A First Course on Kinetics and Reaction Engineering

Example S5.1

Problem Purpose

This example illustrates the use of the MATLAB template file SolvIVDifI.m to solve a set of initial value ordinary differential equations where the final value of the independent variable is known.

Problem Statement

In equations (1) and (2), A is a constant with a value of 0.1597. Calculate the values of z_1 and z_2 at $t = 1$ and the corresponding percentage change in z_1.

$$\frac{dz_1}{dt} = -A\frac{z_1}{z_1 + z_2} \quad ; \quad z_1(0) = 0.103 \tag{1}$$

$$\frac{dz_2}{dt} = 0.5A\frac{z_1}{z_1 + z_2} \quad ; \quad z_2(0) = 0.0 \tag{2}$$

Problem Analysis

Equations (1) and (2) are ordinary differential equations (ODEs), and both of the boundary conditions are applied at the same boundary, namely $t = 0$. This means that they are initial value ODEs. The problem gives us the final value of t, and t is the independent variable. That means that the MATLAB template file SolvIVDifI.m can be used to solve the problem. Here I will follow the step-by-step instructions for using SolvIVDifI.m that are provided with this supplemental unit. Note also that the equations are written in the form shown in equation (3).

$$
\begin{aligned}
\frac{dz_1}{dt} &= f_1(t, z_1, z_2, \cdots, z_n); & z_1(t_0) &= z_1^0 \\
\frac{dz_2}{dt} &= f_2(t, z_1, z_2, \cdots, z_n); & z_2(t_0) &= z_2^0 \\
&\quad\vdots \\
\frac{dz_n}{dt} &= f_n(t, z_1, z_2, \cdots, z_n); & z_n(t_0) &= z_n^0
\end{aligned}
\tag{3}
$$

Problem Solution

A copy of SolvIVDifI.m was saved in the working directory as S5_Example_1.m. The function declaration statement was changed so that the function name was the same as the filename without the ".m" filetype. At the same time, the long initial comment was changed to a shorter comment indicating the purpose of the modified template file. The template file must be modified in four places each time it is used to solve a new problem. The locations where the modifications are required are indicated by comments that begin "% EDIT HERE." The first required modification involves declaring variables for

each constant that appears in the problem and assigning values to those variables in consistent units. Here there is only one constant, A, and it does not have units. All of these changes can be seen in Listing 1.

```
% Modified version of the MATLAB template file SolvIVDifI.m used to solve
% Example 1 of Supplemental Unit S5 of "A First Course on Kinetics and
% Reaction Engineering."
%
function [t_f,z] = S5_Example_1
    % Known quantities and constants (in consistent units)
    A = 0.1597;
```

Listing 1. Modified version of SolvIVDifl.m after renaming and making the first required modification.

The second required modification involves entering the code to evaluate the derivatives, that is, the right hand sides of equations (1) and (2) when they are written in the form of equation (3). This modification appears within the internal function named odeqns. The resulting, modified version of odeqns is shown in Listing 2.

```
% Function that evaluates the ODEs
function dzdt = odeqns(t,z)
    dzdt = [
        -A*z(1)/(z(1) + z(2))
        0.5*A*z(1)/(z(1) + z(2))
    ];
end % of internal function odeqns
```

Listing 2. Internal function odeqns after making the second required modification.

The third required modification involves entering the initial value of the independent variable, t, the initial values of the dependent variables, $\underline{z}$ and the final value of the independent variable, t. Equations (1) and (2) show that for this problem, the initial value of the independent variable is $t = 0$ and the corresponding initial values of the dependent variables are $z_1(0) = 0.103$ and $z_2(0) = 0.0$. These values must be assigned to the variables t0, z0(1) and z0(2), respectively, in the template file at the location indicated by the "%EDIT HERE" comment for the third required modification. The problem asks for the values of z_1 and z_2 at $t = 1$, so tf is set equal to 1.0. Listing 3 shows the section of the template file where this information was entered. The template file also includes a note advising you to change the solver from ode45 to ode15s if the equations being solved are stiff. In this case, the equations are not stiff and the ode45 solver can be used.

```
% Initial and final values
t0 = 0.0;
z0 = [
    0.103
    0.0
];
tf = 1.0;
```

Listing 3. Initial conditions added as the third required modification of the template file.

The fourth and final modification involves adding code to calculate any additional quantities using the results from solving the ODEs. In this problem we are asked to calculate the percentage change in z_1. That is easily done, a can be seen in Listing 4 which shows the last few lines of the modified template file. Notice that I did not put a semicolon at the end of the line that calculates the percentage change; if I did, it would be calculated, but it would not be listed in the output when the file is executed, and I'd never know its value. Any code you enter here should not have a semicolon at the end of the line if you want to see the result. Note also, that this not a returned value; if you wanted to perform calculations at the MATLAB command prompt that used this result, you would need to change the function statement so that, for example, the variable `pct_change` was included among the returned variables.

```
% calculate the percent change in z(1)
pct_change = 100*(z(1)-z0(1))/z0(1)

end % of S5_Example_1.m
```

Listing 4. Partial listing of the template file after the completion of the fourth required modifications.

That completes the required modifications, so once the file is saved to make the changes permanent, it can be executed by typing the first line shown in Listing 5. Doing so produces the remainder of Listing 5. Looking at the output, you can see that z_1 had decreased by 89% at t = 1.0, where z_1 = 0.0113 and z_2 = 0.0459.

```
>> [t_f,z] = S5_Example_1

pct_change =

  -89.0366

t_f =

    1

z =

    0.0113    0.0459
```

Listing 5. Output generated upon execution of the modified template file, S5_Example_1.m