A Unified Vectorial Approach to Difference Point Methods in Stagewise Operations

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A fundamental unified approach from vectorial considerations is presented from which the usual rectangular and triangular difference point methods are derived as special cases. The approach is then extended to yield other difference point methods including some of higher order. Results are applicable to blending, distillation, extraction, foam fractionation, and other operations.

There are a number of difference point methods that are well known. These include that of Ponchon and Savarit (*6*) for distillation, Varteressian and Fenske for liquid extraction (*12*), and others (*4, 5, 7*). It will be the purpose of the present paper to show how the various difference point methods all have a common origin in terms of vector algebra. In addition some new difference point methods will be developed.

Consider first some properties of vectors.

Suppose

$$\overline{AP} = \frac{b}{a}\overline{PB} \qquad (1)$$

where a and b are scalar quantities. It can be readily shown (*2, 9*) that

$$(a + b)\,\overline{OP} = a\overline{OA} + b\overline{OB} \qquad (2)$$

Now, let

$$\overline{OM} = a\overline{OA} \qquad (3)$$

and let

$$\overline{ON} = b\overline{OB} \qquad (4)$$

Also define

$$\overline{OR} = \overline{OM} + \overline{ON} \qquad (5)$$

Then

$$\overline{OR} = a\overline{OA} + b\overline{OB} = (a + b)\overline{OP} \qquad (6)$$

RECTANGULAR DIAGRAMS

If $\overline{OM}$ and $\overline{ON}$ are vectors in a three-dimensional vector space, the orientation of the rectangular coordinate axes can be so chosen that line AB will fall in the cutting plane (projective plane) $X = 1$, as shown in Figure 1.

Representing the vectors in terms of their rectangular components one obtains

$$\overline{OM} = \bar{i}I_M + \bar{j}J_M + \bar{k}K_M \qquad (7)$$

$$\overline{ON} = \bar{i}I_N + \bar{j}J_N + \bar{k}K_N \qquad (8)$$

$$\overline{OR} = \bar{i}I_R + \bar{j}J_R + \bar{k}K_R \qquad (9)$$

so that by Equation (5)

$$\overline{OR} = \bar{i}(I_M + I_N) + \bar{j}(J_M + J_N) + \bar{k}(K_M + K_N) \qquad (10)$$

Then from Equations (3) and (7), and when one notes that pierce point A lies in the plane $X = 1$, it becomes evident that $I_M = a$. Similarly for point B in plane $X = 1$, from Equations (4) and (8) it is evident that $I_N = b$. Dividing one gets

$$I_M/I_N = a/b \qquad (11)$$

From Equation (7) the coordinates of pierce point A are $(1, J_M/I_M, K_M/I_M)$. Similarly from Equation (8) the coordinates of point B are $(1, J_N/I_N, K_N/I_N)$. From Equations (6) and (10) the coordinates for point P are $\left(1, \dfrac{J_M + J_N}{I_M + I_N}, \dfrac{K_M + K_N}{I_M + I_N}\right)$. Thus the vector addition in Equation (5) can be followed in the plane $X = 1$, on line AB, in terms of the pierce point coordinates utilizing Equation (11).

The various difference point methods all have a fundamental characteristic in common. They are based on the accountability (conservation) of certain quantities or components. For example in the Ponchon-Savarit method these components are the enthalpy H, the mass C of one material component, and the combined masses $C + D$ of both material components. When one combines streams, each of these three components is separately accountable. This of course is precisely the same situation as with vectors. Thus any stream can be represented as a vector $\bar{i}(C + D) + \bar{j}H + \bar{k}C$ or $\bar{i}(C + D) + \bar{j}C + \bar{k}H$. The addition (or subtraction) of these streams can then be followed in the plane $X = 1$ as before. Since for either representation $C + D$ is in the X direction, the physical significance of $\bar{i}$ is unit mass of the two material components. The above mentioned plane therefore becomes the enthalpy-concentration diagram itself, and Equation (11) becomes the usual lever law.

A stream which consists only of heat, which in turn is convertible to enthalpy, is represented simply by the vector $\bar{j}H$. This heat vector pierces the plane $X = 1$ at infinity.

The vectorial approach also suggests modifications of the usual Ponchon-Savarit method. Rewriting the stream vector as $\bar{i}C + \bar{j}H + \bar{k}(C + D)$ or $\bar{i}C + \bar{j}(C + D) + \bar{k}H$ changes the basis to unit mass of one material component and of course modifies the lever law accordingly. Rewriting instead as $\bar{i}H + \bar{j}C + \bar{k}(C + D)$ or as $\bar{i}H + \bar{j}(C + D) + \bar{k}C$ changes the basis to unit enthalpy, with each weight for the lever law being a total enthalpy rather than a mass. For certain problems these modifications may be more suitable than the conventional approach.

