperature
X_{cin}	0.959	0.959	0.959	0.959	0.959	Inlet Coolant Temperature
X_{set}	-	-	0.973	0.973	0.973	Setpoint
X_1	0(1)	1(2)	1(2)	0(1)	0(1)	Initial Height
X_2	1	1	1	1	1	Initial Concentration
X_3	1	1	1	1	1	Initial Temperature

(1) To avoid singularity problems, the actual number used was 1×10^{-6}
(2) Liquid level was fixed at constant height while temperature was being controlled

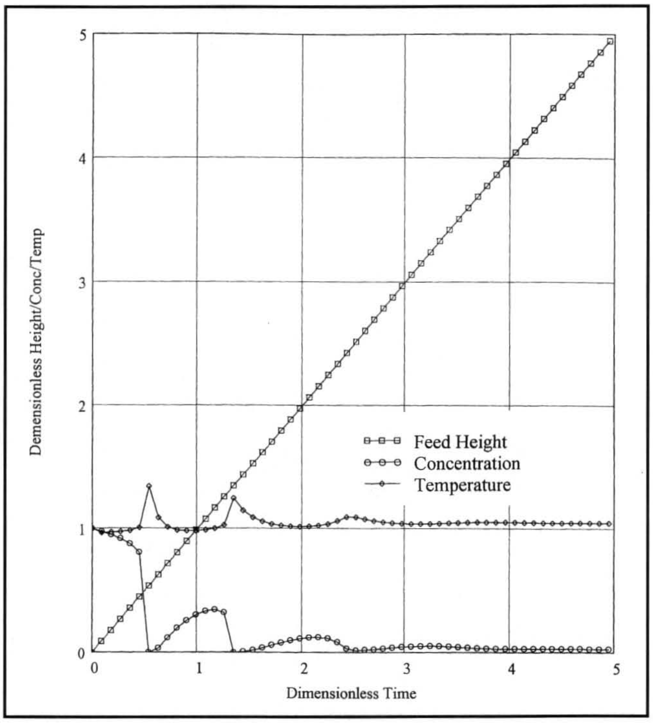

Figure 2. *Case Study I: The dynamic response of the uncontrolled system during startup, with no effluent output. The tank fills at dimensionless time=1.*

observed that the problem assignment formulated in this manner gave the students a lot of confidence by focusing their attention on the subject of the problem, which was to model and simulate the system. There was an opportunity to investigate as many case studies as possible, the result of which advanced general understanding of the concepts that are vital to learning of the course materials.

Toward the end of the assignment, the preconceived notion of the course being a means of learning mathematics was suddenly changed to the use of mathematics as a tool in learning process control. Consequently, there was a general feeling of "I can do it on my own" among many students. This was the kind of confidence we wanted them to develop, and our feeling was overwhelming when we saw it work.

Secondly, breaking up the assignment into various case studies enabled the students to answer simple "what-if" questions associated with them. For example, Case Study I dealt with investigating the dynamics of the uncontrolled system during fill-up, with the outlet valve closed (see Figure 2). It was learned that so long as the valve remained closed, the liquid level in the reactor would continue to rise, the effect of which would possibly lead to overflow. The evidence of the system attaining stability in concentration and temperature, *i.e.*, X_2 and X_3 eventually settling at certain bounded levels as time approached infinity even as the liquid level increased,

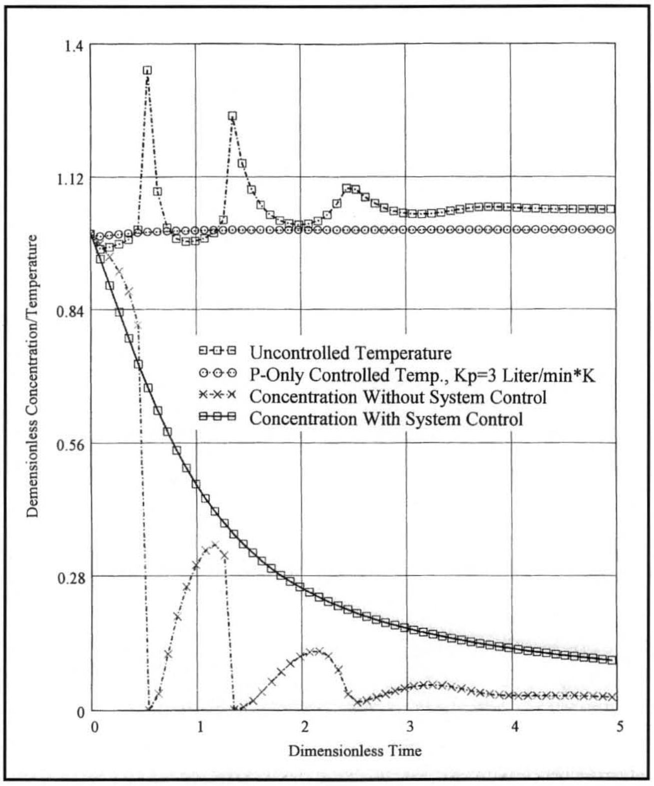

Figure 3. *Comparison of Case Studies I (uncontrolled) and III (controlled) for temperature and concentration dynamics. Application of proportional control effectively removed the oscillations in both variables.*

