# A First Course on Kinetics and Reaction Engineering

# Example 29.1

## Problem Purpose

This problem will help you determine whether you have mastered the learning objectives for this unit. Specifically, it illustrates the analysis of a CSTR cascade. In addition, it highlights the difference between a single CSTR and a CSTR cascade.

## Problem Statement

The rate expression for liquid phase reaction (1) is given in equation (2); the pre-exponential factor is equal to 12,000 mol $L^{-1}$ $min^{-1}$, the activation energy is 6,500 cal $mol^{-1}$ and the constant $K$ is equal to 0.21 mol $L^{-1}$. The reactant A flows into the process at a rate of 9.5 L $min^{-1}$ at a concentration of 1.3 mol $L^{-1}$ and a temperature of 75 °C. The heat of reaction (1) is constant and equal to 4300 cal $mol^{-1}$, and the heat capacity of the solution is also constant and equal to 0.515 cal $cm^{-3}$ $K^{-1}$. Compare the total reactor volume required to convert 99% of the reactant if a single CSTR is used to that when a cascade of three CSTRs of equal volume is used.

$$A \rightarrow Z \tag{1}$$

$$r = k_0 \exp\left\{\frac{-E}{RT}\right\}\frac{C_A}{K + C_A} \tag{2}$$

## Problem Analysis

In this problem we are given the rate expression for the reaction and asked questions about reactor performance, therefore it is a reaction engineering problem and not a kinetics problem. The reactors involved are CSTRs, and they operate adiabatically. Nothing in the problem statement mentions any changes to the reactor or reactors as they are operating, so we will analyze their steady state operation. To answer the questions posed, for each reactor we will write mole balances for every species that appears as either a reactant or a product in at least one reaction, and we will write an energy balance on the reacting fluid. We will solve the resulting set of design equations and use the results to answer the questions asked in the problem statement.

## Problem Solution

The general steady state CSTR mole and energy balance design equations are given in equations (3) and (4). In this problem, there is only one reaction occurring, so the summations over the reactions will reduce to a single term. The reactors operate adiabatically and perform negligible work through moving shafts and boundaries, so the heat input and work terms will equal zero. Finally, we are given a volume-specific heat capacity for the fluid as a whole, so the summation over the individual heat capacities of the species can be replace by a single sensible heat term. With those simplifications, steady state CSTR mole balances for A and Z and a steady state CSTR energy balance will take the form given in equations

(5) through (7). In past problems involving flow reactors, we have used a superscripted zero to denote inlet quantities and no superscript for outlet properties. Now that we are working with multiple reactors, we will need to be more explicit in identifying the specific inlet and outlet streams, so equations (5) through (7) have been written with explicit subscripts denoting inlet ("in") and outlet ("out") streams. The subscript "out" has also been added to the rate because a CSTR is perfectly mixed, meaning that the composition and temperature of the outlet stream is the same as the composition and temperature every where within the reactor, and the rate is evaluated at the conditions in the reactor.

$$0 = \dot{n}_i^0 - \dot{n}_i + V \sum_{\substack{j=all \\ reactions}} \nu_{i,j} r_j \tag{3}$$

$$0 = \sum_{\substack{i=all \\ species}} \left( \dot{n}_i^0 \int_{T^0}^{T} \hat{C}_{pi}\, dT \right) + V \sum_{\substack{j=all \\ reactions}} r_j \Delta H_j(T) - \dot{Q} + \dot{W} \tag{4}$$

$$0 = \dot{n}_{A,in} - \dot{n}_{A,out} - V r_{out} \tag{5}$$

$$0 = \dot{n}_{Z,in} - \dot{n}_{Z,out} + V r_{out} \tag{6}$$

$$0 = \dot{V}_{in} \int_{T_{in}}^{T_{out}} \tilde{C}_p\, dT + V r_{out} \Delta H(T_{out}) = \dot{V}_{in} \tilde{C}_p (T_{out} - T_{in}) + V r_{out} \Delta H(T_{out}) \tag{7}$$

