Deliverable 3

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ABE 30100

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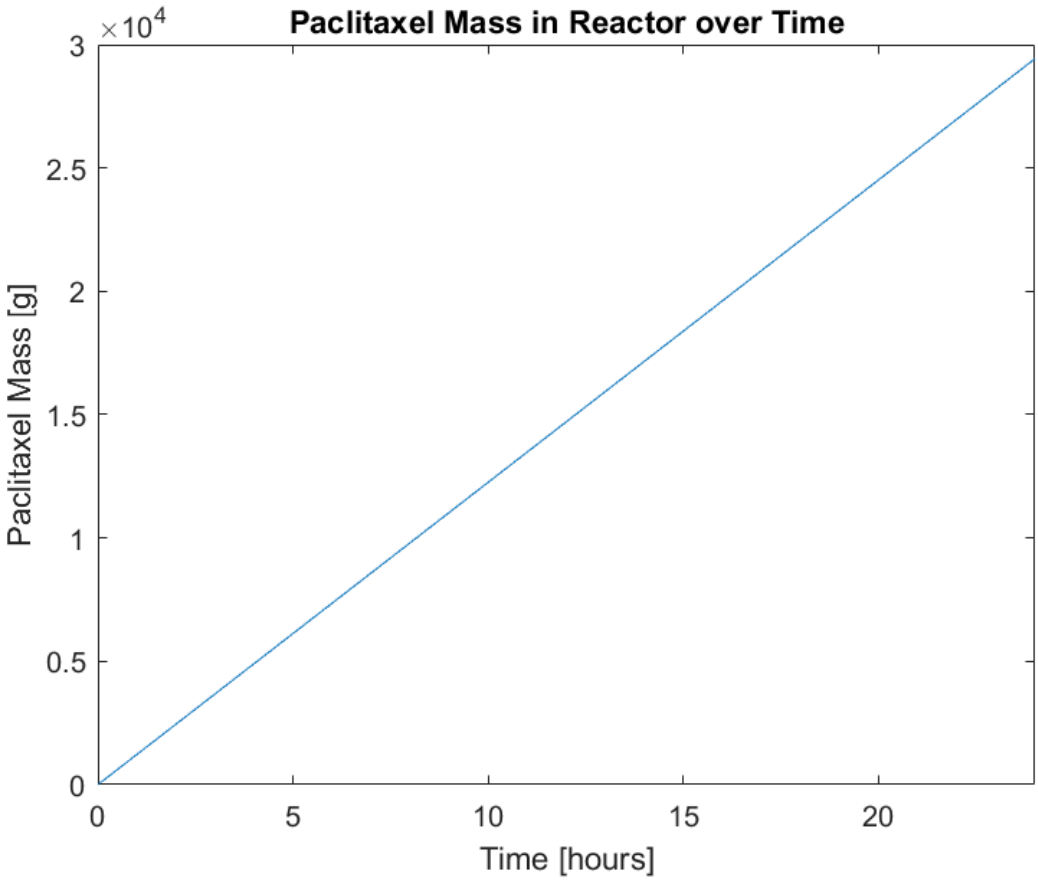
Iteration I

```
clear;
% Constants and Initial Conditions
F1 = 0; % [L/h]
C1 = 5; % [g/L]
F2 = 0; % [L/h]
V = 1; % [L]
T = 273 + 30; % [K]
cp = 4.186; % [J/g-K]

e = 2; % [g/L]
s = 2; % [g/L]
rho_cell = 200; % [g/L]
Vs1 = e * V / rho_cell; % [L]
Vs2 = s * V / rho_cell; % [L]
rho_water = 1000; % g/L

x = 5; % [g/L]
p = 0; % [g/L]
d = 0; % [g/L]
a = 0; % [g/L]

Wx = 150.13; % [g/mol]
Wd = 272.476; % [g/mol]
Wa = 60.052; % [g/mol]
Wp = 853.906; % [g/mol]

Hxd = 15; % [J/mol]
Hxa = 7; % [J/mol]
Hxe = 0; % [J/mol]
Hdp = 8; % [J/mol]
Has = 0; % [J/mol]

m = (e + s + x + p + d + a) * V; % [g]
ms1 = e; % [g]
ms2 = s; % [g]

rxe = 0;
rxd = 1 / 15; % [mol/L-s]
rxd = rxd * 3600; % [mol/L-h]
rxa = 1 / 7; % [mol/L-s]
rxa = rxa * 3600; % [mol/L-h]
```

```
rdp = 1 / 8; % [mol/L-s]
rdp = rdp * 3600; % [mol/L-h]
ras = 0;

time = 0:0.01:24; % [h]
p_t = zeros(length(time),1);
i = 1;
delt = 0.01;

for i = 1:length(time)
    p_t(i) = p; % [g]
    % integrate dxdt = F1 * C1 - (rxe + rxd + rxa) * Wx * Vs1; % [g/h]
    x = x + F1 * C1 * delt - (rxe + rxd + rxa) * Wx * Vs1 * delt; % [g]
    if x < 0
        x = 0;
    end
    % integrate dddt = rxd * Wx * Vs1 - rdp * Wd * Vs2; % [g/h]
    d = d + rxd * Wx * Vs1 * delt - rdp * Wd * Vs2 * delt; % [g]
    if d < 0
        d = 0;
    end
    % integrate dadt = rxa * Wx * Vs1 - ras * Wa * Vs2; % [g/h]
    a = a + rxa * Wx * Vs1 * delt - ras * Wa * Vs2 * delt; % [g]
    if a < 0
        a = 0;
    end
