ASSIGNMENT 1: MIXING TANK WITH A CHEMICAL REACTION

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Contents

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Brief

A $1m^3$ mixing tank with overflow initially filled with water is fed by a stream of 6M $H_2O_{2(aq)}$ solution at 0.5 litres per second. A second stream of pure water is to be used to dilute the $H_2O_{2(aq)}$ solution to 4M, however, this stream contains metal ions which catalyse the decomposition of H_2O_2. This decomposition can be modelled as a first order reaction with a rate constant of $0.00015s^{-1}$. [1]

Results

Hydrogen peroxide decomposes according to:

$$2H_2O_2 \rightarrow 2H_2O + O_2$$

This can be modelled as a first order reaction by the integrated rate law:

$$[A] = [A]_0 e^{-kt}$$

$$\therefore [H_2O_2] = [H_2O_2] \times e^{-0.00015t}$$

From the basic provided equation:

$$Acummulation = In - Out + Generation$$

A differential equation for the evolution of the moles of H_2O_2 in the tank was found to be: [2]

$$\frac{dn(t)}{d(t)} = C_1(t)V_1(t)e^{-kt} - \frac{n(t)}{V}[V_1(t) + V_2(t)]$$

Upon Euler integration, in order to find the number of moles of H_2O_2 in the tank at any time, we get:

$$n(t+1) = n(t) + \left(\frac{((C(t) \times V(t) \times e^{-k}) - n(t)}{Tank\ volume \times (V_1(t) + V_{2\ steady\ state}}\right) \times dt$$

The required steady state flowrate can be found from the differential equation. At steady state:

$$\frac{dn(t)}{d(t)} = 0$$

Hence:

$$C_1(t)V_1(t)e^{-kt} - \frac{n(t)}{V}[V_1(t) + V_2(t)] = 0$$

$$C_1(t)V_1(t)e^{-kt} = \frac{n(t)}{V}[V_1(t) + V_2(t)]$$

$$6 \times 0.5 \times e^{-0.00015} = \frac{4}{1}[0.5 + V_2]$$

$$V_2 = \frac{(6 \times 0.5 \times e^{-0.00015}) - 2}{4} = 0.2498875084L/s$$

With this information, a coded solution was made, and the following results were obtained:

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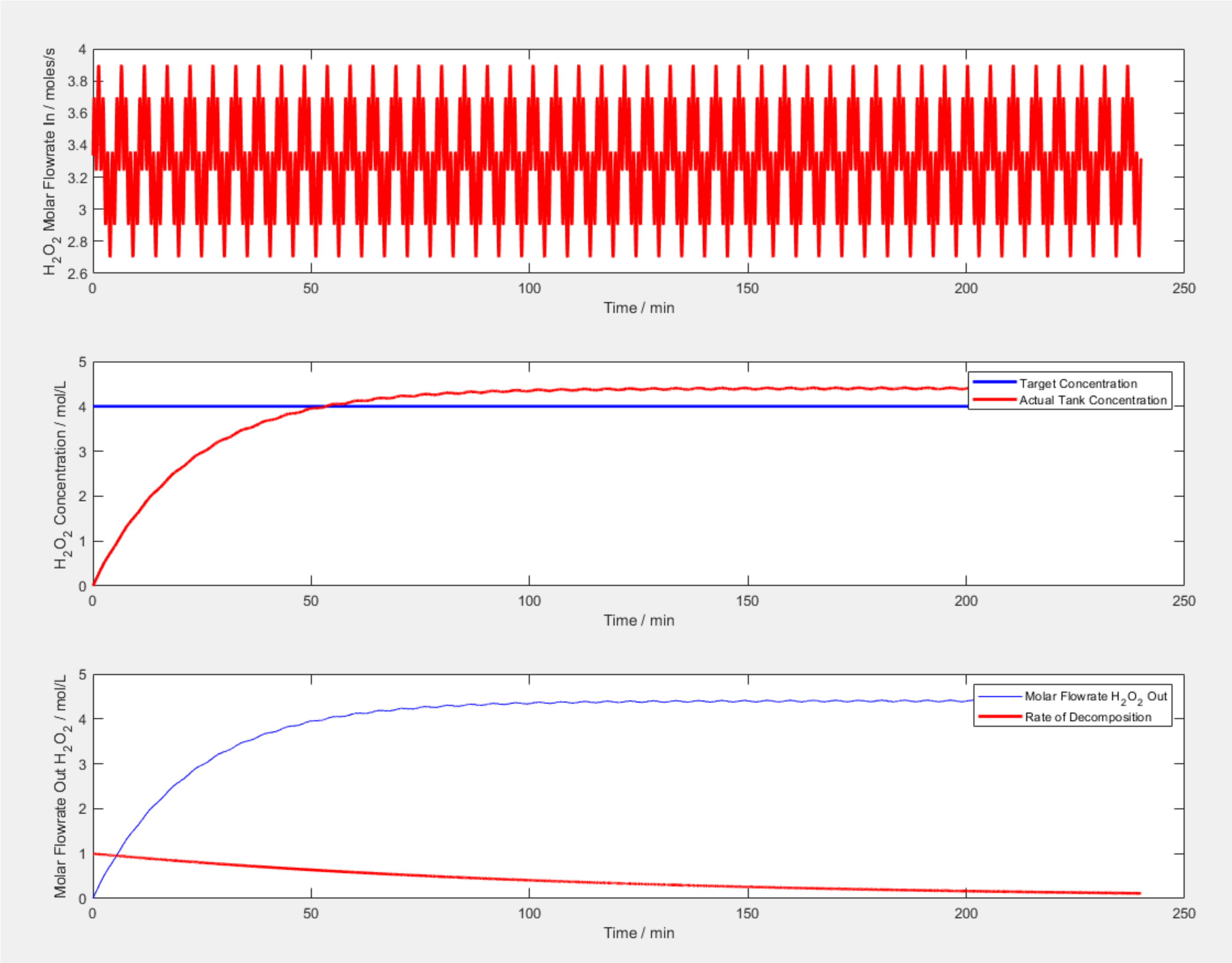

