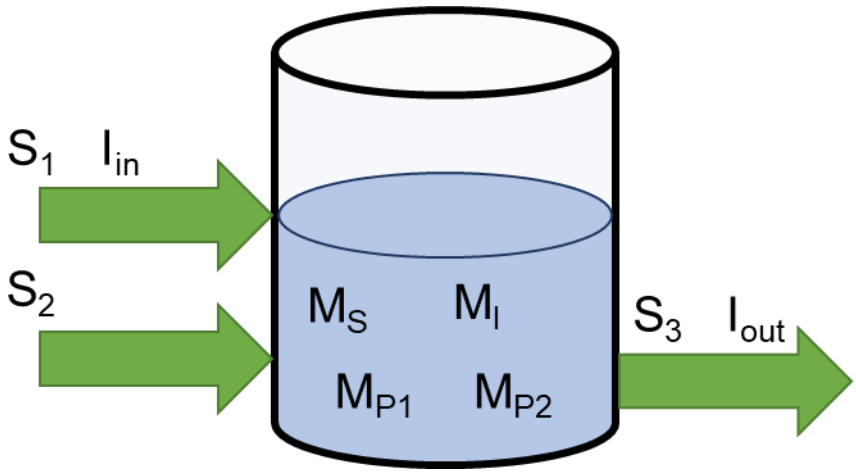
# MATHEMATICAL MODELING

## The goal of this project is to:

- Develop, implement and validate a mathematical model for a simple system in Python. Use dependency graphs to analyse the system

**The System:**

For a continuous stirred tank reactor (CSTR) with two inputs of solvent (S), one containing an impurity (I), and one output, within the reactor there are masses (M) of two species (P1 and P2) of particles that are of interest, the system and its boundaries are defined as:




**Mathematical Equations:**

The liquid level in the reactor is kept constant by having the output flow equal to the inlet flows, i.e.:

$$S_3 = S_1 + S_2$$

Impurity in and out are functions of the inlet flow rate and reactor composition respectively:

$$I_{in} = 0.05 S_1$$

$$I_{out} = S_3 \frac{M_I}{M_S}$$

Birth (B) and death (D) equations for P1 and P2 are defined as follows:

$$B_{P1} = \alpha M_{P1}$$

$$D_{P1} = k M_{P1} M_{P2} + \eta M_I$$

$$B_{P2} = \delta M_{P1} M_{P2}$$

$$D_{P2} = \gamma M_{P2}$$

**Variables:**

| Variable | Value | Unit |
|---|---|---|
| α | 0.0005 | 1/s |
| k | 0.0001 | 1/s |
| η | 0.0004 | 1/s |
| δ | 0.012 | 1/s |
| γ | 0.0002 | 1/s |
| $S_1$ | 0.01 | kg/s |
| $S_2$ | 0.005 | kg/s |
| $M_S$ | 1 | kg |
| $M_I$ | Initial – 0.01 | kg |
| $M_{P1}$ | Initial – 0.07 | kg |
| $M_{P2}$ | Initial – 0.001 | kg |

**Prediction:**

predict the mass of I, P1 and P2 after 1 hr (3600 s)

**Validation:**

Use the following values to validate the model

| Time (s) | Mass P1 (kg) |
|---|---|
| 600 | 0.0769 |
| 1200 | 0.1112 |
| 1800 | 0.1465 |
| 2400 | 0.1629 |
| 3000 | 0.1832 |
| 3600 | 0.3275 |