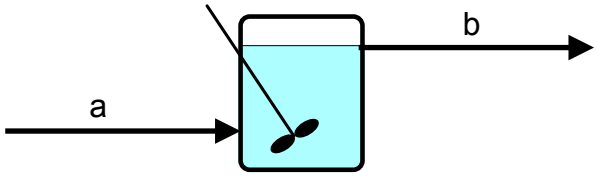


*Figure 1. Schematic diagram for the single reactor case.*

We now can consider the two situations specified in the problem. First, consider a single CSTR as illustrated schematically in Figure 1. Note that in the figure, the inlet stream has been designated as stream $a$ and the outlet stream as stream $b$. Thus, when the design equations (5) through (7) are written for this reactor, they take the form given in equations (8) through (10).

$$0 = f_1(V, \dot{n}_{Z,b}, T_b) = \dot{n}_{A,a} - \dot{n}_{A,b} - V r_b \tag{8}$$

$$0 = f_2(V, \dot{n}_{Z,b}, T_b) = \dot{n}_{Z,a} - \dot{n}_{Z,b} + V r_b \tag{9}$$

$$0 = f_3(V, \dot{n}_{Z,b}, T_b) = \dot{V}_a \tilde{C}_p (T_b - T_a) + V r_b \Delta H(T_b) \tag{10}$$

Equations (8) through (10) are non-linear, non-differential equations. In order to solve them numerically one must (a) identify a set of unknown quantities, equal in number to the number of equations, (b) provide a guess for the value of each unknown, and (c) provide code that when given values for the unknowns, evaluates the equations. You can see in the equations above that I have identified $V$, $\dot{n}_{Z,b}$ and $T_b$ as the unknowns, and I can guess a value for each. The code I provide will need to evaluate the functions $f_1$ through $f_3$, given values for $V$, $\dot{n}_{Z,b}$ and $T_b$. To do that, I'll need to be able to provide or calculate a value for every other quantity that appears in the functions. Looking through the functions, it can be seen that $\dot{V}_a$ = 9.5 L min$^{-1}$, $\tilde{C}_p$ = 0.515 cal cm$^{-3}$ K$^{-1}$, $T_a$ = 75 °C and $\Delta H\left(T_b\right)$ = 4300 cal mol$^{-1}$ are constants given in the problem statement. The inlet molar flow rate of A is also a constant that can be calculated from the inlet volumetric flow rate and the inlet concentration of A ($C_{A,a}$ = 1.3 mol L$^{-1}$) given in the problem statement using equation (11). The inlet molar flow rate of Z is zero since the problem does not mention that any Z is present in the feed.

$$\dot{n}_{A,a} = C_{A,a}\dot{V}_a \tag{11}$$

The outlet molar flow rate of A is also a constant, and once the inlet molar flow rate is found, the outlet molar flow rate of A can be calculated from the conversion ($f_A$ = 0.99) given in the problem statement using equation (12). The rate, $r_a$, can be calculated using equation (2) with the constants $k_0$ = 12,000 mol L$^{-1}$ min$^{-1}$, $E$ = 6,500 cal mol$^{-1}$ and $K$ = 0.21 mol L$^{-1}$, given in the problem statement. As previously noted, the concentration of A appearing in the rate expression is the concentration of A in stream $b$, which can be calculated using equation (13). The rate coefficient in equation (2) will be evaluated at $T_b$, as well. Since the problem specifies that the fluid density is constant, the volumetric flow rate of stream $b$ is equal to the volumetric flow rate of stream $a$, which is given.

$$\dot{n}_{A,b} = \dot{n}_{A,a}\left(1 - f_A\right) \tag{12}$$

$$C_{A,b} = \frac{\dot{n}_{A,b}}{\dot{V}_b} = \frac{\dot{n}_{A,b}}{\dot{V}_a} \tag{13}$$

With that information, code can be written to evaluate the functions $f_1$ through $f_3$, given values for $V$, $\dot{n}_{Z,b}$ and $T_b$, and the design equations (8) through (10) can be solved numerically to find the values of $V$, $\dot{n}_{Z,b}$ and $T_b$. Upon doing so, one finds that the required reactor volume is 284 L.