    % integrate dedt = rxe * Wx * Vs1; % [g/h]
    e = e + rxe * Wx * Vs1 * delt; % [g]
    if e < 0
        e = 0;
    end
    % integrate dsdt = ras * Wa * Vs2; % [g/h]
    s = s + ras * Wa * Vs2 * delt;
    if s < 0
        s = 0;
    end
    C2 = p / V; % [g/L]
    % integrate dpdt = rdp * Vs2 - F2 * C2
    p = p + rdp * Vs2 * Wd * delt - F2 * C2 * delt; % [g]
    if p < 0
        p = 0;
    end

    % integrate dmdt = F1 * C1 - F2 * C2; % [g/h]
    m = m + F1 * C1 * delt - F2 * C2 * delt; % [g]
    if m < 0
        m = 0;
    end
    % integrate dms1dt = F1 * C1 - Vs1 * Wx * (rxd + rxa); % [g/h]
    ms1 = ms1 + F1 * C1 * delt - Vs1 * Wx * (rxd + rxa) * delt; % [g]
    if ms1 < 0
        ms1 = 0;
    end
```

```
    % integrate dms2dt = Vs1 * Wx * (rxd + rxa) - F2 * C2; % [g/h]
    ms2 = ms2 + Vs1 * Wx * (rxd + rxa) * delt - F2 * C2 * delt; % [g]
    if ms2 < 0
        ms2 = 0;
    end

    % Assuming Subsystems Maintain a constant temperature
    % dhs1dt = Vs1 * (Hxd * Wd * rxd + Hxa * Wa * rxa + Hxe * We * rxe) - F6
    F6 = Vs1 * Wx * (Hxd * rxd + Hxa * rxa + Hxe * rxe);
    if F6 < 0
        F6 = 0;
    end
    % dhs2dt = Vs2 * (Hdp * Wp * rdp + Has * Ws * ras) - F7
    F7 = Vs2 * (Hdp * Wd * rdp + Has * Wa * ras);
    if F7 < 0
        F7 = 0;
    end

    % Assume F3 = 0
    F3 = 0; % [J/h]
    dhdt = F6 + F7 - F3;
    if dhdt < 0
        dhdt = 0;
    end
    T = T + dhdt / (e + s + (rho_water - (e + s)) * V * cp); % [K]
end

plot(time, p_t)
title('Paclitaxel Mass in Reactor over Time')
xlabel('Time [hours]')
xlim([0,24])
ylabel('Paclitaxel Mass [g]')
```

