Chemical Kinetic Simulations

By

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What is Chemical Kinetics?

- Chemical Kinetics is the study of the speed with which a chemical reaction occurs and the factors that affect this speed.
- Chemical Kinetics is useful to determine *how* a reaction occurs
- Study of the rate of reactions

Rate Laws

- A Rate Law is an equation that tells us how fast the reaction proceeds and how the reaction rate depends on the concentrations of the chemical species involved.

- Common type of Rate Laws
  - Zero Order $r = -d[A]/dt = k[A]^0 = k$
  - First Order $r = k[A]^1$
  - Second Order $r = k[A]^2$

What is consecutive First Order Reaction

- Consecutive First Order Reaction is a chemical process in which the product of one reaction is the initial material for other reactions.
  - A → B → C
  - A turns into B, with rate constant k_1, which turns into C, with rate constant k_2

What We Did

- Integrated the Rate Laws
  - In order to understand how the concentrations of the chemicals in a chemical reaction changes with time it is necessary to integrate the Rate Law.
  - $[A]_t = [A]_0 * e^{-k*t}$
  - $[B]t = [A]_0 * k * t * e^{-k*t} + [B]_0 * e^{-k*t}$
  - $[C]_t = [A]_0 * (1 - e^{-kt} - k*t*e^{-kt}) + [B]_0 * (1 - e^{-k*t})$

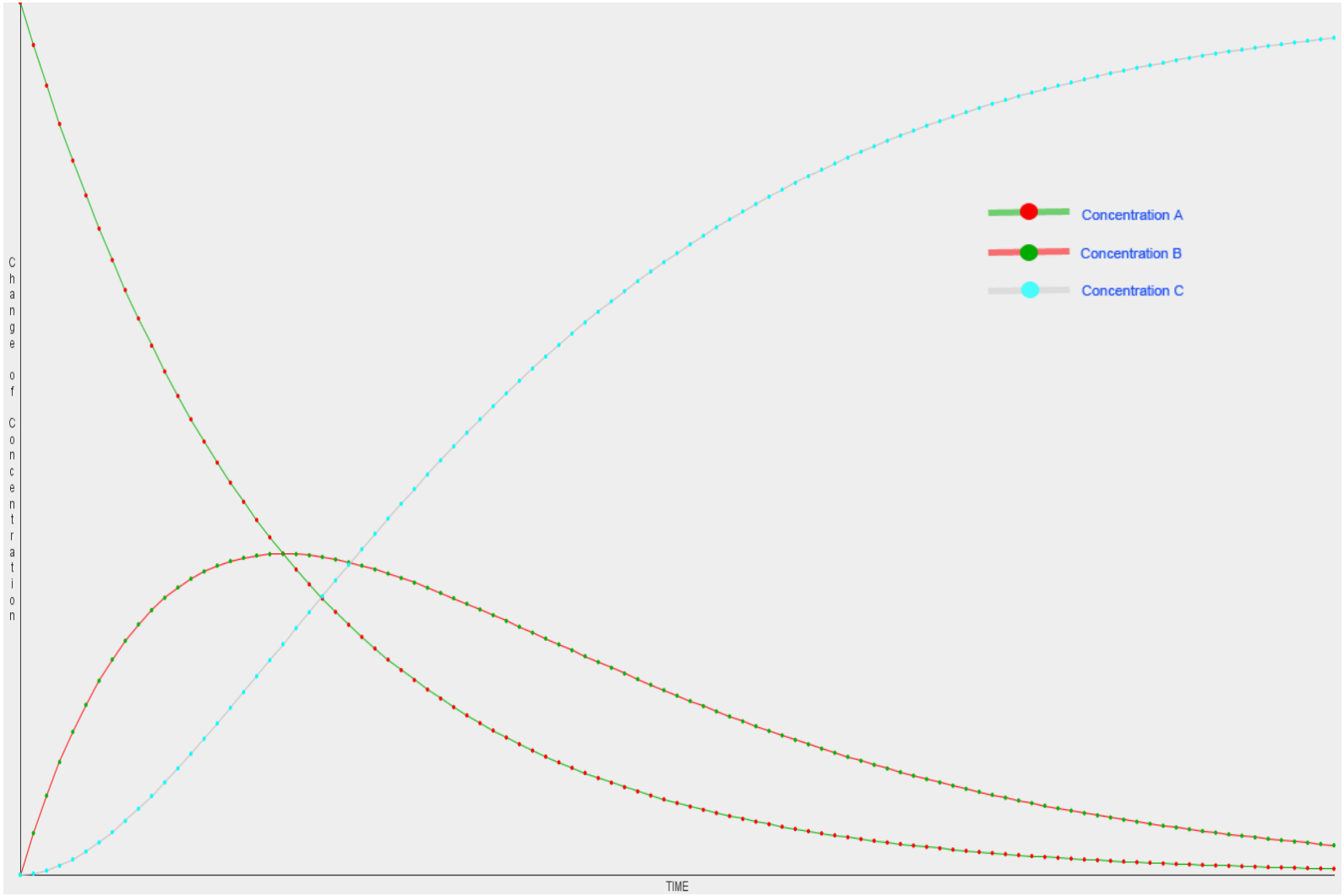
- Used the Integrated forms of Rate Laws for consecutive first order reaction A → B → C and plotted them using a Java Plotter Program.