Of course for any of the above representations $C + D$ may be replaced by D alone to yield still other modifications. In fact all sorts of modifications are possible provided the basic requirement of accountability is fulfilled. It is also evident that the Maloney-Schubert (*5*) solvent content method for liquid extraction, and corresponding modifications, are all attainable by replacing H with solvent S. The graphical calculation of leaching (*7*) also follows from a suitable representation of stream vectors.

The relatively new operation of foam fractionation (*8*) is another case to which the present analysis can be extended. In this operation the two phases are effectively foam and foamate (liquid). The accountable components can be taken as solvent, surfactant, and gas. Via summation other choices of components are possible, such as solution, surfactant, and gas.

EXTENSION TO TRIANGULAR DIAGRAMS

The methods involving triangular diagrams can be arrived at by a somewhat different analysis combined with a different placement of the cutting plane.

For any vector define the scalar terms x, y, z, and W as follows:

$$W = I + J + K \qquad (12)$$

$$x = I/W \qquad (13)$$

$$y = J/W \qquad (14)$$

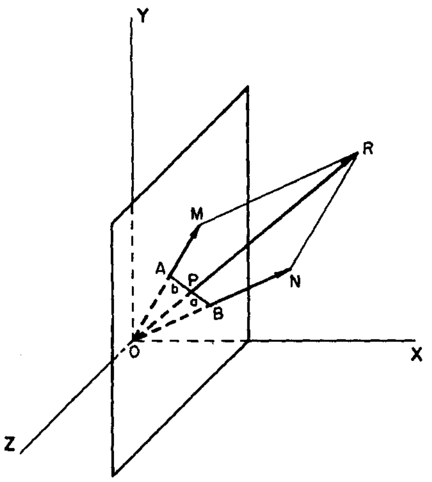

Fig. 1. Placement of cutting plane to yield rectangular coordinate methods.

$$z = K/W \qquad (15)$$

Combining with Equation (7) one gets

$$\overline{OM} = W_M \begin{Bmatrix} x_M \\ y_M \\ z_M \end{Bmatrix} \qquad (16)$$

Now, from Equations (12) through (15)

$$x_M + y_M + z_M = 1 \qquad (17)$$

In three-dimensional rectangular space Equation (17) represents the cutting plane shown in Figure 2. Therefore

$$\overline{OM} = W_M \overline{OA} \qquad (18)$$

where A is the pierce point of OM in the new cutting plane.
Similarly

$$\overline{ON} = W_N \begin{Bmatrix} x_N \\ y_N \\ z_N \end{Bmatrix} = W_N \overline{OB} \qquad (19)$$

where B is the pierce point. For the resultant $\overline{OR}$

$$\overline{OR} = W_R \begin{Bmatrix} x_R \\ y_R \\ z_R \end{Bmatrix} = \begin{bmatrix} W_M x_M + W_N x_N \\ W_M y_M + W_N y_N \\ W_M z_M + W_N z_N \end{bmatrix} = W_R \overline{OP} \qquad (20)$$

where P is the pierce point.

Comparison of Equations (18) and (3) shows that $W_M = a$. Similarly comparison of Equations (19) and (4) shows that $W_N = b$. Dividing one gets

$$W_M/W_N = a/b \qquad (21)$$

Similar comparison of Equations (20) and (6) also shows that $W_R = a + b = W_M + W_N$.

Figure 3 shows a view along a normal to the cutting plane. Triangular coordinates of point A are shown. From geometric considerations of Figures 2 and 3 it is evident that

$$q_M/x_M = s_M/y_M = t_M/z_M \qquad (22)$$

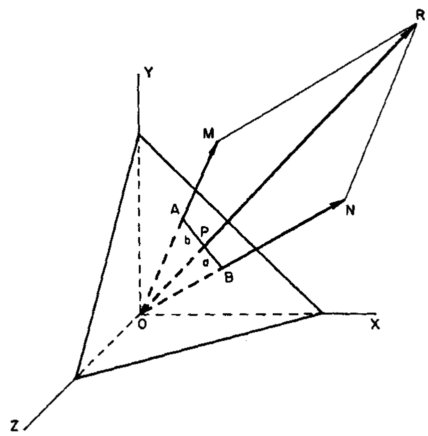

Fig. 2. Placement of cutting plane to yield triangular coordinate methods.

Corresponding expressions can be written for points B and P. Then the vector addition in Equation (5) can be followed in terms of the triangular coordinates of the pierce points in the inclined cutting plane by applying Equation (21) to line AB.

