3.3 Data Reconciliation Supplementary Material: Solution

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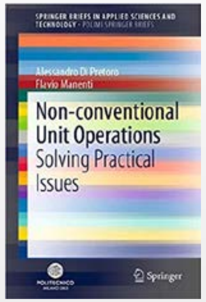
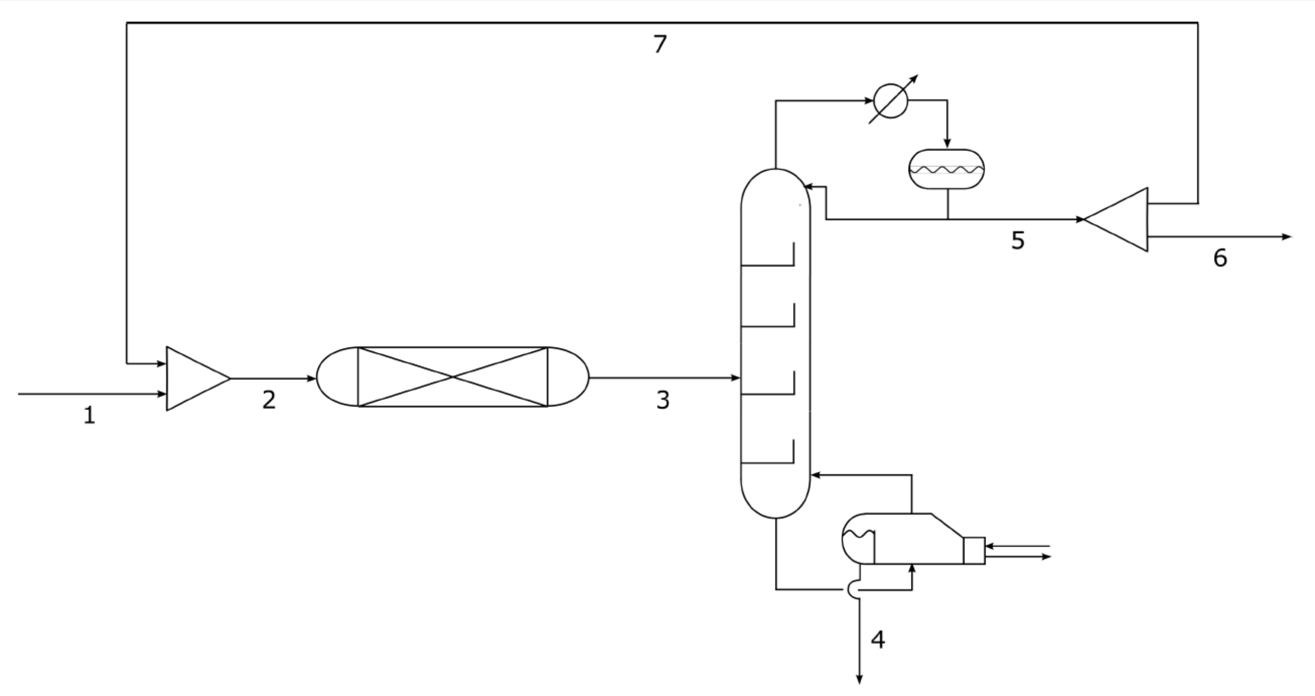
Exercise



Consider the following isomerization process. It consists of synthesis and purification/recycle sections. All the relevant mass flowrates are measured, but balances are not fulfilled.

(I) Reconcile the process data.