Simulations

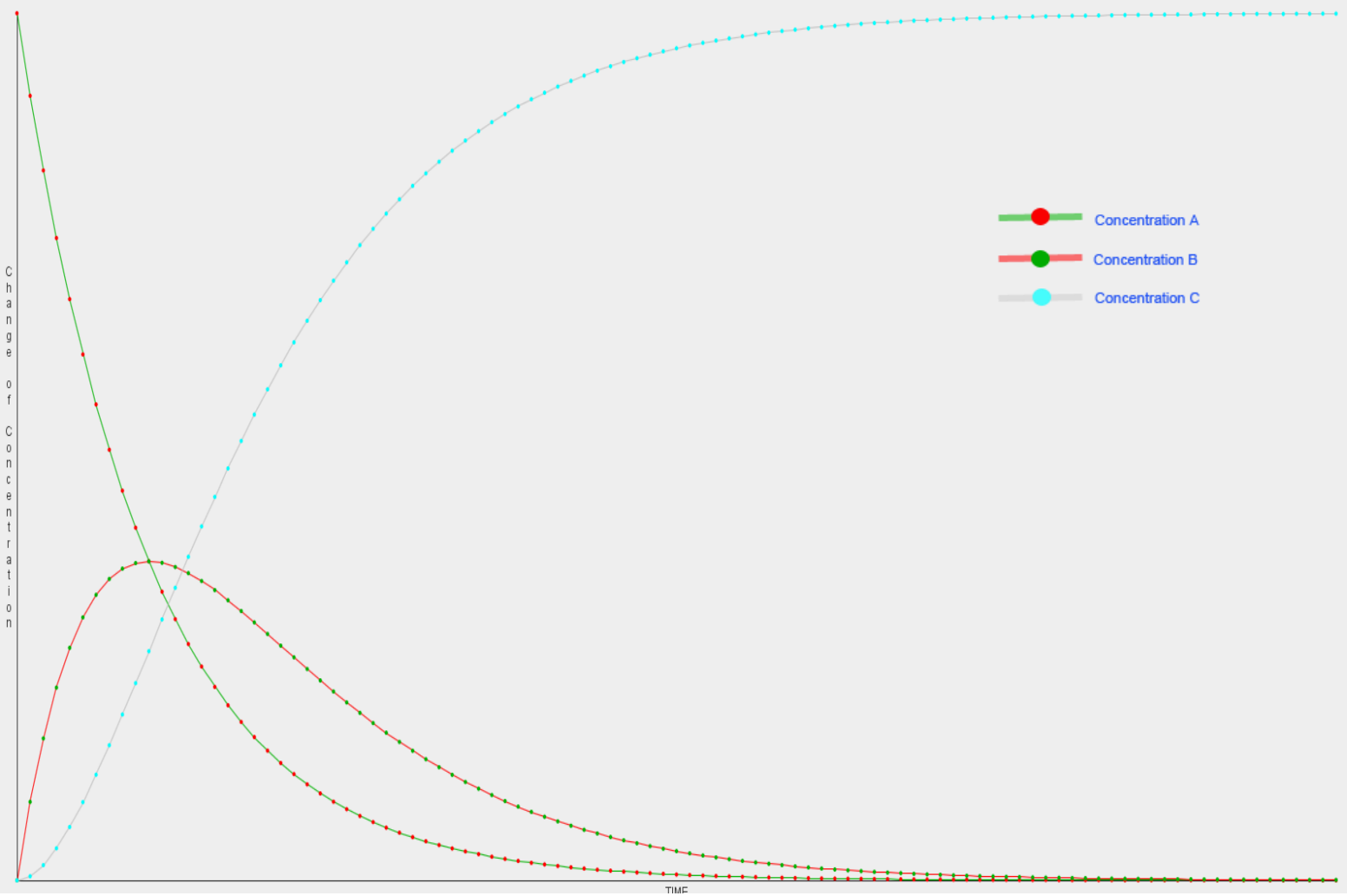
- Coded the Integrated Forms of the Rate Laws in Java.
- Ran Tests using the Integrated Forms of the Rate Laws with Different Constants of k.
  - Ranging from k = .5 to k = 50
- Gathered data from time interval t = .1 to t = 10
- Plotted 100 points for each chemical A, B, and C