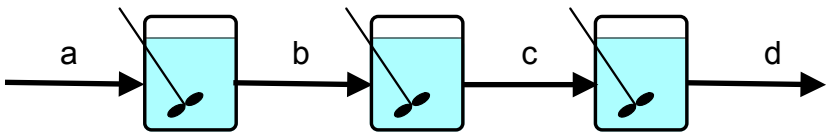


*Figure 2. Schematic diagram for the 3 CSTR cascade.*

Next consider the situation where three CSTRs with equal volumes are used, as shown schematically in Figure 2. As before, each of the flow streams have been numbered. Thus, for example, when the design equations (5) through (7) are written for the middle CSTR, the "in" stream is stream $b$ and the "out" stream is stream $c$. In this way, the design equations for all three reactors can be written as in equations (14) through (22). The problem states that the reactors have equal volumes, so in equations (14) through (22), $V$ represents the volume of one of the CSTRs.

$$0 = f_1\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{n}_{A,a} - \dot{n}_{A,b} - Vr_b \tag{14}$$

$$0 = f_2\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{n}_{Z,a} - \dot{n}_{Z,b} + Vr_b \tag{15}$$

$$0 = f_3\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{V}_a\tilde{C}_p\left(T_b - T_a\right) + Vr_b\Delta H\left(T_b\right) \tag{16}$$

$$0 = f_4\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{n}_{A,b} - \dot{n}_{A,c} - Vr_c \tag{17}$$

$$0 = f_5\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{n}_{Z,b} - \dot{n}_{Z,c} + Vr_c \tag{18}$$

$$0 = f_6\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{V}_b\tilde{C}_p\left(T_c - T_b\right) + Vr_c\Delta H\left(T_c\right) \tag{19}$$

$$0 = f_7\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{n}_{A,c} - \dot{n}_{A,d} - Vr_d \tag{20}$$

$$0 = f_8\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{n}_{Z,c} - \dot{n}_{Z,d} + Vr_d \tag{21}$$

$$0 = f_9\left(V,\dot{n}_{A,b},\dot{n}_{Z,b},T_b,\dot{n}_{A,c},\dot{n}_{Z,c},T_c,\dot{n}_{Z,d},T_d\right) = \dot{V}_c\tilde{C}_p\left(T_d - T_c\right) + Vr_d\Delta H\left(T_d\right) \tag{22}$$

Once again, the design equations are a set of non-linear, non-differential equations. If you look at only the equations for the first reactor, you'll see that there are three equations, but four unknowns ($V$, $\dot{n}_{A,b}$, $\dot{n}_{Z,b}$ and $T_b$). Thus, the equations for the first reactor cannot be solved alone. The same is true for the other two reactors, so all three sets of design equations will need to be solved simultaneously. In order to solve them numerically one must (a) identify a set of unknown quantities, equal in number to the number of equations, (b) provide a guess for the value of each unknown, and (c) provide code that when given values for the unknowns, evaluates the equations. This time there are nine equations, and you can see in the equations above that I have identified $V$, $\dot{n}_{A,b}$, $\dot{n}_{Z,b}$, $T_b$, $\dot{n}_{A,c}$, $\dot{n}_{Z,c}$, $T_c$, $\dot{n}_{Z,d}$ and $T_d$ as the unknowns; I can guess a value for each. The code I provide will need to evaluate the functions $f_1$ through $f_9$, given values for the unknowns. To do that, I'll need to be able to provide or calculate a value for every other quantity that appears in the functions.

As for the single CSTR case, $\dot{V}_a = \dot{V}_b = \dot{V}_c = \dot{V}_d$ = 9.5 L min$^{-1}$, $\tilde{C}_p$ = 0.515 cal cm$^{-3}$ K$^{-1}$, $T_a$ = 75 °C and $\Delta H\left(T_b\right) = \Delta H\left(T_c\right) = \Delta H\left(T_d\right)$ = 4300 cal mol$^{-1}$ are constants given in the problem statement. The inlet molar flow rate of A can be calculated as before using equation (11), and the outlet molar flow rate of

A can be calculated from the given fractional conversion, $f_A$; the only difference is that now the outlet is stream $d$, leading to equation (23).

$$\dot{n}_{A,d} = \dot{n}_{A,a}\left(1 - f_A\right) \tag{23}$$

The rate is again calculated using equation (2) with the constants $k_0$, $E$ and $K$ given earlier (and in the problem statement). In equations (14) through (16), which are balances on the first reactor, the concentration of A is given by equation (24) and the rate coefficient is evaluated at $T_b$. Similarly, in equations (17) through (19) the concentration of A is given by equation (25) and the rate coefficient is evaluated at $T_c$ and in equations (20) through (22) the concentration of A is given by equation (26) and the rate coefficient is evaluated at $T_d$.

