# MATERIAL BALANCE BY LINEAR EQUATIONS

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**ABSTRACT:** *Material balance around process has been conducted by using mixer output equations. A method based on Mason's theory has been proposed to develop mixer output equations.*

**KEY WORDS:** *Numerical method, Material balance, Linear process simulation, Mixer output equations, Mason's theory.*

The steady state solution of material balance problems is important both in the early stages of process simulation and in the advanced stages of design calculations.

Methods presently used to solve material balance problems include 1) the sequential modular approach, 2) the simultaneous modular approach and 3) equation solving approach. For the simultaneous modular approach, this paper develops mixer output equations which results in fast convergence in comparison [1] to Successive substitution, Relaxation, Newton two loops and Newton three loops [2]. The development of these mixer output equations are described here based on Mason's rule [3]. Study of chemical process flowcharts and Mason's theories for calculation of process gains in control has led to the following simple algorithm called linear process simulation or LPS for process simulation and calculation of mixer output flow rates.

In this work, mixer output stream flow rates are represented as a function of the two variables, fresh feed input stream flow rates $X^1$ and split fractions, $F^1$.

A linear mixer output equation can be developed as a function of the two aforementioned variables and any other upstream mixer outputs by doing material balances with linearized equations around each process node. One approach is to solve the set of linear equations simultaneously in blocks. Linear equations for obtaining mixer output stream flow rates for the process shown in Fig. 1 are:

$$X^2 = X^1 + X^8 + X^{11} \quad (1)$$
$$X^8 = F^8 X^4$$
$$X^{11} = F^{11} X^9$$
$$X^9 = F^9 X^2$$

Substituting these equations into equation 1 and simplifying gives:

$$X^2 = X^1 + F^8 X^4 + F^9 F^{11} X^2 \quad (2)$$

Another block of equations is:

$$X^4 = X^3 + X^7 \quad (3)$$
$$X^7 = F^7 X^5$$
$$X^5 = F^5 X^4$$
$$X^3 = F^3 X^2$$

Substituting these equations into equation 3 and

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simplifying gives:

$$X^4 = F^3 X^2 + F^7 F^5 X^4 \quad (4)$$

Equations 2 and 4 are the mixer output equations for Fig. 1 and can be solved simultaneously to give:

$$X^2 = X^1(I - F^5 F^7)(I - F^5 F^7 - F^3 F^8 - F^9 F^{11} + F^5 F^7 F^9 F^{11}) \quad (5)$$

If a mixer output stream equation does not include any other mixer output streams, then it need not to be solved simultaneously with the other mixer equations.

In this study a procedure has been developed to obtain mixer output equations such as equation 5 directly from the process flowsheet without which does not need to solve simultaneous algebraic equations.

### *Development of mixer output vectors*

This approach constructs mixer output vectors using the following equation:

$$L_{ij} = \Sigma M_{ij} P_{ij} [N]^{-1}$$

Where summation is over all possible paths leading from i, fresh feed stream of interest, to j, the mixer output stream of inrest, and

N = I − Product of split fractions of all loops + Product of split fractions of untouching loops taken two at a time − Product of split fractions of untouching loops taken three at a time +··· (untouching loops do not share any node)

$P_{ij}$ = multiples of an identity matrix and split fraction matrices along the path leading from stream i to j.

$M_{ij}$ = function generated from N, by deleting loop terms, containing loops touched by path $P_{ij}$ (i.e., path $P_{ij}$ and the loop are sharing at least one stream).

After calculation of $L_{ij}$, the following equation is used to obtain the mixer output vector of intrest.

$$X^j = \Sigma L_{ij} X^i$$

Where the summation is taken over all the process inputs and reactor outputs.

The following algorithm, is efficient for generation of mixer output vectors and should be followed as:

1- Identify all mixers (MIXR) having at least one stream originating from unit with higher unit number than the mixer unit under consideration (Recycle streams) [4] among their inputs.
2- Multiply all split fractions matrices (ignoring mixers) encountered in tracing all recycle inputs to mixer of type MIXR in all possible (one at a time) upstream direction until the same stream from which tracing was started is reached, name this diagonal matrix $L_1$ and store it. (1 is the loop identification number).
3- List loops associated with each MIXR. Compare loops associated with one MIXR to the ones associated with others, and generate list of untouching loops and possible combinations of these loops.
4- Using combination of untouching loops list and all loops of step 2, construct function N. Register name of individual loops and loops within groups. Calculate N.
5- Starting from a fresh feed or reactor output, continue downstream and multiply an identity matrix and all the split fraction matrices along all possible paths (one at a time) until the desired mixer output stream is reached. Calculate these $P_{ij}$'s and store. Also register stream numbers encountered along the path.
6- Scan the list of loops and loops within groups in function N and eliminate terms that share a stream with path $P_{ij}$ in order to generate function $M_{ij}$. Calculate $M_{ij}$ for all possible paths. Multiply $P_{ij}$ with related $M_{ij}$ and store the result in $P_{ij}$ location.
7- Multiply the result of step 6 by the related $X^i$ (or $X^{ri}$ reactor output). Go back to step 5 as many times as there are process inputs and reactors in the flowsheet.
8- Use equations 6 and 7 for the required mixer output.
9- For other MIXR (mixer) outputs restart from step 5.

Two flowcharts (Figs. 1 and 2) are used to illustrate

the procedure.

From Fig. 1, to obtain $X^2$ the following steps are carried out in the orders described.

1- M1 , M2

2- $L_1 = F^{11} F^9$

$L_2 = F^8 F^3$

$L_3$ = M1($L_1$ , $L_2$)

M2($L_3$)

Untouching loops

$L_1$ , $L_3$

Combinations $L_1L_3$

4- $N = I - L_1 - L_2 - L_3 + L_1L_3$

5- $P_{12} = I$

6- $M_{12} = I - L_3$

7- $M_{12} P_{12} X^1$

8- $X^2 = [M_{12} P_{12} X^1][N]^{-1}$

or

$X^2 = [I - F^7 F^5]X^1[I - F^{11} F^9 - F^8 F^3 - F^7 F^5 + F^{11} F^9 F^5]^{-1}$

For $X^4$ :

5- $P_{14} = F^3$

6- $M_{14} = I$

7- $M_{14}P_{14}X^1$

8- $X^4 = F^3X^1[I - F^{11} F^9 - F^8 F^3 - F^7 F^5 + F^{11} F^9 F^7 F^5]^{-1}$

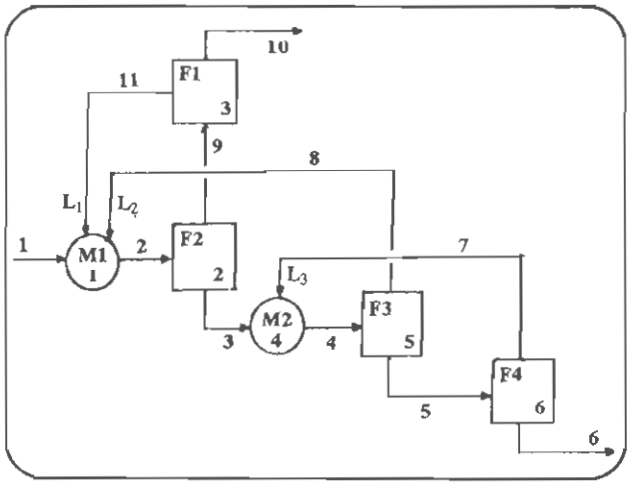


*Fig. 1: Cavett problem flow process*

From Fig. 2, for $X^2$ :

1- M1 , M3

2- $L_1 = F^9 F^6 F^5$

$L_2 = F^{12} F^{14} F^{13}$

$L_3 = F^8 F^6 F^5 F^3$

$L_4 = F^7 F^5 F^3$

$L_5 = F^{17} F^{15} F^{14} F^{13} F^3$

$L_6 = F^{17} F^{11}$

3- M1($L_3$ , $L_4$ , $L_5$ , $L_6$)

M3($L_1$ , $L_2$)

Untouching loops

$L_6$ , $L_1$

$L_6$ , $L_2$

Combinations

$L_1L_6$ , $L_2L_6$

4- $N = I - L_1 - L_2 - L_3 - L_4 - L_5 - L_6 + L_1L_6 + L_2L_6$

5- $P_{12} = I$

6- $M_{12} = I - L_1 - L_2$

7- $M_{12} P_{12} X^1$

8- $X^2 = [I - F^9 F^6 F^5 - F^{12} F^{14} F^{13}] X^1 [I - F^9 F^6 F^5 - F^{12} F^{14} F^{13} - F^8 F^6 F^5 F^3 F^7 F^5 F^3 - F^{17} F^{15} F^{14} F^{13} F^3 - F^{17} F^{11} + F^9 F^6 F^5 F^{17} F^{11} + F^{12} F^{14} F^{13} F^{17} F^{11}]^{-1}$