Simulations for A→B→C

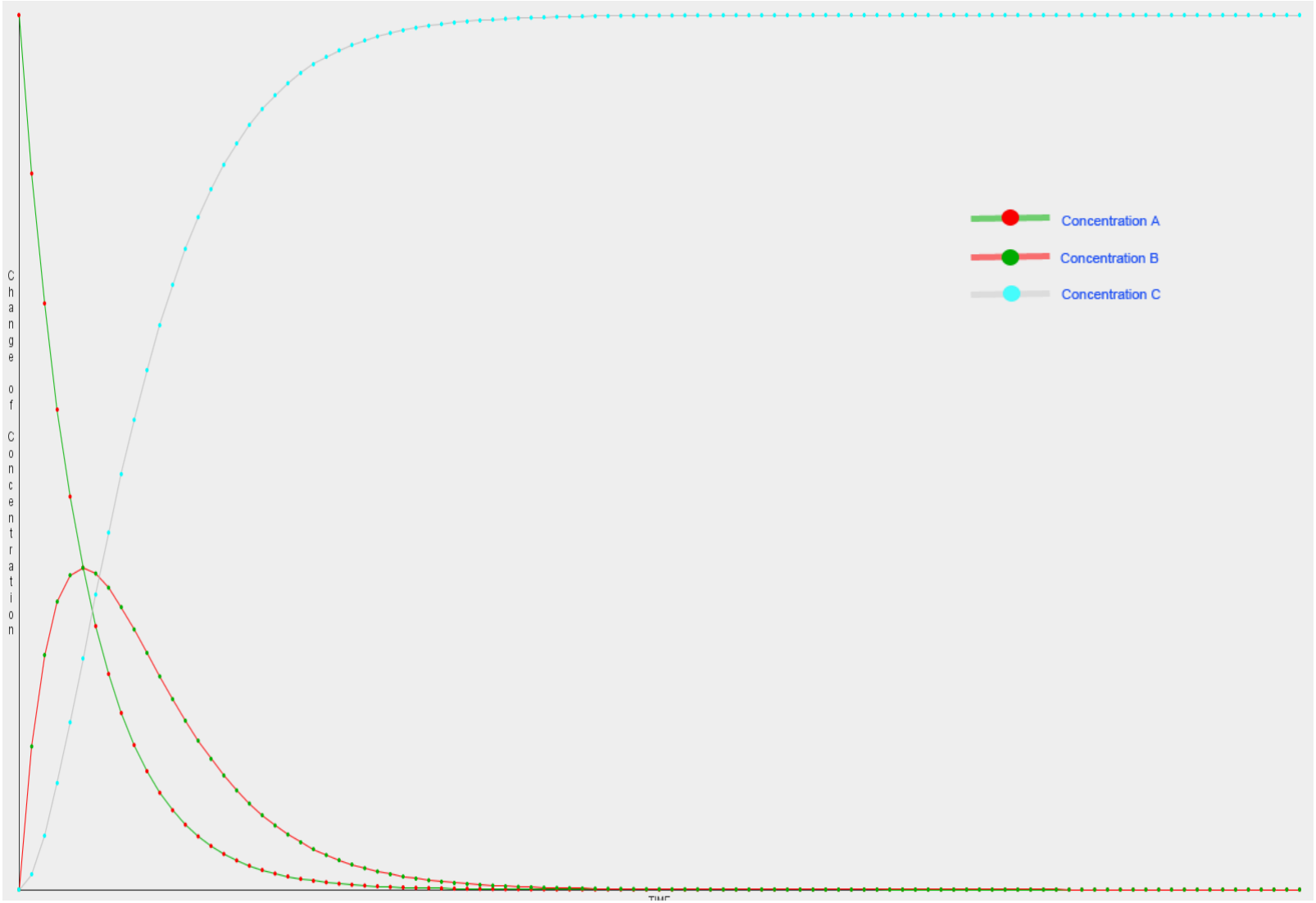
Simulation when constant rate is .5



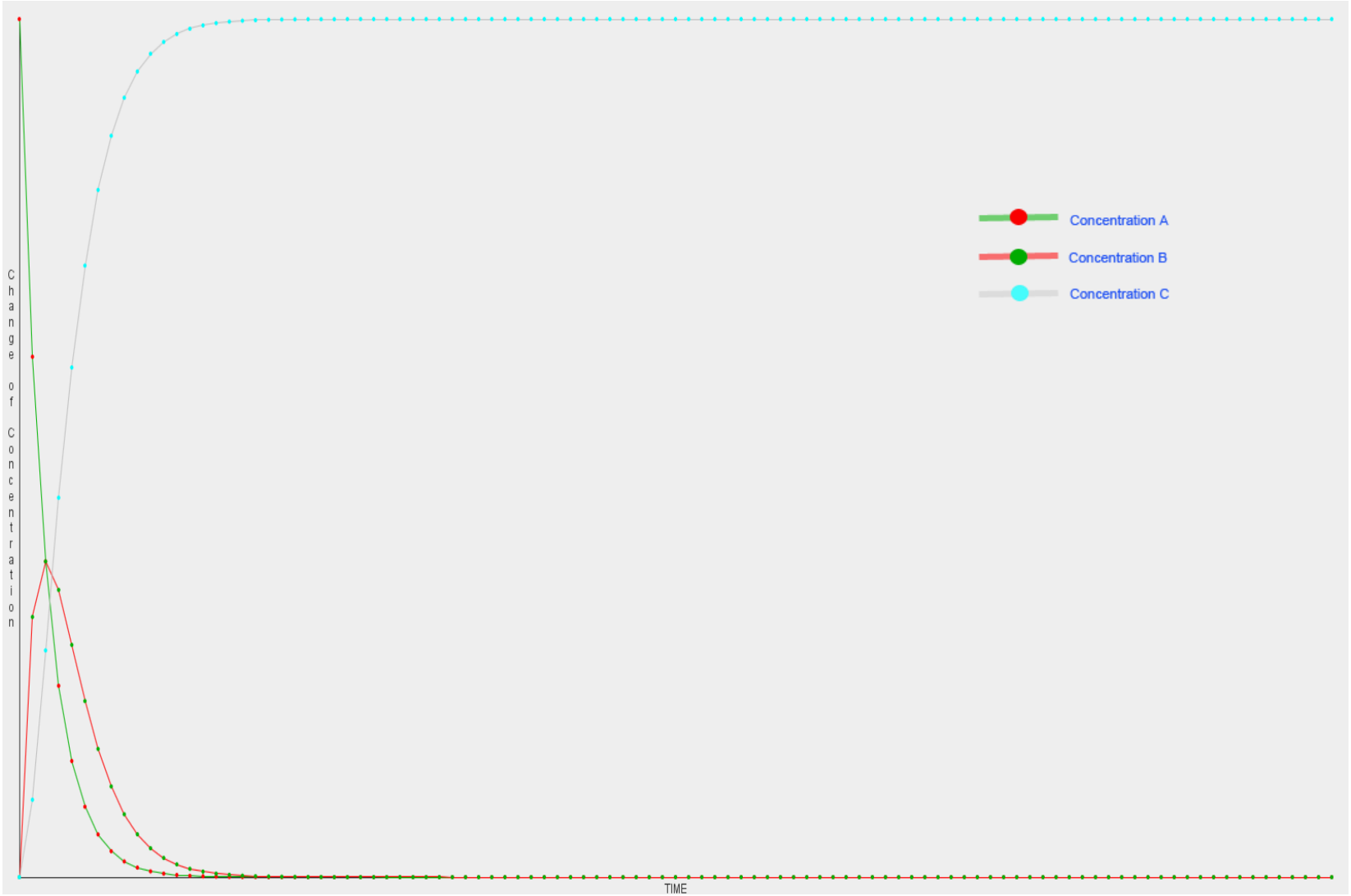
