Indian Institute of Technology,
Delhi

Batch reactor for Nylon 6

An optimisation Study

TTP 311 Assignment 2

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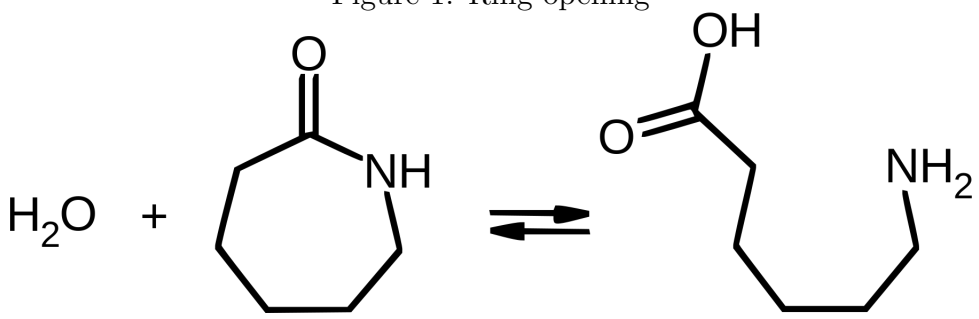
March 26, 2015

Figure 1: Ring opening



Introduction

The aim of this assignment is to simulate the production of Nylon 6 in a batch reactor, and recreate the graphs of L, M_n, M_w, PDI and also figure out an approach to obtain the conditions for maximum polymerisation in minimum time in an industrial setting.

Reactions

Following enlisted are the 3 main reactions involved in the polymerisation.

Ring opening

Ring opening involves breaking of the C-N bond in caprolactam to form, what we will refer to as P1 . Following is a vector image of the reaction, courtesy my(very limited) LaTeXskills.

Polyaddition

Poly addition is a polymerization technique where unsaturated monomer molecules add onto the active site on a growing polymer chain one at a time. There are a limited number of these active sites at any moment during the polymerization which gives this method its key characteristics.

$$P_n + L \rightleftharpoons P_{n+1}$$

Polycondensation

A condensation reaction, also commonly referred to as dehydration synthesis, is a chemical reaction in which two molecules or moieties (functional groups) combine to form a larger molecule, together with the loss of a small molecule.