Process data

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

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Solution

Data reconciliation is a NLP problem with DoR = 4 > 0:

$$\min_{\mathbf{f}_R} \varepsilon^2 (\mathbf{f}_R)$$

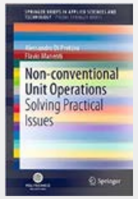
$$s.t.: \mathbf{A} \cdot \mathbf{f}_R + \mathbf{c} = 0$$

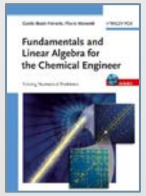
f_R = reconciled flowrate vector

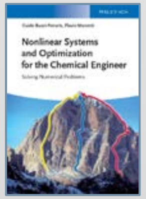
A = process constraints coefficient matrix

With absolute square error:

$$\boldsymbol{\varepsilon}^T \cdot \boldsymbol{\varepsilon} = \sum_{i=1}^{NM=7} \left(\mathbf{f}_{R,i} - \mathbf{f}_{m,i} \right)^2$$







Solution

Process constraints:

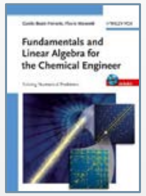
$$\begin{cases} f_1 + f_7 - f_2 = 0 & \textbf{\textit{Mixer}} \\ f_2 - f_3 = 0 & \textbf{\textit{Reactor}} \\ f_3 - f_4 - f_5 = 0 & \textbf{\textit{Column}} \\ f_5 - f_6 - f_7 = 0 & \textbf{\textit{Splitter}} \end{cases}$$

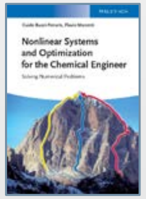
4 equations, 7 unknowns → 3-DoF NLP

Matrix revision:

$$\begin{cases} f_1 = -f_7 + f_3 \\ f_2 = f_3 \\ f_4 = f_3 - f_5 \\ f_6 = f_5 - f_7 \end{cases}$$

Solution





Linear system solution: $\mathbf{A}\cdot\mathbf{f}_R=\mathbf{c}$ $\quad \mathbf{f}_R=\mathbf{A}^{-1}\cdot\mathbf{c}$

Matrix of process coefficients A and measure vector c:

Band matrix

$$\mathbf{A}=\begin{bmatrix} 1 & & -1 & & & & 1 \\ & 1 & -1 & & & & \\ & & 1 & & & & \\ & & -1 & 1 & 1 & & \\ & & & & 1 & & \\ & & & & -1 & 1 & 1 \\ & & & & & & 1 \end{bmatrix}$$

Recycle

$$\mathbf{c}=\begin{bmatrix} 95 \\ 170 \\ 175 \\ 75 \\ 103 \\ 15 \\ 82 \end{bmatrix}$$

Recycles and control actions are spoiling matrices for design/operation manegement purposes

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Solution

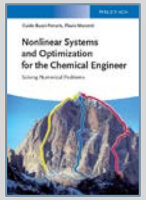
Absolute square error is:

$$\boldsymbol{\varepsilon}^2 = (f_3 - f_7 - 95)^2 + (f_3 - 170)^2 + (f_3 - 175)^2 + $$
$$+ (f_3 - f_5 - 75)^2 + (f_5 - 103)^2 + (f_5 - f_7 - 15)^2 + (f_7 - 82)^2$$

Reconciliation becomes a root-finding problem:

$$\frac{\partial \boldsymbol{\varepsilon}^2}{\partial \mathbf{f}_R} = 0$$

$$\begin{cases} \dfrac{\partial \boldsymbol{\varepsilon}^2}{\partial f_3} = 2 \cdot (f_3 - f_7 - 95) + 2 \cdot (f_3 - 170) + 2 \cdot (f_3 - 175) + 2 \cdot (f_3 - f_5 - 75) \\ \dfrac{\partial \boldsymbol{\varepsilon}^2}{\partial f_5} = -2 \cdot (f_3 - f_5 - 75) + 2 \cdot (f_5 - 103) + 2 \cdot (f_5 - f_7 - 15) \\ \dfrac{\partial \boldsymbol{\varepsilon}^2}{\partial f_7} = -2 \cdot (f_3 - f_7 - 95) - 2 \cdot (f_5 - f_7 - 15) + 2 \cdot (f_7 - 82) \end{cases}$$