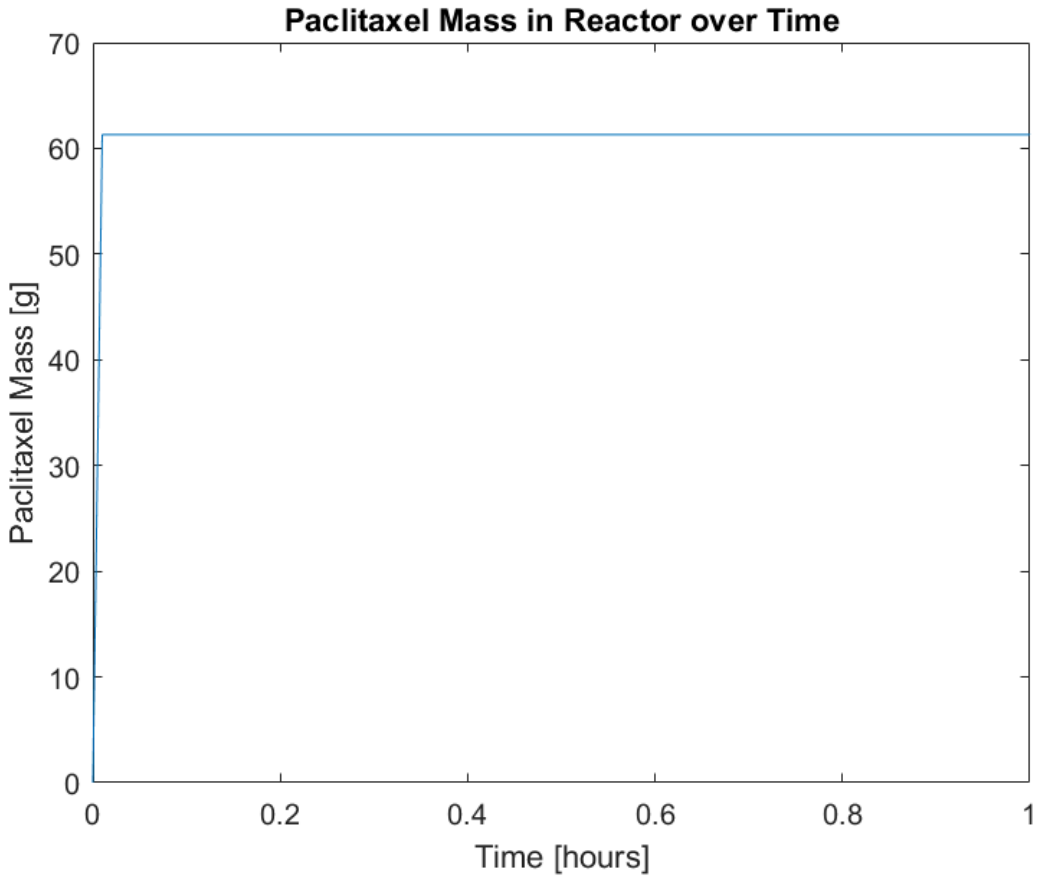


Iteration II

```
clear;
% Constants and Initial Conditions
F1 = 0; % [L/h]
C1 = 5; % [g/L]
F2 = 0; % [L/h]
V = 1; % [L]
T = 273 + 30; % [K]
cp = 4.186; % [J/g-K]

e = 2; % [g/L]
s = 2; % [g/L]
rho_cell = 200; % [g/L]
Vs1 = e * V / rho_cell; % [L]
Vs2 = s * V / rho_cell; % [L]
rho_water = 1000; % g/L

x = 5; % [g/L]
p = 0; % [g/L]
d = 0; % [g/L]
a = 0; % [g/L]

Wx = 150.13; % [g/mol]
```

```
Wd = 272.476; % [g/mol]
Wa = 60.052; % [g/mol]
Wp = 853.906; % [g/mol]

Hxd = 15; % [J/mol]
Hxa = 7; % [J/mol]
Hxe = 0; % [J/mol]
Hdp = 8; % [J/mol]
Has = 0; % [J/mol]

m = (e + s + x + p + d + a) * V; % [g]
ms1 = e; % [g]
ms2 = s; % [g]



time = 0:0.01:24; % [h]
p_t = zeros(length(time),1);
i = 1;
delt = 0.01;

for i = 1:length(time)
    p_t(i) = p; % [g]
    rxe = 0 * x;
    rxd = 1 / 15 * x; % [mol/L-s]
    rxd = rxd * 3600; % [mol/L-h]
    rxa = 1 / 7 * x; % [mol/L-s]
    rxa = rxa * 3600; % [mol/L-h]
    rdp = 1 / 8 * x; % [mol/L-s]
    rdp = rdp * 3600; % [mol/L-h]
    ras = 0 * x;
    % integrate dxdt = F1 * C1 - (rxe + rxd + rxa) * Wx * Vs1; % [g/h]
    x = x + F1 * C1 * delt - (rxe + rxd + rxa) * Wx * Vs1 * delt; % [g]
    if x < 0
        x = 0;
    end
    % integrate dddt = rxd * Wx * Vs1 - rdp * Wd * Vs2; % [g/h]
    d = d + rxd * Wx * Vs1 * delt - rdp * Wd * Vs2 * delt; % [g]
    if d < 0
        d = 0;
    end
    % integrate dadt = rxa * Wx * Vs1 - ras * Wa * Vs2; % [g/h]
    a = a + rxa * Wx * Vs1 * delt - ras * Wa * Vs2 * delt; % [g]
    if a < 0
        a = 0;
    end
    % integrate dedt = rxe * Wx * Vs1; % [g/h]
    e = e + rxe * Wx * Vs1 * delt; % [g]