$$P_n + P_m \rightleftharpoons P_{n+m}$$

Differential Equations

$$\frac{dL}{dt} = -k_1[L][W] + k_1'[P_1] - k_3\mu_0[L] + k_3'[\mu_0 - P_1]$$

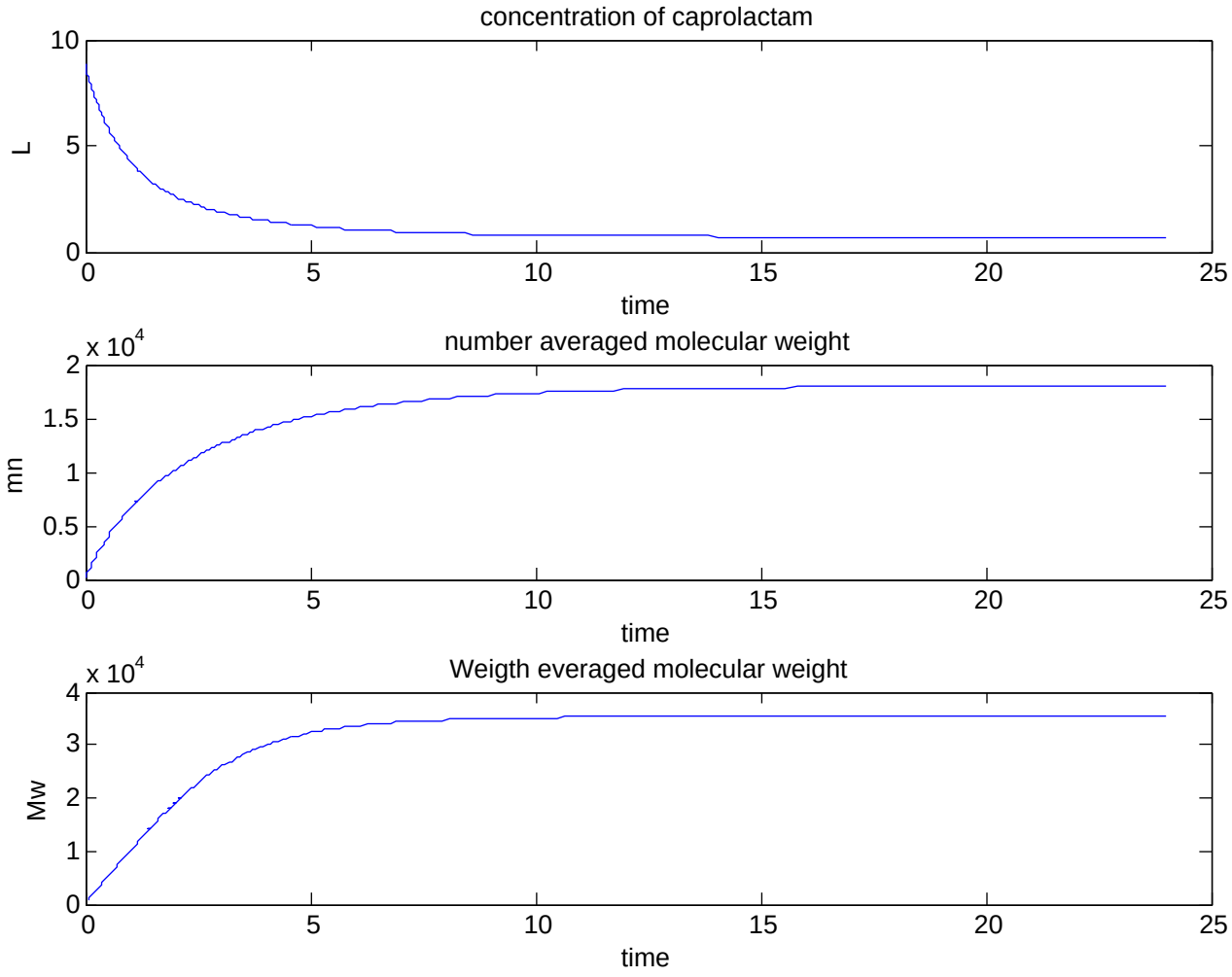
$$\frac{dP_1}{dt} = k_1[L][W] - k_1'[P_1] - 2k_2\mu_0 P_1 + 2k_2'(\mu_0 - P_1) - k_3 P_1 L + k_3' P_1$$