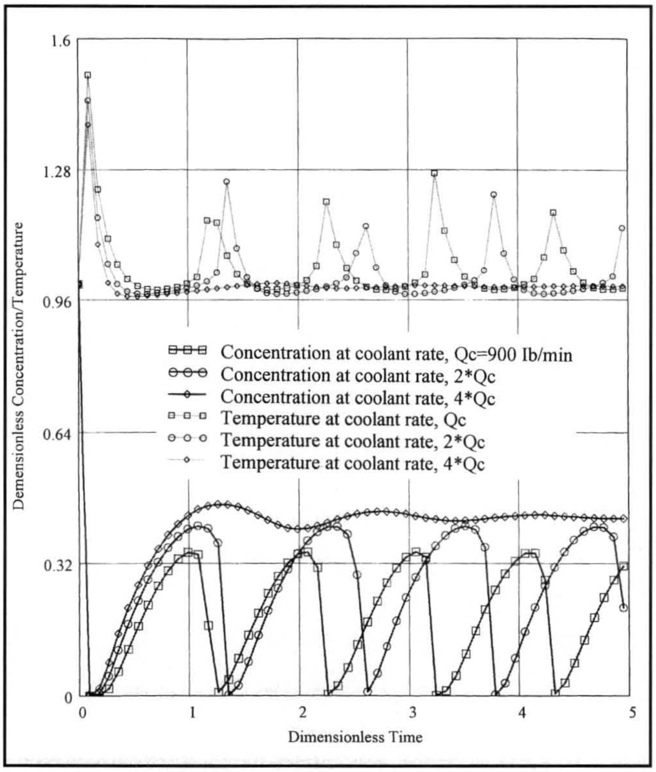

Figure 4. *Case Study V: The effects of multiple-fold increase in flowrate of the coolant is marked by decreased frequency in oscillatory behavior of temperature and concentration, which eventually led to the disappearance of oscillation completely.*

was seen. When a proportional control was applied for control of temperature using the inlet flowrate of the feed as the manipulated variable (see Figure 3), the oscillatory behavior in both concentration (X_2) and temperature (X_3) was removed. The controlled system experienced gradual decay rather than oscillatory changes that marked the behavior of the uncontrolled system.

In Case Study V where the flowrate of the coolant was increased in multiple-fold of up to four, the system experienced pronounced oscillation in temperature and concentration despite the fact that control was applied. But the character of the oscillatory behavior was marked by a decrease in frequency, which eventually disappeared with increase in coolant flowrate (Figure 4). This was an indication that flowrate of the coolant could alternatively be used as a manipulated variable to control the system temperature. The students learned at this point that there was more than one way of achieving control of the system, having discovered the two candidates for manipulated variables, *i.e.,* the feed inlet stream and the flowrate of the coolant.

The assignment also gave the students the opportunity to revisit past courses such as kinetics, heat transfer, and calculus, and gave them the chance to apply the knowledge they have previously learned to this assignment. Since this assignment was given in the first two weeks of the course, many students recognized the need to review some of the earlier course materials they had taken prior to process control.

Overall, this problem assignment received positive commendations from over two-thirds of the class, with many of them stating that it helped them integrate ideas and to use them to study typical problems that occur in many chemical industries. From our point of view, the project was worthwhile, considering the foundation work it laid for better understanding of various topics taught in other courses in the past. Most important in our estimation, however, was its value in fostering understanding of the subject of process control as a course.

ACKNOWLEDGMENTS

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NOMENCLATURE

A	cross sectional area of the tank, cm^2
A_c	surface area for heat transfer, cm^2
a	coefficient (see Eq. 5)
b	coefficient (see Eq. 5)
C_A	concentration of component A in tank (H_2O_2), mole/liter
C_{Ai}	inlet concentration of component A (H_2O_2), mol/liter
C_p	specific heat capacity, J/g K
C_1	parameter associated with heat removal rate, BTU/(hr ft^{2}°F)(lb/min)$^{1/3}$
c	coefficient (see Eq. 5)
D	diameter of the reactor, cm
$D(\theta,X)$	vector valued function of the state-space variables
d	coefficient (see Eq. 5)
E	energy of activation, J/mol
F_c	system parameter associated with cooling, dimensionless
F_{ino}	dimensionless flowrate
F_I	inlet flow rate, liter/min
h	height of the liquid in the tank, cm
J	Jacobian matrix
k_o	pre-exponential factor, 1/sec
K_c	controller gain, liter/min*K
K_p	proportional gain
K_v	valve constant, $cm^{2.5}$/sec
P_1	coefficient (see Eq. 5)
P_2	coefficient (see Eq. 5)
R	universal gas constant, J/mol K
Q_c	coolant volumetric flowrate, liter/min
T	temperature of the reacting mixture in the tank, °C
T_c	temperature of the coolant in the jacket, °C
T_i	inlet temperature of the reacting mixture in the tank, °C
T_{set}	setpoint temperature of the reacting mixture in the tank, °C
U	overall heat transfer coefficient, J/cm^2 K
V	volume of the reacting mixture, liters
X_1	dimensionless height
X_2	dimensionless concentration
X_3	dimensionless temperature
X_{2in}	dimensionless inlet concentration
X_{3in}	dimensionless inlet temperature
X_{Cin}	dimensionless inlet temperature of the coolant
X_{set}	dimensionless temperature setpoint
γ	Arrhenius number, dimensionless
ΔH	enthalpy of reaction, J/mol
ρ	density of the reacting mixture in the tank, g/cm^3
θ	residence time, min

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