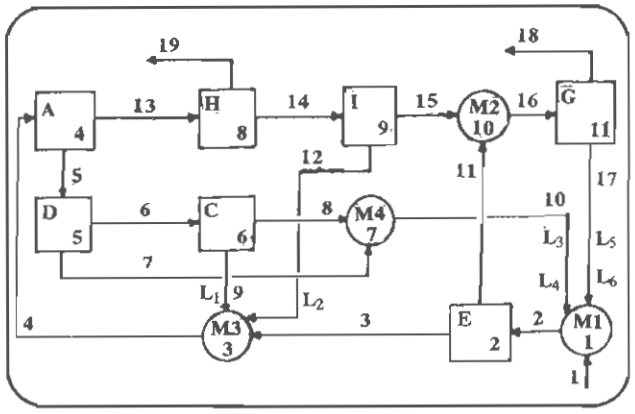


*Fig. 2: Nitric acid flowsheet [5]*

All the matrices involved in the method just described are diagonal (even for systems with reactors) which leads to considerable simplifications in the calculations. Diagonal elements are stored in vectors and no matrix inversion or multiplication is necessary and as a result the order of multiplication of split fractions in certain operations is of no importance.

### *Example*

The *Cavett* [2] problem shown in Fig. 1 was chosen to illustrate the Linear Process Simulation. This problem has 16 components (Table 1).

The results of analysis of this process by LPS are shown in Fig. 3. The convergence routine of this process by LPS is compared to some other simulation techniques [2] in Fig. 3.

These methods include Relaxation, Successive substitutions, the Newton method with two loops and a three loops version (the difference is in the consideration of each of the streams 8 and 11 as a separate loop or addition of these two streams and considering their sum as one loop).

The mixer output equations developed by the method described, provide rapid convergence of recycle computations [1] and the method of development of these equations is simple and can be programmed.

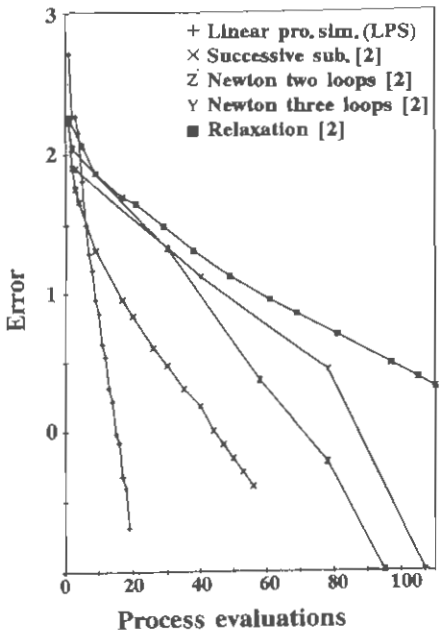


*Fig. 3: Comparison of convergence routines.*

*Table 1:*

| Component | Feed | Product 1 | Product 2 |
|---|---|---|---|
| 1. Nitrogen and helium | 358.2 | 358.2 | 0 |
| 2. Carbon dioxide | 4965.6 | 4963.7 | 1.9 |
| 3. Hydrogen sulfide | 339.4 | 334.4 | 5.0 |
| 4. Methane | 2995.5 | 2995.4 | 0.1 |
| 5. Ethane | 2395.5 | 2380.6 | 14.9 |
| 6. Propane | 2291.0 | 1843.5 | 447.5 |
| 7. *iso*-Butane | 604.1 | 158.4 | 445.7 |
| 8. *n*-Butane | 1539.9 | 245.4 | 1294.5 |
| 9. *iso*-Pentane | 790.4 | 25.7 | 764.7 |
| 10. *n*-Pentane | 1129.9 | 25.1 | 1104.8 |
| 11. Hexane | 1764.7 | 7.0 | 1757.7 |
| 12. Heptane | 2606.7 | 1.9 | 2604.8 |
| 13. Octane | 1844.5 | 0.3 | 1844.2 |
| 14. Nonane | 1669.0 | 0.1 | 1668.9 |
| 15. Decane | 831.7 | 0 | 831.7 |
| 16. Undecane plus | 1214.5 | 0 | 1214.5 |
| Total | 27340.6 | 13339.7 | 14000.9 |

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