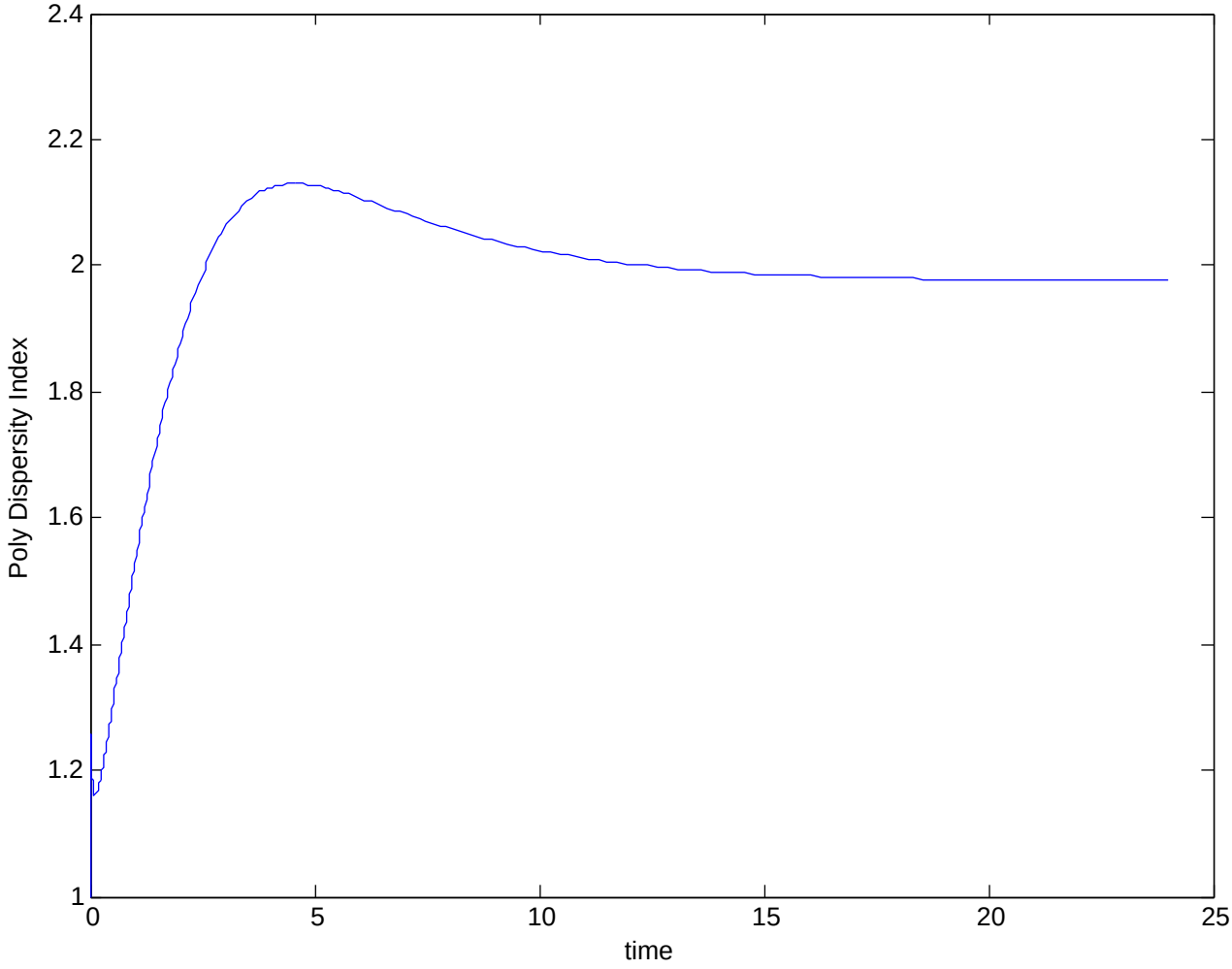
$$\frac{d\mu_0}{dt} = k_1[L][W] - k_1'[P_1] - k_2\mu_0^2 + k_2' W(\mu_1 - \mu_0) - k_3'(\mu_0 - P_1)$$