$$C_{A,b} = \frac{\dot{n}_{A,b}}{\dot{V}_b} = \frac{\dot{n}_{A,b}}{\dot{V}_a} \tag{24}$$

$$C_{A,c} = \frac{\dot{n}_{A,c}}{\dot{V}_c} = \frac{\dot{n}_{A,c}}{\dot{V}_a} \tag{25}$$

$$C_{A,d} = \frac{\dot{n}_{A,d}}{\dot{V}_d} = \frac{\dot{n}_{A,d}}{\dot{V}_a} \tag{26}$$

With that information, code can be written to evaluate the functions $f_1$ through $f_9$, given values for the unknowns ($V$, $\dot{n}_{A,b}$, $\dot{n}_{Z,b}$, $T_b$, $\dot{n}_{A,c}$, $\dot{n}_{Z,c}$, $T_c$, $\dot{n}_{Z,d}$ and $T_d$), and the design equations (14) through (22) can be solved numerically to find the values of those unknowns. Upon doing so, one finds that the individual reactors have a volume of 15.3 L each giving a total required reactor volume of 45.9 L.

We have just seen that for this particular reaction, using a cascade of three CSTRs reduces the total reactor volume from 284 L to 46 L. Each of the three reactors in the cascade is much smaller than the volume that would be required for a single CSTR. This is not a particularly surprising result. We have a typical reaction where the rate will decrease as the reaction progresses due to reactant concentration decreases. That reaction is also endothermic, so if the reactor is adiabatic, the temperature will decrease as the reaction progresses, causing the rate to decrease even more. In a single CSTR, the reaction occurs at the final conditions where the rate is very low. A low rate per unit volume leads to the need for a large reactor. By using three CSTRs in series, the concentration of reactant and the temperature are larger in the first reactor, leading to a higher rate and smaller required volume. In the second reactor the reactant concentration and temperature are smaller, but still larger than in the single CSTR. So in the second reactor the rate is also greater than in the single CSTR, and again less volume is needed. Since the overall conversion is fixed, the third CSTR in the cascade will be at the same temperature and reactant concentration as the single CSTR, so only this third reactor is equivalent to the single CSTR in terms of reaction rate. If one were designing a reactor and needed to specify the kind of reactor to use, a simple qualitative analysis would show that either a PFR or a cascade of CSTRs will outperform a single CSTR.

**Calculation Details Using MATLAB**

Supplemental Unit S2 describes how to solve sets of non-differential equations numerically using MATLAB, and it provides a template file named SolvNonDif.m for doing so. Before it can be used to solve a problem, that template file must be modified in four places, each indicated by a comment that begins "% EDIT HERE". In addition to those required modifications I made a few additional modifications that will be described here along with the required modifications.

I recommend that you work with a copy of the file that has been given a more meaningful name; I made two copies of SolvNonDif.m, saving one as Example_29_1_a.m (for the single CSTR case) and the other as Example_29_1_b.m (for the CSTR cascade case). Since the function name must match the filename, I changed the names accordingly. At the same time, knowing that I won't need to use the results from these calculations in subsequent calculations, I changed both functions so that they do not return any values. The template file begins with a long set of comments describing what it does and how to use it; I replaced these comments with a brief comment stating the purpose of the modified version. None of these modifications were required.

The first ***required*** modification is to enter the values of all universal and problem-specific constants at the point indicated. At the same time these are entered, they should be converted to a consistent set of units. I also entered the ideal gas constant and the three constant quantities (inlet and final molar flow rates of A and final concentration of A) that can be calculated using equations (11), (12), (13), (23) and (26). In the single CSTR case, the final values correspond to stream $b$, while in CSTR cascade, they correspond to stream $d$, so their names are different in the two files. Listings 1 and 2 show the relevant parts of the two MABLAB files.

```
% Modified version of the AFCoKaRE MATLAB template file SolvNonDif.m used
% in the solution of the first part of Example 29.1 of "A First Course on
% Kinetics and Reaction Engineering."
%
function Example_29_1_a
    % Known quantities and constants
    k0 = 12000.0; % mol/L/min
    E = 6500.0; % cal/mol
    K = 0.21; % mol/L
    VFR = 9.5; % L/min
    CAa = 1.3; % mol/L
    nZa = 0; % mol/min
    Ta = 75 + 273.15; % K
    dH = 4300.0; % cal/mol
    cP = 0.515*1000.0; % cal/L/K
    fA = 0.99;
    % Gas constant
    R = 1.987; % cal/mol/K
    % Calculated constants
    nAa = VFR*CAa;
    nAb = nAa*(1-fA);
    CAb = nAb/VFR;
```

