Mathematical modeling of Continuous distillation Column

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The numerical simulation of multi-component separation process requires the following points:-

- Reliable predictive method for computing phase equilibrium, more particularly for calculating equilibrium constant & enthalpies.
- A realistic mathematical model with good flexibility & generalization properties.
- A reliable and efficient numerical method for computing the solution.
- The capability of using the method for design purposes.

Steady state modeling:-

The mathematical relations describing the counter current separation process like distillation consists of four sets of basic equations, called mesh equations:

- Mass balance equation(M)
- Equilibrium relations(E)
- Sum(or conservation) equation(S)
- Enthalpy balance relations(H)

Presentation and arrangement depend on the chosen iterative variable and on the balance formulation; so various numerical methods have been proposed. An analysis of their advantages and disadvantages was reviewed by Wang et.al.(1981). The method can be classified into two main categories:-

- Partitioning and coupling methods.
- Global and simultaneous procedures.

In each class the algorithms can differ from one another according to the following criteria:-

1. The iterative variable chosen and mathematical model used.
2. The way of arranging the equations and the procedure implemented for their solution.

3. The convergence method and the convergence promoters.

Partitioning and coupling methods: -The mesh equations are grouped either by stage or by type. Initials estimates for some variables are required for starting the calculations. For a given set of variables the groups of equations are solved in a predetermined order, the other variables being kept constant. These last variables are updated according to the previous result by using direct substitution method. This procedure is continued until a convergence is achieved. Within this category the different approaches can be used.

1. **Stage to stage methods: -** In this class of methods, the procedure of Lewis and Matheson, Thiele and Geddes, and the Θ method of Holland are used. The mesh equations are grouped stage to stage and solved from bottom to top.
2. **Partitioned by type of equation: -** in this approach temperature and flow rates must be initialised. The mass balance equations are combined with the equilibrium equations to form the first set of equations. These equations are linearised by keeping the constant flow rates and equilibrium constants, and then they are solved component by component. By using the new values of compositions, the sum and enthalpy balance equations can be solved either simultaneously or separately in order to obtain the new temperature & flow rates profiles.

Global and simultaneous procedures: -

In this class of methods, the mesh equations are linearized and simultaneously solved by means of Newtons-Raphson Method. A Jacobian matrix containing a large number of partial derivatives (numerically or analytically) must be generated and the equations are solved with the initial set of variable.

Mathematical model: -

Consider the column shown in following figure, involves N plates numbered from top to bottom, including a condenser (total or partial) numbered 1(one) and a reboiler numbered N. The liquid (molar flow L_j) and vapour (molar flow V_j) coming from the stage j from a liquid – vapour equilibrium. On each stage j, a feed stream F_j and liquid (SL_j) and vapour (SV_j) side stream are planned. Heat supplies or losses Q_j on each plate are taken into account, so non-adiabatic column can be studied.