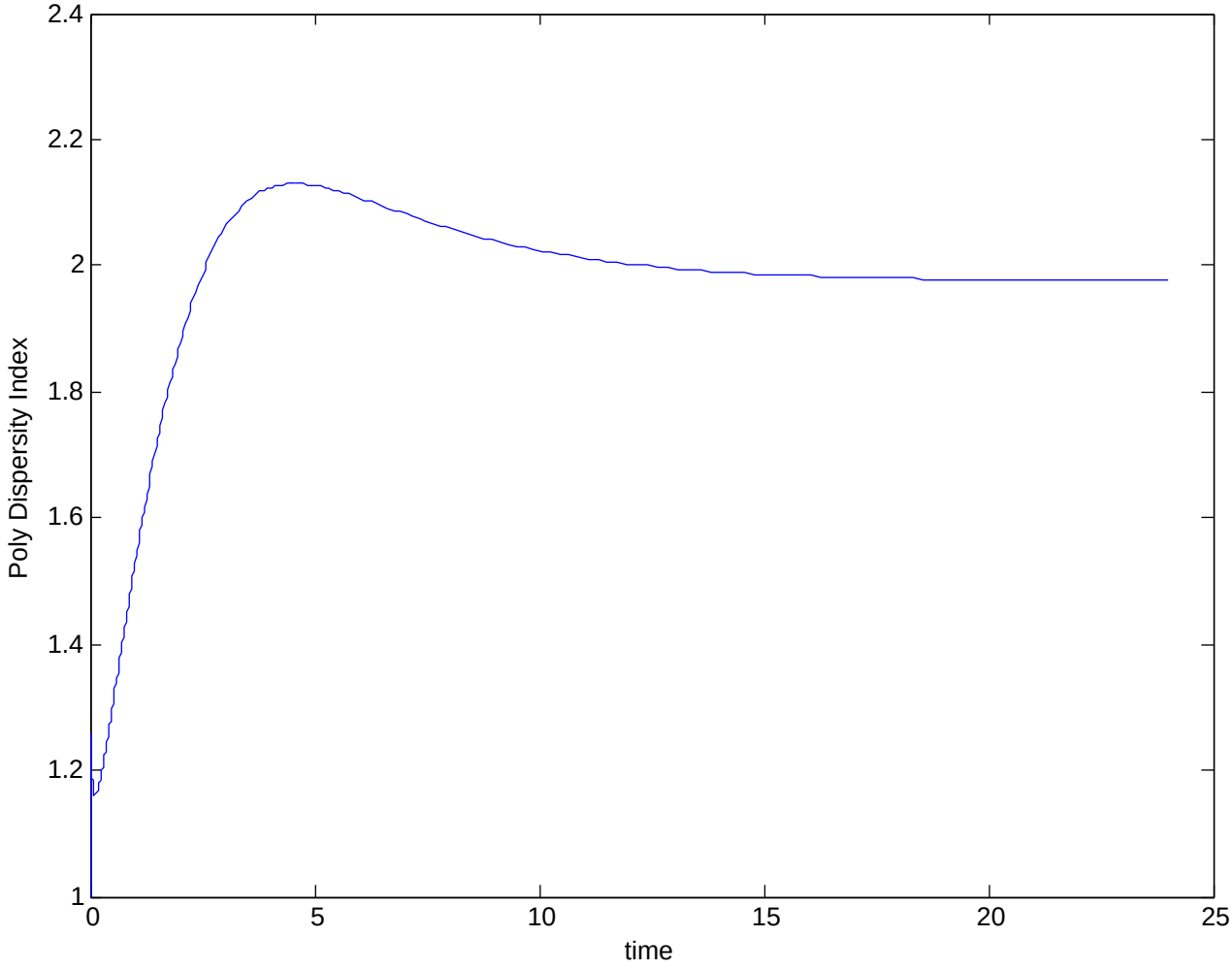
$$\frac{d\mu_1}{dt} = k_1[L][W] - k_1'[P_1] + k_3 L\mu_0 - k_3'(\mu_0 - P_1)$$

$$\frac{d\mu_2}{dt} = k_1[L][W] - k_1'[P_1] + 2k_2\mu_1^2 + \frac{k_2' W(\mu_1 - \mu_3)}{3} + k_3 L(\mu_0 + 2\mu_1) + k_3'(\mu_0 - 2\mu_1 + P_1)$$

Graphs


concentration of caprolactam
L
time
number averaged molecular weight
x 10^4
mn
time
Weigth everaged molecular weight
x 10^4
Mw
time