For a stream consisting of three material components, the masses of which are C, D, and S respectively, the stream vector can be written $\bar{i}C + \bar{j}D + \bar{k}S$ or in one of five other forms obtainable by simple permutation. For any of these permuted vector forms Equation (12) states that W numerically equals the mass of the stream. Similarly Equations (13), (14), and (15) state that x, y, and z are the mass fractions of the respective components in the stream. Thus, in accordance with Equation (22), the triangle of Figure 3 becomes the usual triangular composition diagram, and Equation (21) becomes the usual lever law for this diagram. Operations on the triangular diagram are of course the basis for the previously mentioned Varteressian-Fenske method for liquid extraction and Elgin's method (*4*) for leaching. Properly inclining the equilateral triangle of Figure 3 to the plane of view yields the usual right-triangle modification (*11*). Some related considerations are examined from the point of view of projective geometry by Spalding (*10*) whose results are obtainable by shifting the cutting plane of the present vectorial analysis to different positions.

As was the case with the vertical cutting plane, numerous variations are possible for the inclined plane. The stream vector can be written with components defined as sums or differences of the material components. Examples include $\bar{i}(C + D) + \bar{j}D + \bar{k}S$, $\bar{i}S + \bar{j}(C + D) + \bar{k}(C + D + S)$, $\bar{i}(S - C) + \bar{j}(S - D) + \bar{k}(C + D)$, and others, all of which satisfy the

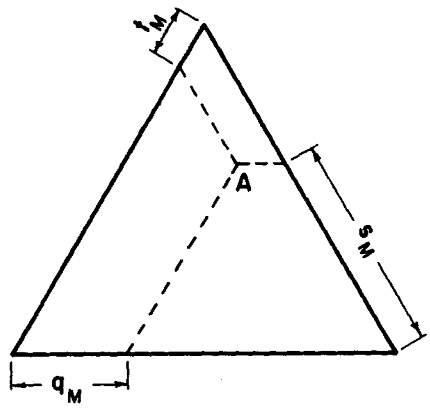

Fig. 3. Triangular coordinates.

basic requirement of accountability. Since H is also accountable, it may be taken as the third component in a system of two material components. This yields the less usual triangular method for solving distillation and other vapor-liquid problems.

In applying the triangular method to a system involving very low concentrations, the practical problem arises of distinguishing from zero on the chart. This problem can be met by appropriately diminishing the unit quantity defined as equal to the coordinate unit vector. This magnifies the corresponding vector component of the stream. To illustrate, in foam fractionation the concentration of surfactant and gas are naturally low. Accordingly, the three coordinate unit vectors might be chosen as 1-g. solvent, 0.1-g. surfactant, and 0.01-g. gas, respectively. The physical significance of x, y, z, and W would thus be changed accordingly. For example W would no longer equal the total number of grams of stream but would equal instead the number of grams of solvent, plus the number of decigrams of surfactant, plus the number of centigrams of gas.

HIGHER-ORDER SYSTEMS

By including additional dimensions the vectorial approach can be applied to higher order systems, that is streams of more than three accountable components. Thus for a four-component stream a four-dimensional vector is employed. Extending Equation (7) one obtains

$$\overline{OM} = \bar{i}I_M + \bar{j}J_M + \bar{k}K_M + \bar{v}V_M \qquad (23)$$

The cutting solid (projective solid) can then be chosen as $X = 1$. In rectangular four-dimensional space this physically represents a three-dimensional rectangular solid. The pierce point of $\overline{OM}$ then has the four-dimensional coordinates $(1, J_M/I_M, K_M/I_M, V_M/I_M)$. Addition and subtraction of four-dimensional vectors, and therefore of streams with four accountable components, can be followed in the three-dimensional cutting solid by applying the lever law to their pierce points.

As a more specific case consider a stream which consists of say the three-material components C, D, and E and the enthalpy H. Equation (23) might then be written as

$$\overline{OM} = \bar{i}(C + D + E) + \bar{j}H + \bar{k}C + \bar{v}D \quad (24)$$

Operating with the pierce points of vectors in this form amounts to extending the usual two-dimensional Ponchon-Savarit method to three-dimensional rectangular space. The three mutually perpendicular axes would physically correspond to the mass fraction of C, the mass fraction of D, and the specific enthalpy.

The vectorial approach also enables triangular coordinate methods to be extended to higher dimensions. For a four-component stream define

$$u = V/W \quad (25)$$

with W redefined as

$$W = I + J + K + V \quad (26)$$

Then when one combines with Equations (13), (14), and (15), the cutting solid for $\overline{OM}$ is represented by

$$x_M + y_M + z_M + u_M = 1 \quad (27)$$

Physically this is a tetrahedron bounded by the coordinate planes of three-dimensional rectangular space plus the plane

$$x_M + y_M + z_M = 1 \quad (28)$$

(Difference points of course can reach beyond these boundaries.) Expressions analogous to Equations (16) to (22) can then be derived, thus extending the use of triangular methods to space.

