Linear Material Balances in Process Flowsheet

Bruno Abreu Calfa

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1 System of Linear Equations Example

1.1 Problem Definition

Adapted from: Biegler, L. T., Grossmann, I. E., Westerberg, A. W. (1997) *Systematic Methods of Chemical Process Design*. Prentice Hall.

The flowsheet in block-diagram form for the production of ethanol is given below.

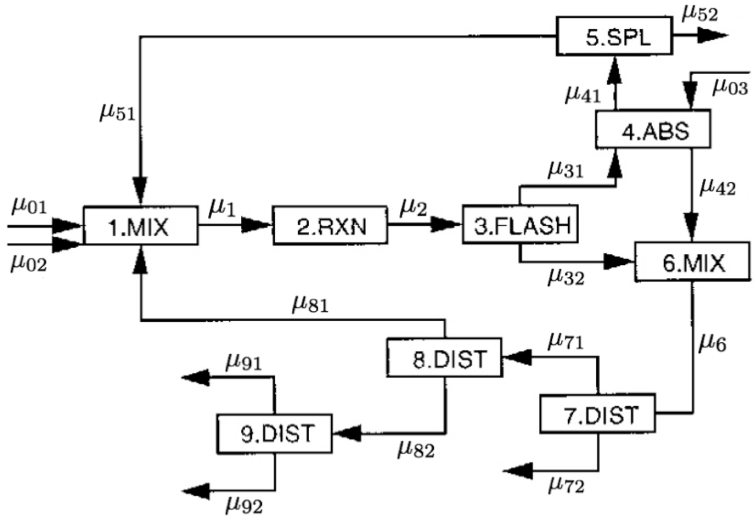

Figure 1: Flowsheet for the production of ethanol. μ_{ij} represents molar flows from unit i and j-th output stream (if more than one).

We want to perform a mass balance on ethylene and then calculate all its flowrates. Using the *split fractions* of each unit, we derive the following linear equations (for ethylene):

$$
\begin{aligned}
\mu_1 &= \mu_{81} + \mu_{01} + \mu_{51} \\
\mu_2 &= 0.93\mu_1 \\
\mu_{31} &= 0.985\mu_2 \\
\mu_{32} &= 0.015\mu_2 \\
\mu_{41} &= 0.979\mu_{31} \\
\mu_{42} &= 0.021\mu_{31} \\
\mu_{51} &= 0.995\mu_{41} \\
\mu_{52} &= 0.005\mu_{41} \\
\mu_6 &= \mu_{32} + \mu_{42} \\
\mu_{71} &= \mu_6 \\
\mu_{81} &= \mu_{71}
\end{aligned}
$$

where $\mu_{01} = 96\,\mathrm{gmol\,s^{-1}}$. Notice that the system has 11 variables and 11 equations.

1.2 Matrix Form

The system of linear equations above can be conveniently written in matrix form, *i.e.* using vectors and matrices. The general form of linear systems is:

$$Ax = b$$

where x is a vector of variables (unknowns), A is a matrix of coefficients of each variable in each equation, and b is a vector of constant numbers also known as the right-hand side (RHS).

Let us write the above system in matrix form by putting all the terms containing the variables to the left-hand side and all the constant terms to the right-hand side of the equations:

$$
\begin{aligned}
\mu_1 - \mu_{51} - \mu_{81} &= \mu_{01} \\
0.93\mu_1 - \mu_2 &= 0 \\
0.985\mu_2 - \mu_{31} &= 0 \\
0.015\mu_2 - \mu_{32} &= 0 \\
0.979\mu_{31} - \mu_{41} &= 0 \\
0.021\mu_{31} - \mu_{42} &= 0 \\
0.995\mu_{41} - \mu_{51} &= 0 \\
0.005\mu_{41} - \mu_{52} &= 0 \\
\mu_{32} + \mu_{42} - \mu_6 &= 0 \\
\mu_6 - \mu_{71} &= 0 \\
\mu_{71} - \mu_{81} &= 0
\end{aligned}
$$

which is equivalent to

$$
\underbrace{\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 \\
0.93 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.985 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0.015 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.979 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0.021 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.995 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0.005 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1
\end{bmatrix}}_{A}
\underbrace{\begin{bmatrix}
\mu_1 \\ \mu_2 \\ \mu_{31} \\ \mu_{32} \\ \mu_{41} \\ \mu_{42} \\ \mu_{51} \\ \mu_{52} \\ \mu_6 \\ \mu_{71} \\ \mu_{81}
\end{bmatrix}}_{x}
=
\underbrace{\begin{bmatrix}
\mu_{01} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0
\end{bmatrix}}_{b}
$$

The system in the previous page can be solved using Linear Algebra theory. By pre-multiplying both sides with the inverse of A, denoted by A^{-1}, and using the definition of the identity matrix, I, the solution is given by:

$$\begin{aligned} Ax &= b \\ A^{-1}Ax &= A^{-1}b \\ Ix &= A^{-1}b \end{aligned}$$

$$\boxed{x = A^{-1}b}$$

However, for numerical stability reasons it is not recommended to explicitly calculate A^{-1} and then multiply it by b. There are better (faster and more stable) ways of solving a linear system (*e.g.*, Gaussian Elimination) and more will be covered in a later course.

1.3 Solving $Ax = b$ in MATLAB

The linear system can be easily solved in MATLAB by simply defining matrix A and vector b, and executing the so-called "backslash operation". The following code demonstrates how to solve the above system in MATLAB.

```
>> A = [1 0 0 0 0 0 -1 0 0 0 -1; 0.93 -1 0 0 0 0 0 0 0 0 0; ...
0 0.985 -1 0 0 0 0 0 0 0 0; 0 0.015 0 -1 0 0 0 0 0 0 0; ...
0 0 0.979 0 -1 0 0 0 0 0 0; 0 0 0.021 0 0 -1 0 0 0 0 0; ...
0 0  0 0 0.995 0 -1 0 0 0 0; 0 0 0 0 0.005 0 0 -1 0 0 0; ...
0 0 0 1 0 1 0 0 -1 0 0; 0 0 0 0 0 0 0 0 1 -1 0; 0 0 0 0 0 0 0 0 0 1 -1]

>> b = [96; 0; 0; 0; 0; 0; 0; 0; 0; 0; 0]

>> x = A\b
```

The solution, x, is (flowrates of ethylene):

$$\boxed{x = \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_{31} \\ \mu_{32} \\ \mu_{41} \\ \mu_{42} \\ \mu_{51} \\ \mu_{52} \\ \mu_6 \\ \mu_{71} \\ \mu_{81} \end{bmatrix} = \begin{bmatrix} 1288.87 \\ 1198.65 \\ 1180.67 \\ 17.98 \\ 1155.87 \\ 24.79 \\ 1150.09 \\ 5.78 \\ 42.77 \\ 42.77 \\ 42.77 \end{bmatrix} \text{gmol s}^{-1}}$$