Question 1

Part (a)

For the reaction, $\dot{\xi} = kn_A$, $\nu_A = -1$ and $\nu_B = 1$.

Balance equations:

$$\frac{dn_A}{dt} = \dot{n}_{A,in} - \dot{n}_{A,out} + \nu_A\dot{\xi}$$

$$\frac{dn_B}{dt} = -\dot{n}_{B,out} + \nu_B\dot{\xi}$$

Since $n_A = AV$, $n_B = BV$, $\dot{n}_{A,in} = A_0F_0$, $\dot{n}_{A_{out}} = AF_0$ and $n_{B,out} = BF_0$, we have

$$V\frac{dA}{dt} = A_0F_0 - AF_0 - kAV$$

$$V\frac{dB}{dt} = -BF_0 + kAV$$

So, the system of ODEs required is

$$\frac{dA_1(t)}{dt} = \frac{A_0F_0}{V} - \left(k + \frac{F_0}{V}\right)A_1(t)$$

$$\frac{dB_1(t)}{dt} = kA_1(t) - \frac{F_0}{V}B_1(t)$$

Assumptions:

- The tank is well-stirred.
- There are no other chemical reactions besides the reaction that converts A in to B.

Initial conditions: $A_1(0) = 0$ and $B_1(0) = 0$.

Part (b)

Steady state:

$$0 = \frac{dA_1(t)}{dt} = \frac{A_0F_0}{V} - \left(k + \frac{F_0}{V}\right)A_1(t) \Longrightarrow A_1(t) = \frac{A_0F_0}{kV + F_0}$$

$$0 = \frac{dB_1(t)}{dt} = \frac{dB_1(t)}{dt} = kA_1(t) - \frac{F_0}{V}B_1(t) \Longrightarrow B_1(t) = \frac{kV}{F_0}A_1(t) = \frac{kV_0A_0}{kV + F_0}$$

Part (c)

For reactor 1, the equations are given in (a), except we replace V by V/n:

$$\frac{dA_1(t)}{dt} = \frac{nA_0F_0}{V} - \left(k + \frac{nF_0}{V}\right)A_1(t)$$

$$\frac{dB_1(t)}{dt} = kA_1(t) - \frac{nF_0}{V}B_1(t)$$

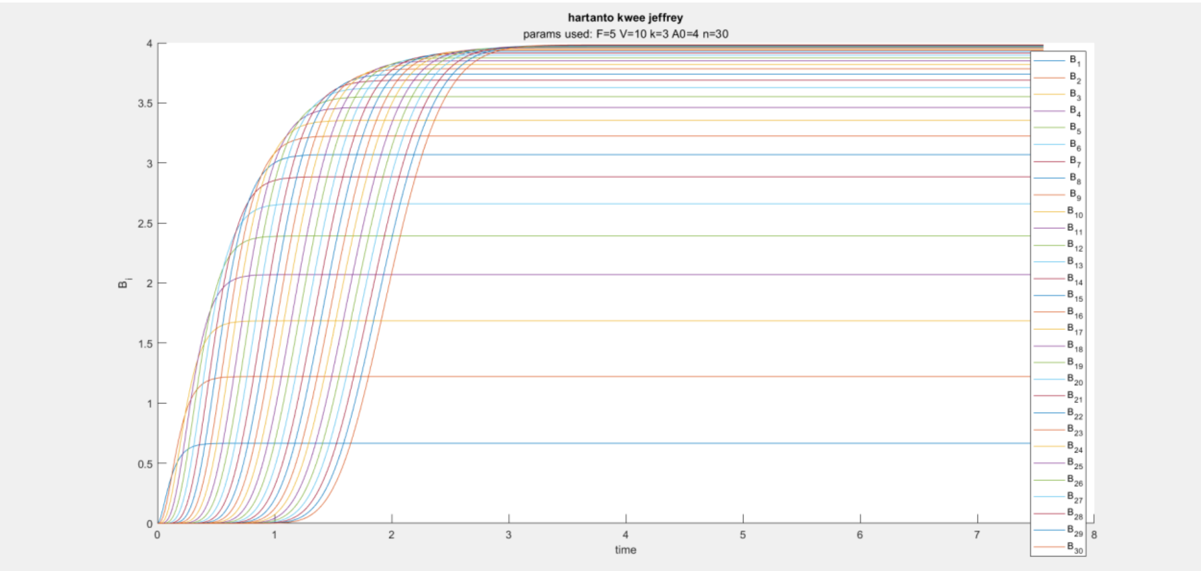
For reactors 2 to n,

$$\frac{dA_i(t)}{dt} = \frac{nA_{i-1}F_0}{V} - \left(k + \frac{nF_0}{V}\right)A_i(t)$$

$$\frac{dB_i(t)}{dt} = \frac{nB_{i-1}(t)F_0}{V} + kA_i(t) - \frac{nF_0}{V}B_i(t)$$