*Listing 1. Changes to the first part of SolvNonDif.m for use in solving the single CSTR case.*

```
% Modified version of the AFCoKaRE MATLAB template file SolvNonDif.m used
% in the solution of the second part of Example 29.1 of "A First Course on
% Kinetics and Reaction Engineering."
%
function Example_29_1_b
    % Known quantities and constants
    k0 = 12000.0; % mol/L/min
    E = 6500.0; % cal/mol
    K = 0.21; % mol/L
    VFR = 9.5; % L/min
    CAa = 1.3; % mol/L
    nZa = 0; % mol/min
    Ta = 75 + 273.15; % K
    dH = 4300.0; % cal/mol
    cP = 0.515*1000.0; % cal/L/K
    fA = 0.99;
    % Gas constant
    R = 1.987; % cal/mol/K
    % Calculated constants
    nAa = VFR*CAa;
    nAd = nAa*(1-fA);
    CAd = nAd/VFR;
```

*Listing 2. Changes to the first part of SolvNonDif.m for use in solving the CSTR cascade case.*

The second ***required*** modification involves entering the code to evaluate functions $f_1$ through $f_3$ (equations (8) through (10)) or $f_1$ through $f_9$ (equations (14) through (22)). In the code, this occurs within an internal function named evalEqns; within evalEqns, both the unknowns and the equations are provided as vector quantities named z and f, respectively. Thus, it is necessary to map the unknowns in this problem solution ($V$, $\dot{n}_{Z,b}$ and $T_b$ for the single CSTR and $V$, $\dot{n}_{A,b}$, $\dot{n}_{Z,b}$, $T_b$, $\dot{n}_{A,c}$, $\dot{n}_{Z,c}$, $T_c$, $\dot{n}_{Z,d}$ and $T_d$ for the CSTR cascade) to a vector z, and to return the values of the functions in the vector f. I find it useful at the start of the internal function that will evaluate the functions, to define local variables with the names used in the problem statement. This modification is not required, but in my opinion, it makes the code more readable and easier to debug. In addition, the list of variables here serves as a reminder of the mapping of the problem solution variables to the vector z.

Recall from the solution that in order to evaluate the functions it is first necessary to calculate the rate using equation (2). For the single CSTR and the last CSTR in the cascade, that can be done directly since the concentration of A in the outlet stream is a known constant. However, for the first and second CSTRs in the cascade, it is first necessary to calculate the concentrations of A using equations (24) and (25). Once the rates have been calculated the functions can next be evaluated. The code containing all these modifications is shown in Listing 3 for the single CSTR case and in Listing 4 for the CSTR cascade.

```
% Function that evaluates the equations
function f = evalEqns(z)
    V = z(1);
    nZb = z(2);
    Tb = z(3);
    ra = k0*exp(-E/R/Tb)*CAb/(K + CAb);
    f = [
        nAa - nAb - V*ra
        nZa - nZb + V*ra
        VFR*cP*(Tb - Ta) + V*ra*dH
    ];
end % of internal function evalEqns
```

*Listing 3. Internal function that evaluated the equations being solved for the single CSTR case.*

```
% Function that evaluates the equations
function f = evalEqns(z)
    V = z(1);
    nAb = z(2);
    nAc = z(3);
    nZb = z(4);
    nZc = z(5);
    nZd = z(6);
    Tb = z(7);
    Tc = z(8);
    Td = z(9);
    CAb = nAb/VFR;
    CAc = nAc/VFR;
    ra = k0*exp(-E/R/Tb)*CAb/(K + CAb);
    rb = k0*exp(-E/R/Tc)*CAc/(K + CAc);
    rc = k0*exp(-E/R/Td)*CAd/(K + CAd);
    f = [
        nAa - nAb - V*ra
        nZa - nZb + V*ra
        VFR*cP*(Tb - Ta) + V*ra*dH
        nAb - nAc - V*rb
        nZb - nZc + V*rb
        VFR*cP*(Tc - Tb) + V*rb*dH
        nAc - nAd - V*rc
        nZc - nZd + V*rc
        VFR*cP*(Td - Tc) + V*rc*dH
    ];
end % of internal function evalEqns
```

