1 Data reconciliation

Both during the design phase and after the plant is operable there's the need to deal with a certain amount of data. Design or calculated data can be input in process simulator, they can undergo several calculations and then they'll always give us (hopefully !) a correct and coherent result, they are somehow "perfect". However "perfection" has a price and usually this price is that it doesn't exist.

Real data can be either directly or indirectly measured, the price of their existence is the error the measurements always bring with them, no matter their typology. Biased data clearly cannot satisfy conservation laws as well as other physical principles, therefore in order to have a more accurate estimation of what's actually happening to the system we need to reconcile them.

Reconciling means to estimate and minimize the errors so that the data fulfill the physical principles. In short data reconciliation is nothing but a constrained optimization.

1.1 Flowrates mass reconciliation

The system under analysis consists of a PF reactor and a distillation column (cf. Figure 1.1.1) whose distillate is recycled back to the reactor.

All the mass flowrates have been measured as listed in Table 1.1. Their reconciliation is requested.

Furthermore the most critical instrumentation functioning in the system has to be identified.

Stream #	**Flowrate** $[kg/h]$
1	95.00
2	170.00
3	175.00
4	75.00
5	103.00
6	15.00
7	82.00

Table 1.1: Measured stream flowrates

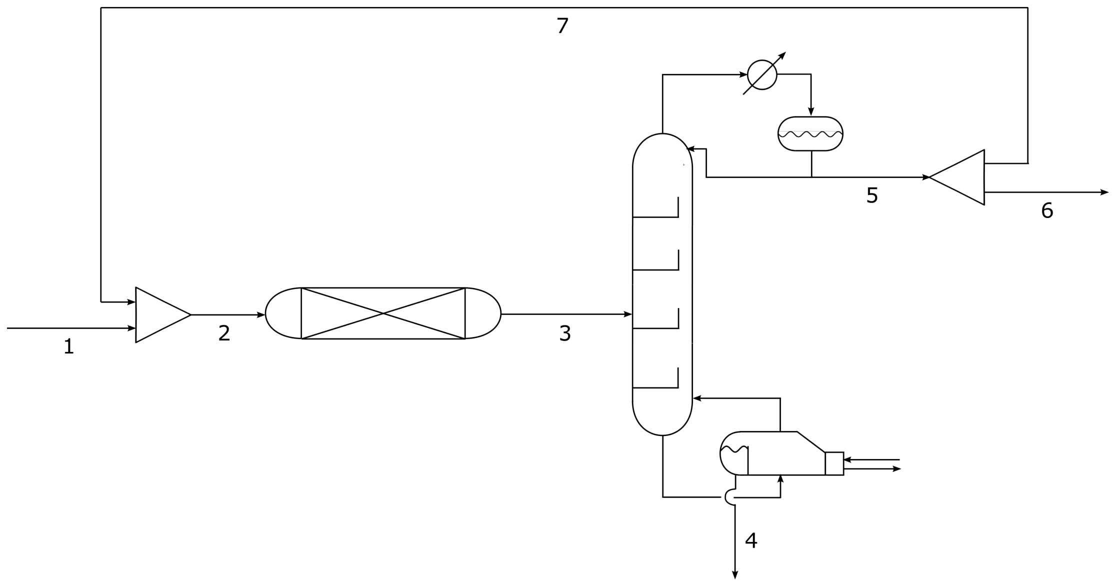

Figure 1.1.1: Process Flowsheet

Solution I

Data reconciliation is a constrained optimization. The problem can be formalized as:

$$\min_{\overline{F}_R} \varepsilon^2(\overline{F}_R) \tag{1.1.1}$$

$$s.t.\, A \cdot \overline{F}_R + c = 0 \tag{1.1.2}$$

where $\overline{F}_R$ is the reconciled flowrates vector, ε is the error and A is the constraints coefficients matrix.

The absolute square error is explicitly expressed as:

$$\overline{\varepsilon}^T \cdot \overline{\varepsilon} = \sum_{i=1}^{7} (\overline{F}_{Ri} - \overline{F_i})^2 \tag{1.1.3}$$

The physical constraints to fulfill are given by the mass balance equations for each unit:

$$\begin{cases} F_1 + F_7 - F_2 = 0 & Mixer \\ F_2 - F_3 = 0 & Reactor \\ F_3 - F_4 - F_5 = 0 & Column \\ F_5 - F_6 - F_7 = 0 & Splitter \end{cases} \tag{1.1.4}$$

As it can be noticed there are 7 unknown variables but only 4 equations, that means the system has 3 degrees of freedom and we're asked to solve a 3 dimensional optimization problem.

The simplest way to solve the reconciliation will be presented first. However, the price of its simplicity is paid by the cumbersome calculations required. It consists of the application of the substitution method and it's performed by substituting 4 selected dependent variables into the absolute square error expression. Since the absolute square error is a quadratic function the minimization can be finally performed by zeroing the gradient of the resulting expression.

First of all the "most comfortable" variables can be made explicit from the 1.1.4.

$$\begin{cases} F_1 = -F_7 + F_3 \\ F_2 = F_3 \\ F_4 = F_3 - F_5 \\ F_6 = F_5 - F_7 \end{cases} \tag{1.1.5}$$

the new absolute square error can then be written as:

$$\bar{\varepsilon}^2 = (F_3 - F_7 - 95)^2 + (F_3 - 170)^2 + (F_3 - 175)^2 + (F_3 - F_5 - 75)^2 + (F_5 - 103)^2 + (F_5 - F_7 - 15)^2 + (F_7 - 82)^2 \tag{1.1.6}$$

Its gradient results to be:

$$\begin{cases} \frac{\partial \bar{\varepsilon}^2}{\partial F_3} = 2 \cdot (F_3 - F_7 - 95) + 2 \cdot (F_3 - 170) + 2 \cdot (F_3 - 175) + 2 \cdot (F_3 - F_5 - 75) \\ \frac{\partial \bar{\varepsilon}^2}{\partial F_5} = -2 \cdot (F_3 - F_5 - 75) + 2 \cdot (F_5 - 103) + 2 \cdot (F_5 - F_7 - 15) \\ \frac{\partial \bar{\varepsilon}^2}{\partial F_7} = -2 \cdot (F_3 - F_7 - 95) - 2 \cdot (F_5 - F_7 - 15) + 2 \cdot (F_7 - 82) \end{cases} \tag{1.1.7}$$

It can be set it equal to zero and the corresponding system of equations can be solved:

$$\begin{cases} (F_3 - F_7 - 95) + (F_3 - 170) + (F_3 - 175) + (F_3 - F_5 - 75) = 0 \\ -(F_3 - F_5 - 75) + (F_5 - 103) + (F_5 - F_7 - 15) = 0 \\ -(F_3 - F_7 - 95) - (F_5 - F_7 - 15) + (F_7 - 82) = 0 \end{cases} \iff \begin{cases} 4 \cdot F_3 - F_5 - F_7 = 515 \\ -F_3 + 3 \cdot F_5 - F_7 = 43 \\ -F_3 - F_5 + 3 \cdot F_7 = -28 \end{cases}$$