Simulation when constant rate is 1



Simulation when constant rate is 2

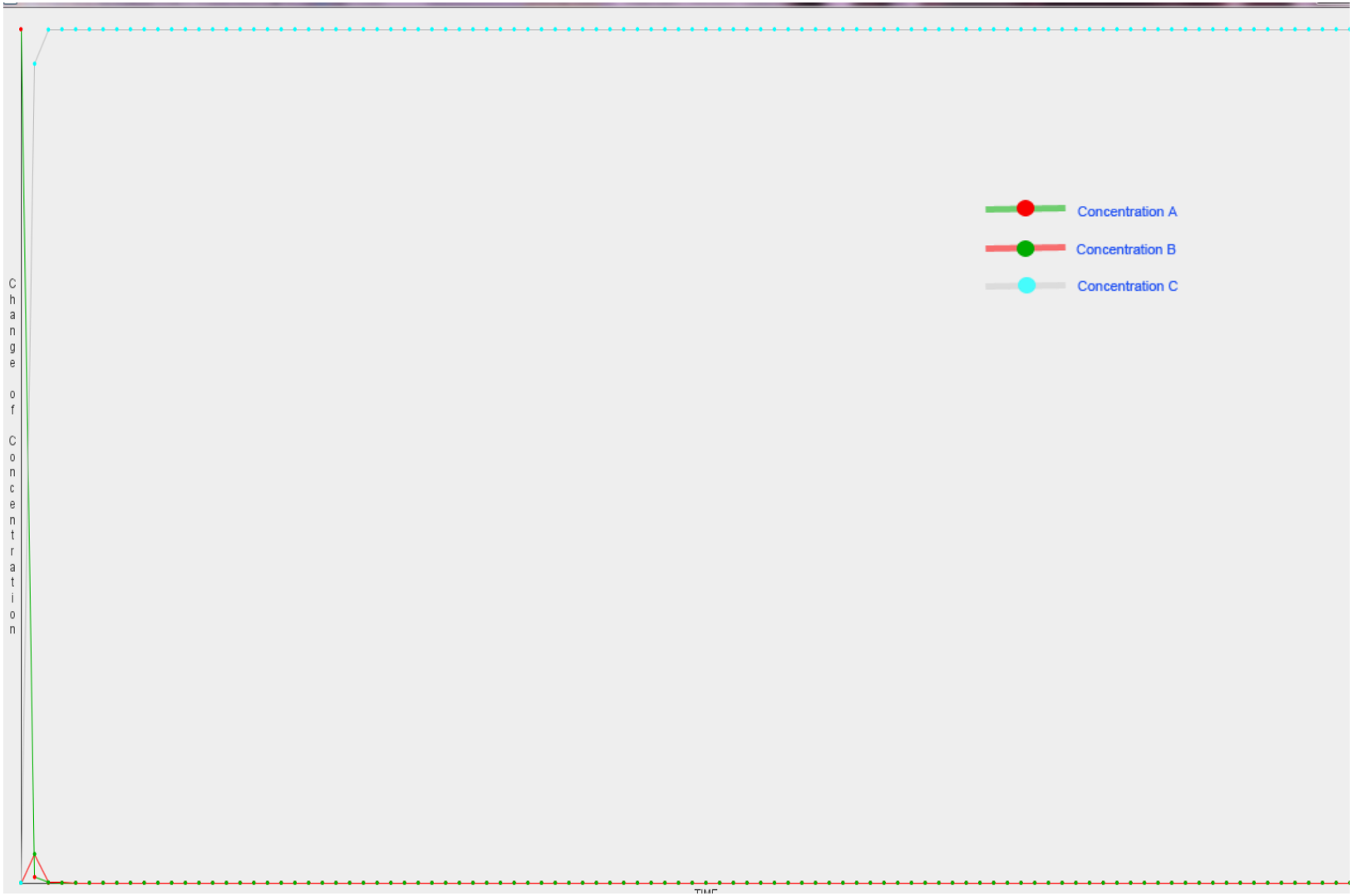


Simulation when constant rate is 5