Poly Dispersity Index
time
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0
5
10
15
20
25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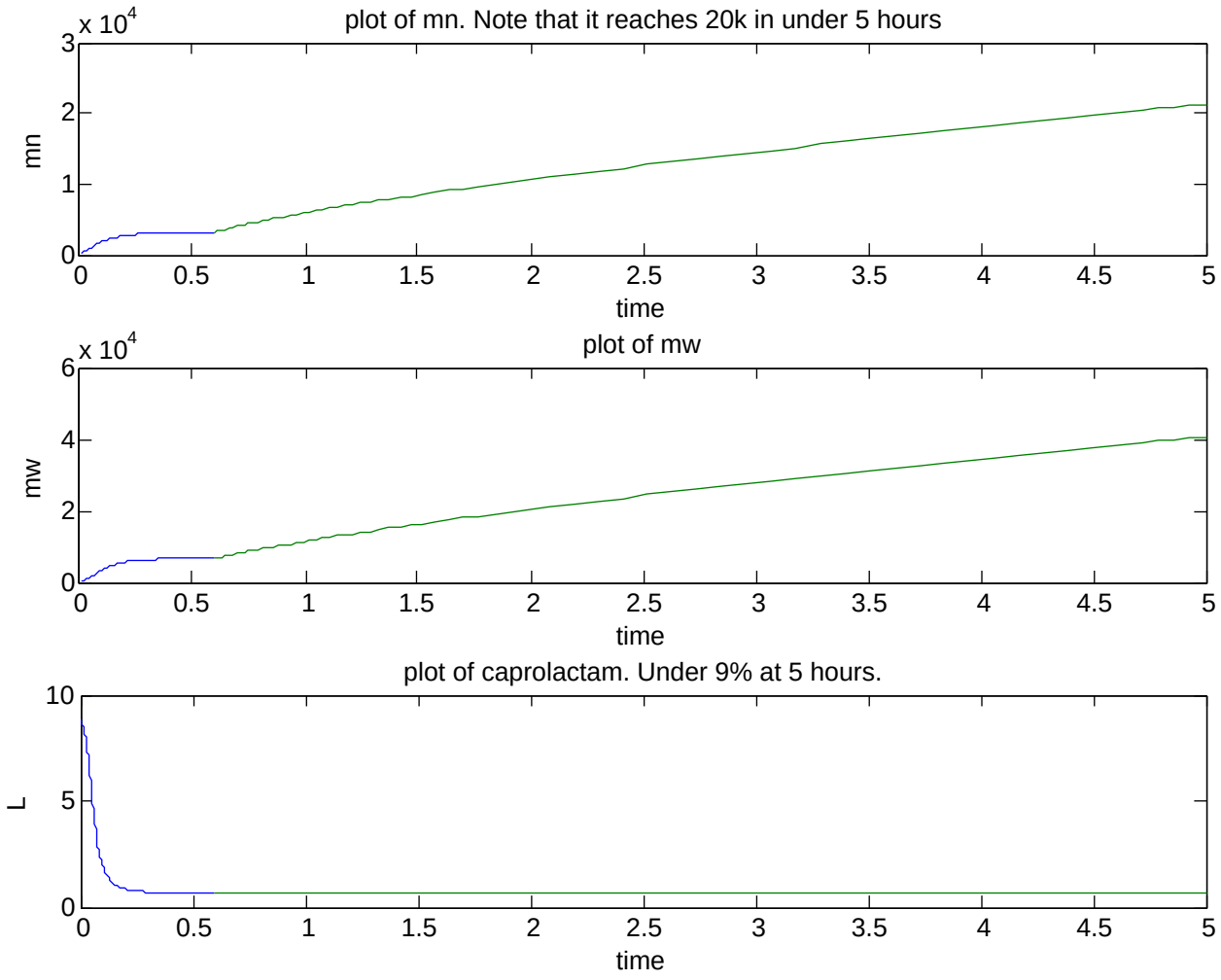
plot of mn. Note that it reaches 20k in under 5 hours
x 10^4
mn
time
plot of mw
x 10^4
mw
time
plot of caprolactam. Under 9% at 5 hours.
L
time

Approach for part 2

For obtaining an optimised process, I iterated over several possible reactions and stored the ones which satisfied the conditions, i.e final caprolactam concentration <9% and the final number averaged molecular weight should be greater than 20000.

We keep the initial conditions within a reasonable limit, temperature between 240 and 270 degrees celsius, a water concentration of 4 moles/litre and P=0.1. The second reactor is running at 240 degrees celsius and has a water concentration of 0, which is reasonable assuming current dehumidifier technology.

After taking these conditions into account and making a second round of filtering, we then use a hit and trial method to find the appropriate timeline for both reactions. It is observed that the first reactor reaches equilibrium very quickly, so we can immediately transfer the contents to the second reactor.

These conditions are then taken into account when developing the final program.

Results

1. Temperature for first reactor= 270 degrees celsius
2. Temperature for second reactor= 240 degrees celsius
3. Water for first reactor= 4 moles/litre
4. Water for second reactor= 0 moles/litre
5. time for first reactor= 0.6 hours
6. time for second reactor= 4.4 hours