    if e < 0
        e = 0;
    end
    % integrate dsdt = ras * Wa * Vs2; % [g/h]
    s = s + ras * Wa * Vs2 * delt;
```

```
    if s < 0
        s = 0;
    end
    C2 = p / V; % [g/L]
    % integrate dpdt = rdp * Vs2 - F2 * C2
    p = p + rdp * Vs2 * Wd * delt - F2 * C2 * delt; % [g]
    if p < 0
        p = 0;
    end

    % integrate dmdt = F1 * C1 - F2 * C2; % [g/h]
    m = m + F1 * C1 * delt - F2 * C2 * delt; % [g]
    if m < 0
        m = 0;
    end
    % integrate dms1dt = F1 * C1 - Vs1 * Wx * (rxd + rxa); % [g/h]
    ms1 = ms1 + F1 * C1 * delt - Vs1 * Wx * (rxd + rxa) * delt; % [g]
    if ms1 < 0
        ms1 = 0;
    end
    % integrate dms2dt = Vs1 * Wx * (rxd + rxa) - F2 * C2; % [g/h]
    ms2 = ms2 + Vs1 * Wx * (rxd + rxa) * delt - F2 * C2 * delt; % [g]
    if ms2 < 0
        ms2 = 0;
    end

    % Assuming Subsystems Maintain a constant temperature
    % dhs1dt = Vs1 * (Hxd * Wd * rxd + Hxa * Wa * rxa + Hxe * We * rxe) - F6
    F6 = Vs1 * Wx * (Hxd * rxd + Hxa * rxa + Hxe * rxe);
    if F6 < 0
        F6 = 0;
    end
    % dhs2dt = Vs2 * (Hdp * Wp * rdp + Has * Ws * ras) - F7
    F7 = Vs2 * (Hdp * Wd * rdp + Has * Wa * ras);
    if F7 < 0
        F7 = 0;
    end

    % Assume F3 = 0
    F3 = 0; % [J/h]
    dhdt = F6 + F7 - F3;
    if dhdt < 0
        dhdt = 0;
    end
    T = T + dhdt / (e + s + (rho_water - (e + s)) * V * cp); % [K]
end

plot(time, p_t)
title('Paclitaxel Mass in Reactor over Time')
xlabel('Time [hours]')
xlim([0,1])
ylabel('Paclitaxel Mass [g]')
```


Paclitaxel Mass in Reactor over Time
Paclitaxel Mass [g]
Time [hours]
0
10
20
30
40
50
60
70
0
0.2
0.4
0.6
0.8
1