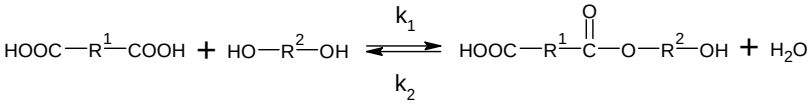
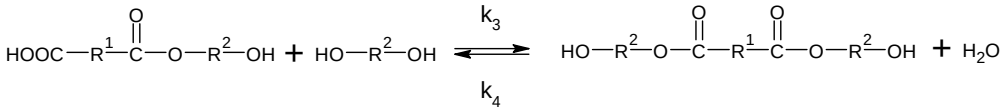
The project guidelines

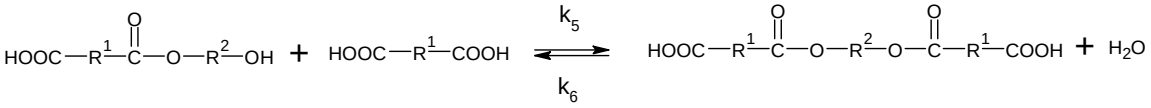
Esterification reactions play a key role in the preparation of certain polymers. In a system containing, for example, a dicarboxylic acid (A) and a diol (B), an equilibrium is established between the starting materials, esters (AB, ABA, BAB) and water (W). The initial stage of this process can be very simply written as:



(1)



(2)



(3)

The aim of the project is to implement in Python (NumPy + SciPy + Matplotlib) models of the system using (a) extent of reaction method, and (b) kinetic approach, and to investigate of the models.

After developing of the models please answer the following questions:

Q1: How to validate both models? Demonstrate the code showing the correctness of models.

Q2: Assuming that $k_1=k_3=k_5=10^{-3}$ *L/mol·s*, $k_2=k_4=k_6=10^{-4}$ *L/mol·s*, $[A]_0$= *2 mol/L* and $[B]_0$=*1 mol/L,* what are the equilibrium concentrations and the time for equilibrium to be reached in the system?

Q3: Knowing that $k_1=k_3=k_5=10^{-3}$ *L/mol·s*, $k_2=k_4=k_6=10^{-4}$ *L/mol·s* and $[A]_0=[B]_0$=*1 mol/L* how does the initial water concentration affect the equilibrium concentration of esters? Assume that initially the system is esters free.

Q4: Estimate (any approach) what is the highest possible concentration of AB in the system and after what time it is reached, assuming $k_1=k_3=k_5=5.0\cdot10^{-4}$ *L/mol·s*, $k_2=k_4=k_6=1.0\cdot10^{-5}$ *L/mol·s* and knowing that $[A]_0$, $[B]_0$ and $[W]_0$ may vary in a range from *0* to *2 mol/L.*

Your project as a Word document or a Jupyter notebook should consist: brief introduction, reaction scheme, the source code (with comments) of models (a and b), and answers to the questions illustrated by plots, tables or the Python code (if necessary) and providing your assumptions.

Evaluation: Q1 – 50pt, Q2 – 10pt, Q3 – 20pt, Q4 – 20pt.

References: 1) Hans Fangohr, Python for Computational Science and Engineering, https://fangohr.github.io/teaching/python/book.html; 2) Martin Schmal, Chemical Reaction Engineering: Essentials, Exercises and Examples, 2020, CRC; 3) Robert J. Silbey, Robert A. Alberty, Moungi G. Bawend, Physical Chemistry, Wiley, 2005; 4) https://github.com/sbednarz/modeling