CP409 Problem Solving Block A – Week 1

In the preparatory tasks, you have encountered three fundamental aspects of modelling:

- Using a material balance to derive a differential equation that describes the rates of change of materials in a system (e.g. batch reactor);
- You can solve the equations using basic mathematical skills, remembering to apply suitable boundary conditions;
- Or you can solve the equations numerically, which is a good way to check that your analytical solutions are correct.

In this first week's task we will apply the same ideas to a new situation; you have all the tools to solve the problems set, you just need to use them correctly!

Task A1

You may be familiar with the story of Apollo 13, the NASA flight to the Moon in 1970. Two days into the mission, an oxygen tank exploded, causing a loss of power and limited resources for removing carbon dioxide from the air the astronauts were breathing inside the capsule. Carbon dioxide is dangerous when it reaches a volumetric concentration of about 4%, after which brain function starts to be affected. If you are trying to land a space ship, you need all your faculties!

We will model how the carbon dioxide level increases with time in the capsule. Let the capsule have a volume V, with N astronauts each breathing 6 litres of air per minute, with exhaled air containing 5% more CO_2 (and 5% less O_2) by volume than inhaled air.

(a) At the time of the accident, the concentration of CO_2 can be assumed to be zero. How does its concentration vary over time without any removal system?

(b) The astronauts managed to rig up the CO_2 removal system, which comprised canisters of lithium hydroxide adsorbent. The relevant reaction is

$$2LiOH + CO_2 \rightarrow Li_2CO_3 + H_2O$$

We can model the rate of CO_2 adsorption as being proportional to its concentration in the atmosphere (the reaction is linear in CO_2 concentration). Use a material balance to derive a differential equation for the evolution of the CO_2 concentration over time. Find the analytical solution for this differential equation.

(c) More modern spacecraft use lithium peroxide (Li_2O_2) as the adsorbent. The relevant reaction is

$$2Li_2O_2 + 2CO_2 \rightarrow 2Li_2CO_3 + O_2$$

This is second order in the concentration of CO_2, hence modify your differential equation for the evolution of the concentration CO_2 to model the adsorption rate as the square of the concentration. Find your analytical solution for this case.

For the Friday zoom session:

(d) Using the Euler Method in Matlab, find numerical solutions to your differential equation from part (b) and compare to your analytical ones.

To do this you need to use typical numbers for the various parameters. Try $N = 3$ astronauts, $V = 30m^3$, and a range for the rate constant of the CO_2 adsorption process. What rate constant keeps the astronauts alive for 4 days so that they can make it safely back home?

(e) Again use the Euler Method in Matlab to find numerical solutions to your differential equation in part (c) to check your analytical work.