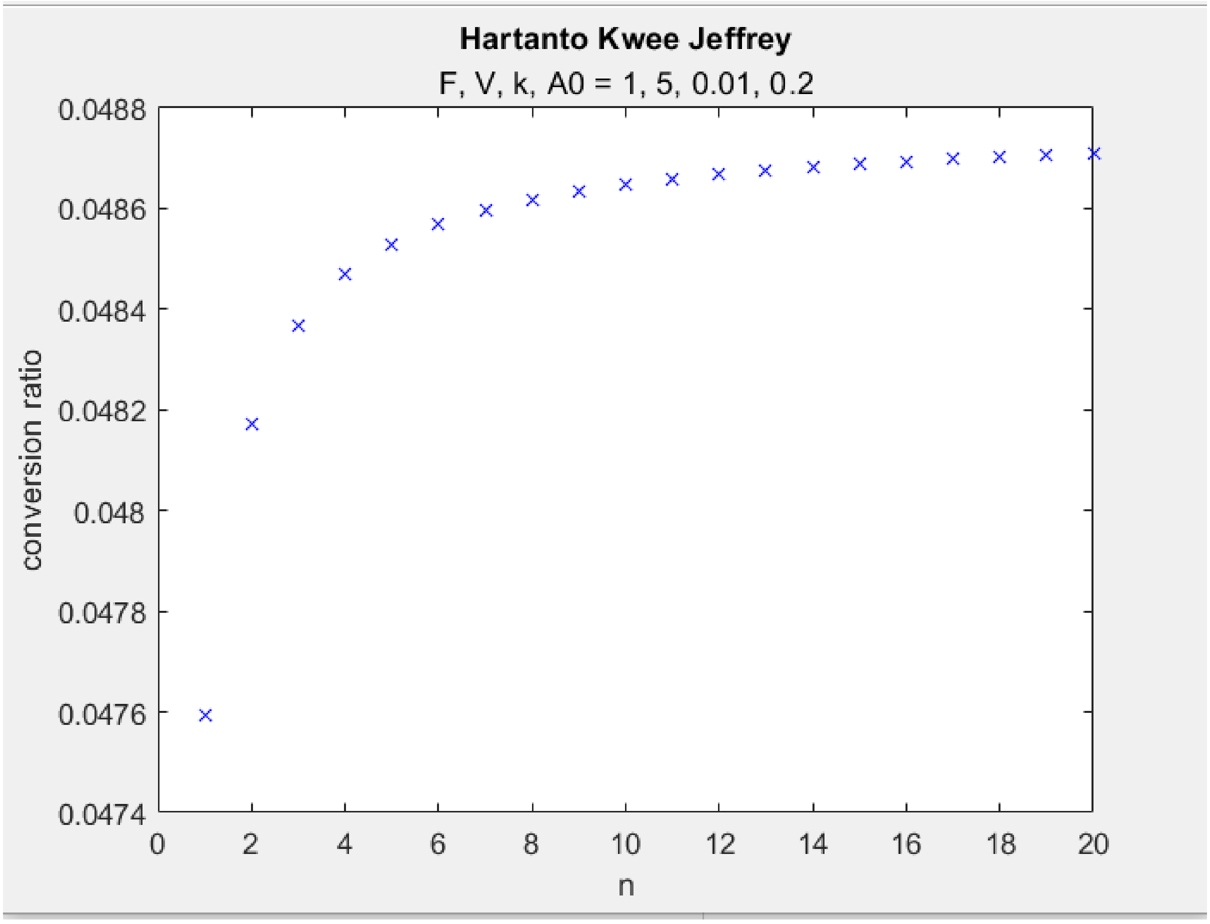
The initial condition is $A_i(0) = B_i(0) = 0$ for $i = 1, 2, \dots, n$.

Part (d)



Part (e)

I agree with the supervisor since the conversion ratio B_n/A_n does increase with n.



Question 2

BS: bloodstream

BR: brain

Assumption:

- The distribution of A and B in blood is uniform
- The volume of blood remains constant at V
- The blood reaches the brain and the liver immediately after injection.

