Chapter 04.00B

Physical Problem for Simultaneous Linear Equations
Chemical Engineering

Problem Statement: Liquid-liquid extraction depends on the ability of some metal ions to form metal complexes with organic acids. The method is used to separate, concentrate, and purify metals and organic compounds. Liquid-liquid extraction was the technique used to produce weapon grade uranium during the arms race (cold war) era. The technique is also used to recover noble metals used in catalytic processes such as oil refining etc.

In liquid-liquid extraction, the metal ion in the aqueous phase is recovered by mixing the aqueous phase with an organic phase. The metal ion forms a complex with the organic phase and floats on top of the aqueous phase. The organic phase can be decanted and separated from the aqueous phase and the complexed metal ion recovered in a useful form using an acid (nitric acid for nitrates, sulfuric acid for sulfates etc).

A liquid-liquid extraction process conducted in the Electrochemical Materials Laboratory involved the extraction of nickel from the aqueous phase into an organic phase. A typical experimental data from the laboratory is given in Table 1.

Table 1 Aqueous and organic phase concentration of nickel.

Ni aqueous phase (g/l)	2	2.5	3	3.5	4
Ni organic phase (g/l)	8.57	10	12	14	15.66

Estimate the amount of nickel in organic phase when 2.3 g/l is in the aqueous phase. Use quadratic interpolation.

Solution

The polynomial is going through three data points (a_1, g_1), (a_2, g_2), and (a_3, g_3) where from the above table

$$a_1 = 2, g_1 = 8.57$$
$$a_2 = 2.5, g_2 = 10$$
$$a_3 = 3, g_3 = 12$$

Requiring that $g = x_1 a^2 + x_2 a + x_3$ passes through the three data points gives

$$g(a_1) = g_1 = x_1 a_1^2 + x_2 a_1 + x_3$$

$$g(a_2) = g_2 = x_1 a_2^2 + x_2 a_2 + x_3$$
$$g(a_3) = g_3 = x_1 a_3^2 + x_2 a_3 + x_3$$

Substituting the data $(a_1, g_1), (a_2, g_2), (a_3, g_3)$

$$x_1(2)^2 + x_2(2) + x_3 = 8.57$$
$$x_1(2.5)^2 + x_2(2.5) + x_3 = 10$$
$$x_1(3)^2 + x_2(3) + x_3 = 12$$

gives

$$4x_1 + 2x_2 + x_3 = 8.57$$
$$6.25x_1 + 2.5x_2 + x_3 = 10$$
$$9x_1 + 3x_2 + x_3 = 12$$

This set of equations can be rewritten in the matrix form as

$$\begin{bmatrix} 4x_1 + & 2x_2 + & x_3 \\ 6.25x_1 + & 2.5x_2 + & x_3 \\ 9x_1 + & 3x_2 + & x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ 10 \\ 12 \end{bmatrix}$$

The above equations can be written as a linear combination as follows

$$x_1 \begin{bmatrix} 4 \\ 6.25 \\ 9 \end{bmatrix} + x_2 \begin{bmatrix} 2 \\ 2.5 \\ 3 \end{bmatrix} + x_3 \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 8.57 \\ 10 \\ 12 \end{bmatrix}$$

and further using matrix multiplication gives

$$\begin{bmatrix} 4 & 2 & 1 \\ 6.25 & 25 & 1 \\ 9 & 3 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 8.57 \\ 10 \\ 12 \end{bmatrix}$$

The solution of the above simultaneous linear equations will give the value of x_1, x_2, x_3.

QUESTIONS:

1. Verify if you get back the value of the Ni organic phase when the Ni aqueous phase is 2.5 g/l.
2. Estimate the value of the Ni organic phase when the Ni aqueous phase is 2.78 g/l
3. Estimate the error between linear interpolation and quadratic interpolation values obtained for nickel in organic phase when 2.78 g/l is in the aqueous phase.

SIMULTANEOUS LINEAR EQUATIONS	
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