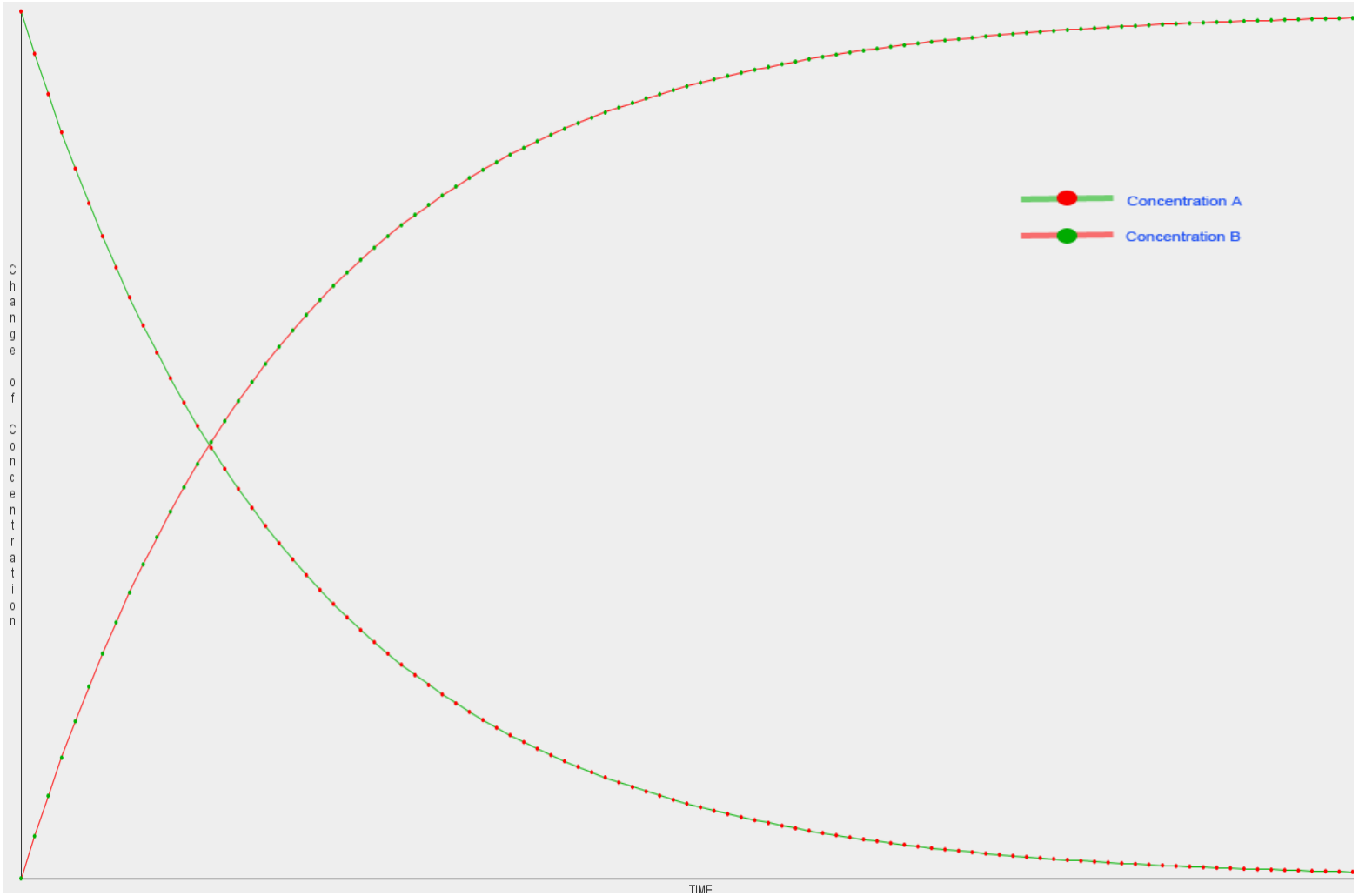
Simulation when constant rate is 10

Simulation when constant rate is 50



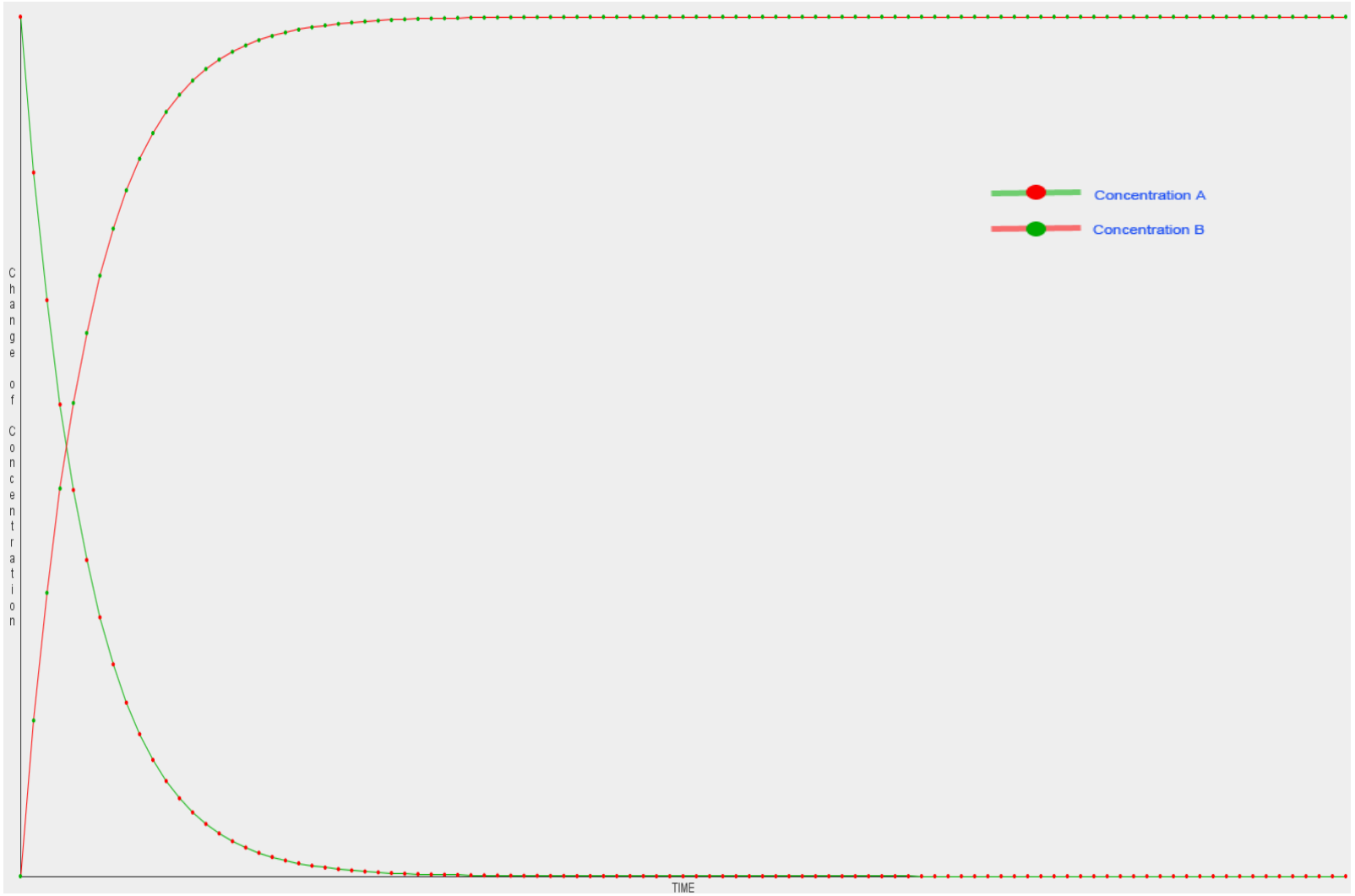
Simulations for A→B