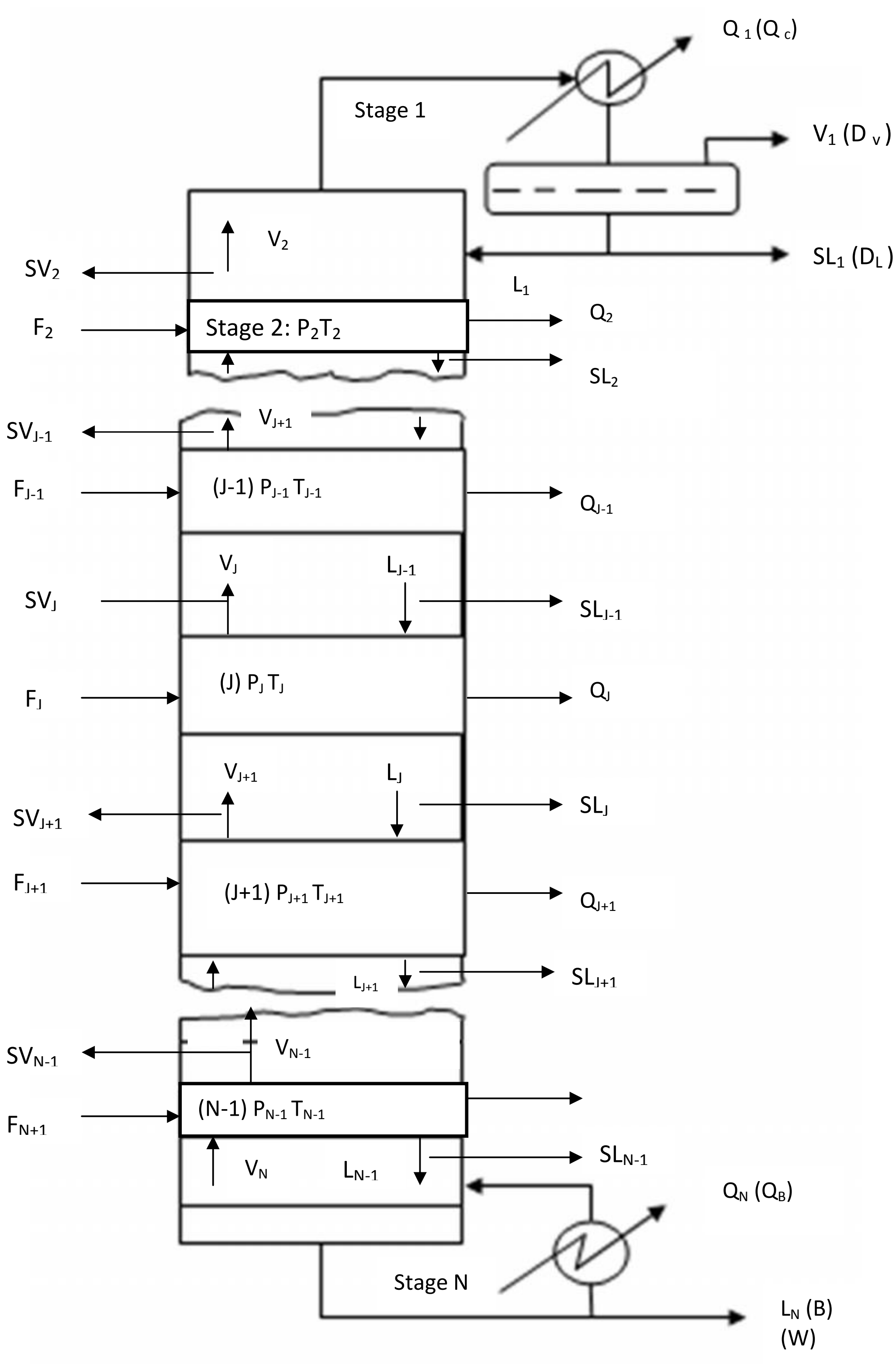

Fig. 26.1: Continuous Distillation Column

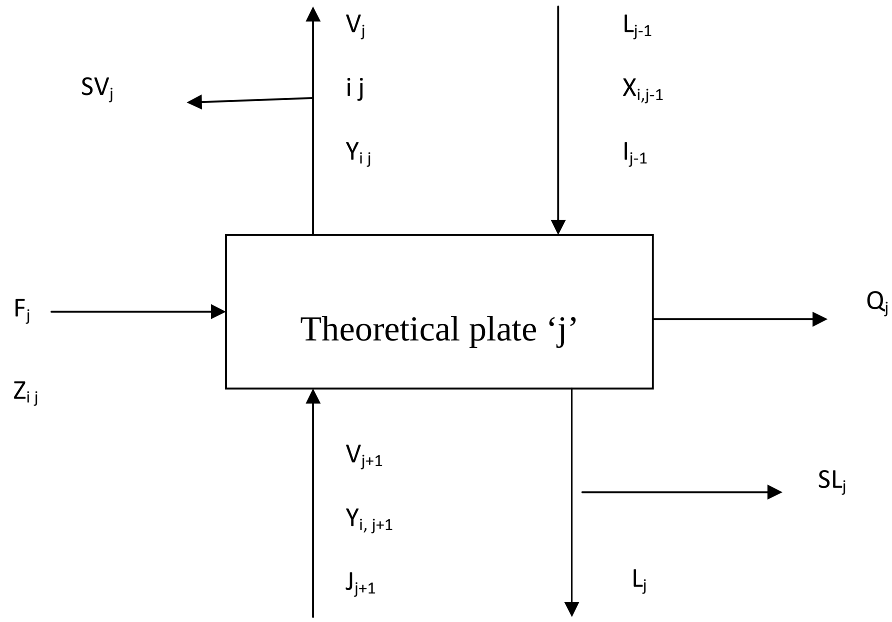

Fig. 26.2: Theoretical Plate of a Continuous Column

When the configuration of the column is fixed, the steady state mesh equations can be expressed as follows for a mixture involving C components:

- Mass balance equation(M) (j=1,N)

a) Overall mass balance:

$$L_{j-1} + V_{j+1} + F_j - L_j - SL_j - V_j - SV_j = 0 \quad \ldots 26.1$$

b) Partial mass balance(i=1,C)

$$L_{j-1} . X_{i,\, j-1} - (L_j + SL_j). X_{i\,j} - (V_j + SV_j). Y_{i\,j} + V_{j+1} . Y_{i,\, j+1} + F_j . Z_{i,\, j} = 0 \quad \ldots 26.2$$

- Equilibrium equations(E) (i=1,C; j=1,N)

$$Y_{i\,j} - K_{i\,j} . X_{i\,j} = 0 \quad \ldots 26.3$$

This equation is based on the assumption that each plate is a theoretical plate, that is to say that liquid vapour equilibrium exists on each plate between the two phases coming from it.

- Sum equations(S)

$$\sum_{i=1}^{C} (X_{i\,j} - Y_{i\,j}) = 0 \quad \ldots 26.4$$

- Enthalpy balance equations (H) (j=1, N)

$$L_{j-1} .H_{j-1} + V_{j+1} .H_{j+1}+F_j .H_{F j} – (L_j +SL_j) .H_j – (V_j +SV_j) .H_{v j} –Q_j =0 \quad \ldots 26.5$$

This enthalpy balance is based on the assumption of an ideal heat transfer, i.e. the vapour and liquid stream coming from each plate have the same temperature. In addition to these equations, and correlations are required to predict the equilibrium constants and the enthalpies. These correlations are often complex equations describing relations between thermodynamic properties and state variable.

Degree of freedom:

In order to define the problem, all the feed flows F_j feed composition $Z_{i\,j}$ (i=1, C), feed temperatures and pressure are fixed. All the liquid and vapour side stream flows SL_j , SV_j , as well as the amounts of heat supplied Q $(2 \leq j \leq N - 1)$ and the pressure P_j are also fixed.

In the case of a total condenser V_1 =0, the heat Q_N supplied to the reboiler is fixed and the reflux ratio, $R=L_1/SL_1$, is also fixed when the side stream flow rate is given. In the case of a partial condenser Q_N and the heat supplied to the condenser Q_1 are fixed. So the unknowns of the problem are liquid and vapour compositions $X_{i\,j}$, $Y_{i\,j}$, the temperature T_j on each plate, the liquid(L_1 to L_N) and vapour(V_1 to V_N) molar flow i.e t_o.

Source:
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