Balance Equations

$$\frac{dn_{A,BS}}{dt} = -k_b V - k_r A_{BS} V - e_a A_{BS} V$$

$$\frac{dn_{B,BS}}{dt} = k_r A_{BS} V - e_B B_{BS} V$$

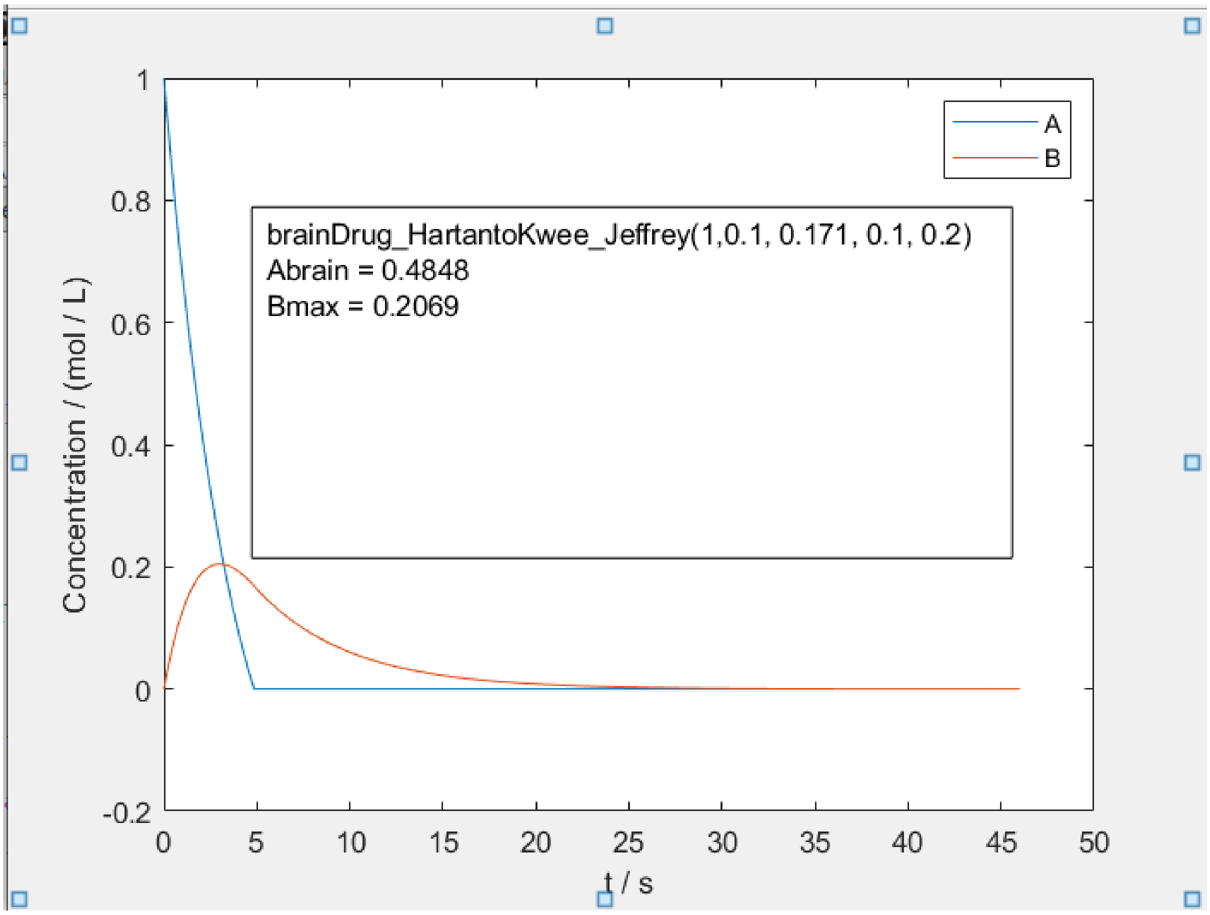
$$\frac{dn_{A,BR}}{dt} = k_b V$$

We can rewrite them into

$$\frac{dA_{BS}}{dt} = -k_b - k_r A_{BS} - e_a A_{BS}$$

$$\frac{dB_{BS}}{dt} = k_r A_{BS} - e_B B_{BS}$$

$$\frac{dA_{BR}}{dt} = k_b$$


brainDrug_HartantoKwee_Jeffrey(1,0.1, 0.171, 0.1, 0.2)
Abrain = 0.4848
Bmax = 0.2069
A
B
Concentration / (mol / L)
t / s
1
0.8
0.6
0.4
0.2
0
-0.2
0
5
10
15
20
25
30
35
40
45
50