*Listing 4. Internal function that evaluated the equations being solved for the CSTR cascade case.*

The third ***required*** modification is where guesses for the unknowns are provided. The guesses are entered in the array named z_guess. They must be entered using the same mapping of the unknowns to the vector `z` as was used in the internal function `evalEqns`. The previous modification, where variables with more meaningful names were defined, serves as a key to remind you which variable is `z(1)`, which

is z(2), and so on. Listing 5 shows the guesses used for the single CSTR case and Listing 6 shows the guesses for the CSTR cascade.

```
    % guesses for the solution
    z_guess = [
        100.
        nAa - nAb
        Ta + 10
    ];
```

*Listing 5. Guesses for the values of the unknowns used in the single CSTR case.*

```
    % guesses for the solution
    z_guess = [
        50.
        0.3*nAa
        0.6*nAa
        nAa - 0.3*nAa
        nAa - 0.6*nAa
        nAa - nAd
        Ta + 10
        Ta + 20;
        Ta + 30;
    ];
```

*Listing 6. Guesses for the values of the unknowns used in the single CSTR case.*

The final ***required*** modification only applies if you need to use the results from solving the set of equations to calculate other quantities. For the single CSTR case, there are no additional calculations needed, but I did put in a statement that will print the value of the reactor volume, as can be seen in Listing 7. For the CSTR cascade, it is necessary to calculate the total reactor volume. As Listing 8 shows, I also added a statement that calculates and displays the total reactor volume.

```
    % Solve the set of algebraic equations
    z = fsolve(@evalEqns, z_guess);
    display('The solver found the following values for the unknowns:');
    z
    display('The corresponding values of the functions being solved are
as follows:');
    f = evalEqns(z)
    V = z(1)
```

*Listing 7. Final part of the MATLAB file used to solve the single CSTR design equations.*

```
    % Solve the set of algebraic equations
    z = fsolve(@evalEqns, z_guess);
    display('The solver found the following values for the unknowns:');
    z
    display('The corresponding values of the functions being solved are
as follows:');
    f = evalEqns(z)
    V_cstr = z(1)
    V_total = 3*z(1)
```

*Listing 8. Final part of the MATLAB file used to solve the CSTR cascade design equations.*

At this point, the modified template files can be used to solve the equations. To do so, the function name is typed at the MATLAB command prompt. The resulting output in Listings 9 and 10 shows that solver did successfully converge to a solution to the design equations for both cases.

```
>> Example_29_1_a

Equation solved.

fsolve completed because the vector of function values is near zero
as measured by the default value of the function tolerance, and
the problem appears regular as measured by the gradient.

<stopping criteria details>

The solver found the following values for the unknowns:

z =
  283.8797
   12.2265
  337.4042

The corresponding values of the functions being solved are as follows:

f =
   1.0e-09 *

    0.0000
   -0.0000
   -0.1310

V =
  283.8797
```

*Listing 9. Output from the execution of Example_29_1_a.m.*

```
>> Example_29_1_b

Equation solved, fsolve stalled.

fsolve stopped because the relative size of the current step is less than the
default value of the step size tolerance squared and the vector of function values
is near zero as measured by the default value of the function tolerance.

<stopping criteria details>

The solver found the following values for the unknowns:

z =
   15.3015
    4.0208
    0.7825
    8.3292
   11.5675
   12.2265
  340.8295
  337.9834
  337.4042

The corresponding values of the functions being solved are as follows:

f =
   1.0e-09 *

   -0.0000
    0.0000
    0.0946
    0.0000
   -0.0000
   -0.1583
    0.0000
    0.0000
   -0.0146

V_cstr =
   15.3015

V_total =
   45.9045
```

*Listing 10. Output from the execution of Example_29_1_b.m.*