Simulation when constant rate is .5

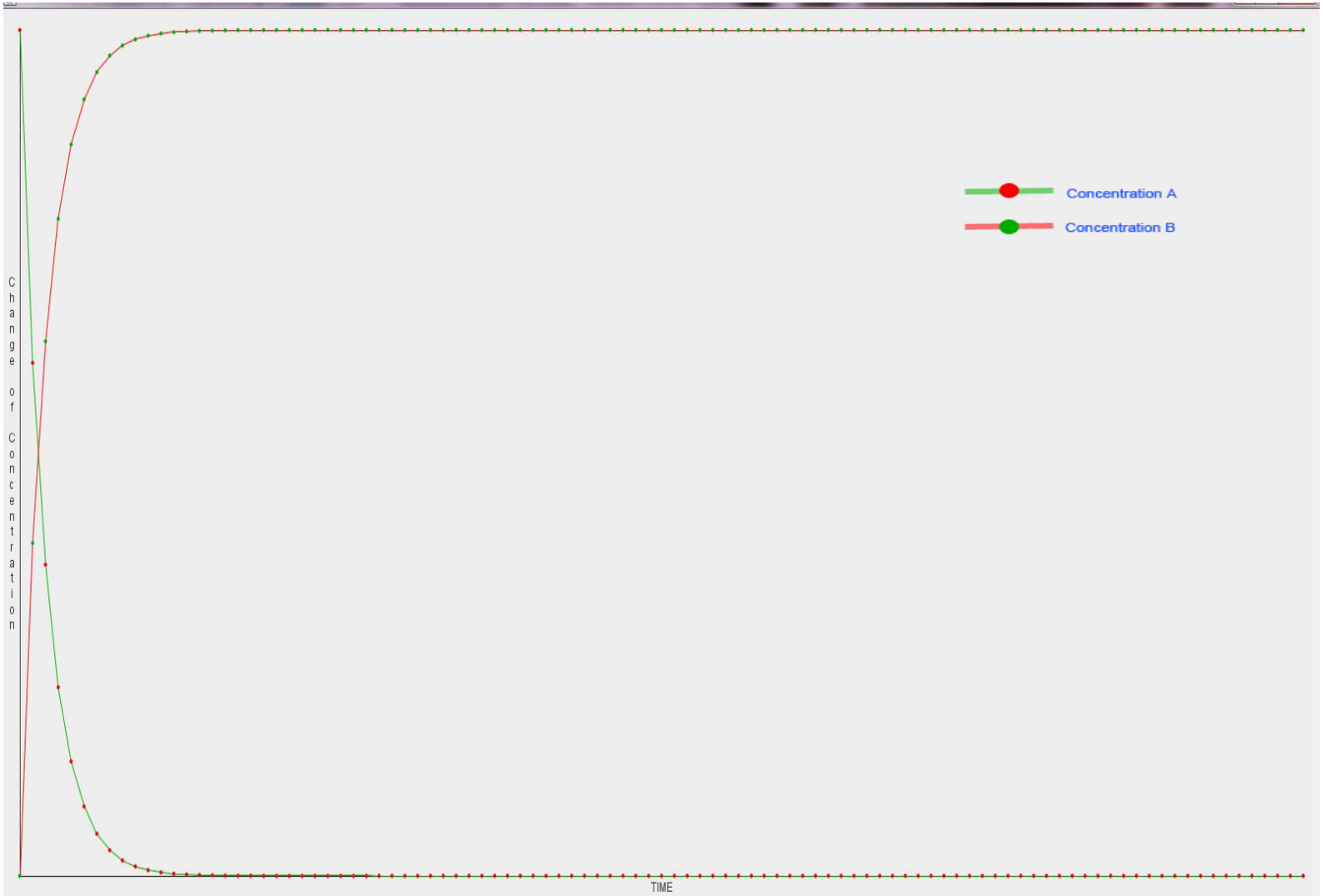


Simulation when constant rate is 1

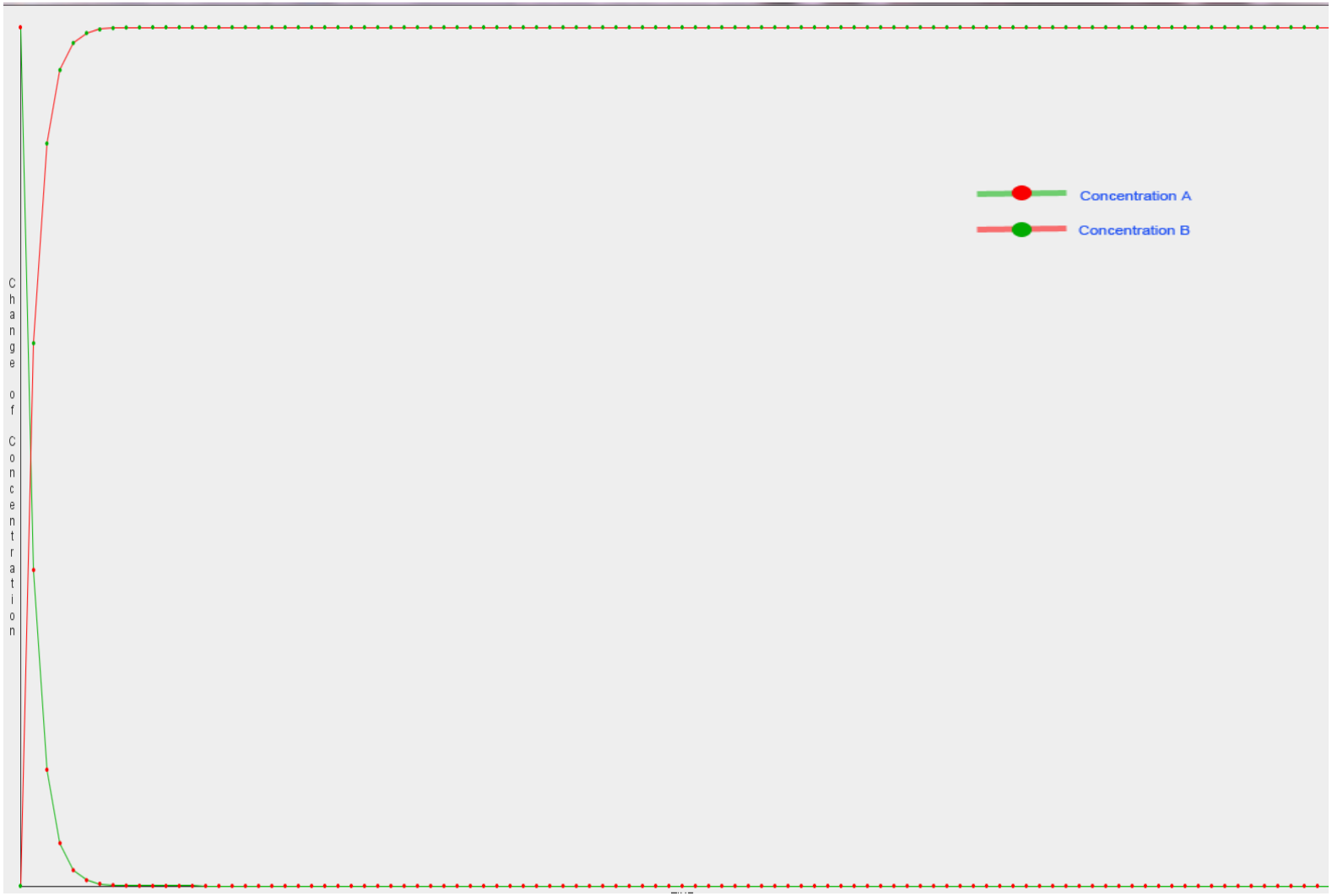