The time needed for the system to reach 90% of the target concentration from start-up was found to be 37.9 minutes.

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Full Code

```
clear
clf

C_start    =  0;
C_target   =  4;
V2_stst    =  0.000249887504;
KP         =  0.00005;
V_tank     =  1;
V1_base    =  0.0005;
C1_base    =  6;
f_step     =  1.2;
t_step     =  0.5;
dt         =  1.0;
t_max      =  8;
t_max      =  t_max    * 3600;
t_step     =  t_step   * 3600;
C1_base    =  C1_base  * 1000;
C_start    =  C_start  * 1000;
C_target   =  C_target * 1000;

i_max      = ceil(t_max/dt)+1;
i_step     = round(t_step/dt);
t          = 0.0:dt:(i_max-1)*dt;

for i = 1:1:i_max-1
V1(i)  = V1_base;
C1(i)  = C1_base;
V1(i)  = V1_base*(1+0.1*(sin(i/(10))+sin(i/(50))));
C1(i)  = C1_base*(1.1+0.1*(sin(i/(10))+sin(i/(50))));

    if i < i_step
        V1(i)  = V1_base;
    else
        V1(i)  = f_step*V1_base;
    end
end

n1(1)  = C1(1)*V1_base;
n2(1)  = C_start*V_tank;
for i = 1:1:i_max-1
    n1(i+1)  = V1(i)*C1(i);
    n2(i+1)  = n2(i)+(C1(i)*V1(i)*exp(-0.00015)-n2(i)/V_tank*(V1(i)+V2_stst))*dt;
    V1(i+1)  = KP*(n2(i)/V_tank-C_target);
    V1(i+1)  = max(V1(i),0);
    V1(i+1)  = min(V1(i),V1_base);
end
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```
C_target = C_target/1000;
t        = t /60;
V_tank   = V_tank*1000;

near_target = 0;
for i = 1:1:i_max
  if (abs((n2(i)/(V_tank*1000))-C_target)/C_target < 0.1) && near_target == 0
    near_target = 1;
    fprintf('System has reached within 90 percent of target concentration in: %f minutes.\n',(i-1)*dt/60)
  end
end

for i = 1:1:i_max
    loss(i) = exp(-0.00015*(i));
end

conc(1:i_max) = n2/(V_tank*1000);
ct(1:i_max)   = C_target;
subplot(3,1,1)
  plot(t,n1,'r','LineWidth',2) ; hold on
  xlabel('Time / min')
  ylabel('H_{2}O_{2} Molar Flowrate In / moles/s')
  hold off
subplot(3,1,2)
  plot(t,ct,'b-','LineWidth',2) ; hold on
  plot(t,conc,'r','LineWidth',2) ; hold on
  xlabel('Time / min')
  ylabel('H_{2}O_{2} Concentration / mol/L')
  legend('Target Concentration','Actual Tank Concentration')
  hold off
subplot(3,1,3)
  plot(t,n2/1000,'b-') ; hold on
  plot(t,loss,'r','LineWidth',2) ; hold on
  xlabel('Time / min')
  ylabel('Molar Flowrate Out H_{2}O_{2} / mol/L')
  legend('Molar Flowrate H_{2}O_{2} Out','Rate of Decomposition')
  hold off
```

[1]

[2]

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Line-By-Line Explanation

Line	Explanation
1-2	Clears all variables and figures
4-14	Definition of variables
15-19	Conversion of variables
21-23	Defines the maximum time and time step
25-29	Simulates a smooth flow and concentration
31-36	If the current iteration exceeds the step change time, flowrate increases by the flowrate step change
38-41	Defines base values for molar flow in the influx and within the tank
42	Euler integration
43-46	Controls the flow, if target concentration is reached, flow is 0, else maximum flow
48-50	Conversion of variables
52-58	Once the system is within 90% of the target concentration, the time taken for this to occur is printed to the user
60-62	Calculates the rate of decomposition
64-65	Calculates the tank concentration at every time and defines the target concentration for each time as a setpoint
66-84	Multiplot function

References

[1] H. Bock, Assignment 1: Mixing Tank with a Chemical Reaction, Edinburgh: Heriot-Watt University.

[2] Heriot-Watt University, *B49CF2 Computational Simulation and Control: Exercise 4 Summary and Exercise 5 (Project 6): Dilution Tank with Storage,* Edinburgh: Heriot-Watt University, 2018.

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