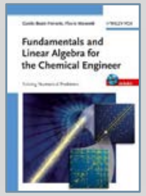


Solution

$$\frac{\partial \boldsymbol{\varepsilon}^2}{\partial \mathbf{f}_R} = 0$$

$$\begin{cases} (f_3 - f_7 - 95) + (f_3 - 170) + (f_3 - 175) + (f_3 - f_5 - 75) = 0 \\ -(f_3 - f_5 - 75) + (f_5 - 103) + (f_5 - f_7 - 15) = 0 \\ -(f_3 - f_7 - 95) - (f_5 - f_7 - 15) + (f_7 - 82) = 0 \end{cases}$$

$$\begin{cases} 4 \cdot f_3 - f_5 - f_7 = 515 \\ -f_3 + 3 \cdot f_5 - f_7 = 43 \\ -f_3 - f_5 + 3 \cdot f_7 = -28 \end{cases} \Rightarrow \begin{cases} f_3 = 174.17 kg/h \\ f_5 = 99.71 kg/h \\ f_7 = 81.96 kg/h \end{cases}$$



Solution

Stream #	Measured kg/h	Reconciled kg/h	Error %
1	95	92.21	3.03
2	170	174.17	–2.39
3 ^{OPT}	***175***	***174.17***	***0.48***
4	75	74.46	0.73
5 ^{OPT}	***103***	***99.71***	***3.30***
6	15	17.75	–15.49
7 ^{OPT}	***82***	***81.96***	***0.05***

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Solution

Stream #	Measured kg/h	Reconciled kg/h	Error %	
1	95	92.21	3.03	
2	170	174.17	–2.39	
3 OPT	***175***	***174.17***	***0.48***	
4	75	74.46	0.73	
5 OPT	***103***	***99.71***	***3.30***	
6	15	17.75	–15.49	???
7 OPT	***82***	***81.96***	***0.05***	

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Solution

Minimization of relative square error (balancing)

Among nany possibilities:

$$\boldsymbol{\varepsilon}_n^T \cdot \boldsymbol{\varepsilon}_n = \sum_{i=1}^{NM=7} \frac{\left(\mathbf{f}_{R,i} - \mathbf{f}_{m,i}\right)^2}{\mathbf{f}_{m.i}^2}$$

$$\boldsymbol{\varepsilon}_n^2 = \frac{\left(f_3 - f_7 - 95\right)^2}{95^2} + \frac{\left(f_3 - 170\right)^2}{170^2} + \frac{\left(f_3 - 175\right)^2}{175^2} + \frac{\left(f_3 - f_5 - 75\right)^2}{75^2} + \frac{\left(f_5 - 103\right)^2}{103^2} + \frac{\left(f_5 - f_7 - 15\right)^2}{15^2} + \frac{\left(f_7 - 82\right)^2}{82^2}$$

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Solution

Stream #	Measured kg/h	Reconciled kg/h	Error %
1	95	91.41	3.78
2	170	174.98	–2.93
3^{OPT}	***175***	***174.98***	***0.01***
4	75	76.27	1.69
5^{OPT}	***103***	***98.71***	***4.17***
6	15	15.14	–0.95
7^{OPT}	***82***	***83.57***	***1.91***

Solution references

1. Di Pretoro A., Manenti F. (2020). Non-conventional Unit Operations: Solving Practical Issues, Springer Briefs in Applied Sciences and Technology series, Springer.

2. Buzzi Ferraris G., Manenti F. (2010). Fundamentals and Linear Algebra for the Chemical Engineer: Solving Numerical Problems, Vol. 1, Wiley-VCH, Weinheim, Germany

3. Buzzi Ferraris G., Manenti F. (2013). Nonlinear Systems and Optimization for the Chemical Engineer: Solving Numerical Problems, Vol. 3, Wiley-VCH, Weinheim, Germany

4. BzzMath Digitalization Library at https://super.chem.polimi.it, in download section, freely available for academies (Digitalization branches: DA, AI, ML, DoE, DT, DM)