Simulation when constant rate is 2



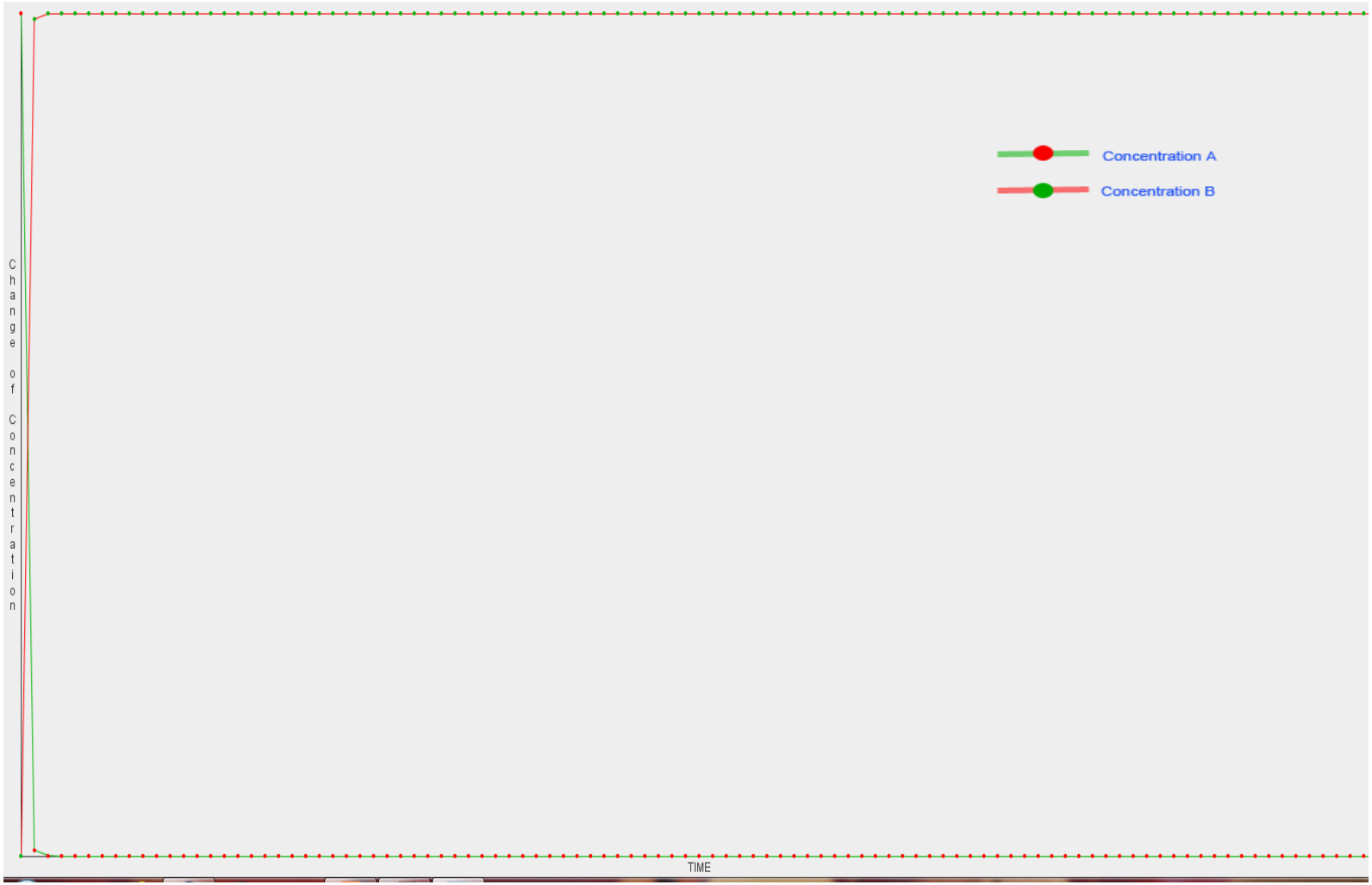
Simulation when constant rate is 5



Simulation when constant rate is 10



Simulation when constant rate is 50



Future Work

- Run Simulations for A → B → C → D
- Run Simulations for different values of k, l, and m

Questions