As a final illustration of extension to a higher dimension a combination triangular-rectangular method for a four-component system will be considered.

Combining Equation (23) with Equations (12) to (15) one obtains

$$\overline{OM} = W_M(\bar{i}x_M + \bar{j}y_M + \bar{k}z_M) + \bar{v}V_M \quad (29)$$

Equation (17) is now selected as the cutting solid. In four-dimensional space this is physically a three-dimensional equilateral triangular prism, although, as before, difference points can fall outside. By Equation (18)

$$\overline{OA} = \bar{i}x_M + \bar{j}y_M + \bar{k}z_M + \bar{v}(V_M/W_M) \quad (30)$$

Operations can now be followed in terms of A and other pierce points via the lever law. Letting x_M, y_M, and z_M be mass fractions, and setting $V_M = H_M$ so that the axial direction of the prism corresponds to specific enthalpy, one gets the method of Clare, et al. (3) for enthalpy-concentration calculations with streams containing three material components. For diagramatic representation the interested reader is referred to this reference wherein the specific system argon-oxygen-nitrogen-enthalpy is considered.

Further extension of the vectorial approach to five or more dimensions is difficult in practice. The pierce points would necessarily appear in four or higher dimensional cutting solids, which makes their physical representation awkward.

A more fruitful direction in which to extend the present analysis might be the application of vector calculus to processes involving continuous change. Matrix calculus has been suggested (1) for certain related problems.

APPLICATION TO PROBLEM SOLVING

The ease and convenience of representing process streams in terms of vectors, and then applying vector algebra to the addition and subtraction of streams entering and leaving their corresponding envelopes, can simplify certain complex problems. For example a Ponchon-Savarit calculation for a distillation column with several feed streams and side streams can be handled by judiciously drawing appropriate envelopes and writing corresponding vector equations for the streams involved. Then by transposing terms and combining equations as necessary difference points for the several sections of the column can be found. The entire calculation can thus be carried out simply and systematically.

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NOTATION

a = scalar, or line segment
A = point
b = scalar, or line segment
B = point
C = mass of a material component
D = mass of a material component
E = mass of a material component
H = enthalpy
$\bar{i}$ = unit vector in X direction
I = scalar for X direction
$\bar{j}$ = unit vector in Y direction
J = scalar for Y direction
$\bar{k}$ = unit vector in Z direction
K = scalar for Z direction
M = point
N = point
O = origin
P = point
q = triangular coordinate
R = point
S = mass of a material component, especially solvent
s = triangular coordinate
t = triangular coordinate
u = scalar fraction for the fourth-dimensional component
$\bar{v}$ = unit vector in the direction of the fourth dimension
V = scalar for the direction of the fourth dimension
W = sum of component scalars
x = scalar fraction for the X component
X = coordinate
y = scalar fraction for the Y component
Y = coordinate
z = scalar fraction for the Z component
Z = coordinate

Subscripts

M = vector $\overline{OM}$, or stream M
N = vector $\overline{ON}$, or stream N
R = vector $\overline{OR}$, or stream R

LITERATURE CITED

1. Acrivos, Andreas, and N. R. Amundson, *Ind. Eng. Chem.*, **47**, 1533 (1955).
2. Brand, Louis, "Vectorial Mechanics," p. 8. Wiley, New York (1930).
3. Clare, L. E. A., G. G. Haselden, and R. A. Nottle, *Trans. Inst. Chem. Engrs.*, **31**, 234 (1953).
4. Elgin, J. C., *Trans. Am. Inst. Chem. Engrs.*, **32**, 451 (1936).
5. Maloney, J. O., and A. E. Schubert, *ibid.*, **36**, 741 (1940).
6. McCabe, W. L., and J. C. Smith, "Unit Operations of Chemical Engineering," p. 708, McGraw-Hill, New York (1956).
7. *Ibid.*, p. 762.
8. Gaden, E. L., and V. Kevorkian, *Chem. Eng.*, **63**, No. 10, p. 173 (1956).
9. Sokolnikoff, I. S., and R. M. Redheffer, "Mathematics of Physics and Engineering," p. 289, McGraw-Hill, New York (1958).
10. Spalding, D. B., *Chem. Eng. Sci.*, **11**, No. 3, p. 183 (1959); No. 4, p. 225 (1960).
11. Treybal, R. E., "Mass Transfer Operations," p. 391, McGraw-Hill, New York (1955).
12. Varteressian, K. A., and M. R. Fenske, *Ind. Eng. Chem.*, **28**, 1353 (1936).

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