

Example 1

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 set of experimental data from the laboratory is given below.

Ni aqueous phase, a (g/l)	2	2.5	3
Ni organic phase, g (g/l)	8.57	10	12

Assuming g is the amount of Ni in the organic phase and a is the amount of Ni in the aqueous phase, the quadratic interpolant that estimates g is given by

$$g = x_1 a^2 + x_2 a + x_3, \quad 2 \leq a \leq 3$$

The solution for the unknowns x_1 , x_2 , and x_3 is given by

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

Find the values of x_1 , x_2 , and x_3 using the Gauss-Seidel method. Estimate the amount of nickel in the organic phase when 2.3 g/l is in the aqueous phase using quadratic interpolation. Use

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

as the initial guess and conduct two iterations.

Solution:-

Rewriting the equations gives

$$\begin{aligned} x_1 &= \frac{8.57 - 2x_2 - x_3}{4} \\ x_2 &= \frac{10 - 6.25x_1 - x_3}{2.5} \\ x_3 &= \frac{12 - 9x_1 - 3x_2}{1} \end{aligned}$$

Iteration #1

Given the initial guess of the solution vector as

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Philippe G. Ciarlet, Jacques-Louis Lions



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containing extra information can be found via www.springer.com

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Problem Solving in Chemical Engineering with Numerical Methods Michael B. Cutlip, Mordechai Shacham, 1999 A companion book including interactive software for students and professional engineers who want to utilize problem solving software to effectively and efficiently obtain solutions to realistic and complex problems An Invaluable reference book that discusses and Illustrates practical numerical problem solving in the core subject areas of Chemical Engineering Problem Solving in Chemical Engineering with Numerical Methods provides an extensive selection of problems that require numerical solutions from throughout the core subject areas of chemical engineering Many are completely solved or partially solved using POLYMATH as the representative mathematical problem solving software Ten representative problems are also solved by Excel Maple Mathcad MATLAB and Mathematica All problems are clearly organized and all necessary data are provided Key equations are presented or derived Practical aspects of efficient and effective numerical problem solving are emphasized Many complete solutions are provided within the text and on the CD ROM for use in problem solving exercises BOOK JACKET Title Summary field provided by Blackwell North America Inc All Rights Reserved

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Introduction to Numerical Analysis Francis Begnaud Hildebrand, 1987-01-01 The ultimate aim of the field of numerical analysis is to provide convenient methods for obtaining useful solutions to mathematical problems and for extracting useful information from available solutions which are not expressed in tractable forms This well known highly respected volume provides an introduction to the fundamental processes

of numerical analysis including substantial grounding in the basic operations of computation approximation interpolation numerical differentiation and integration and the numerical solution of equations as well as in applications to such processes as the smoothing of data the numerical summation of series and the numerical solution of ordinary differential equations Chapter headings include 1 Introduction 2 Interpolation with Divided Differences 3 Lagrangian Methods 4 Finite Difference Interpolation 5 Operations with Finite Differences 6 Numerical Solution of Differential Equations 7 Least Squares Polynomial Approximation In this revised and updated second edition Professor Hildebrand Emeritus Mathematics MIT made a special effort to include more recent significant developments in the field increasing the focus on concepts and procedures associated with computers This new material includes discussions of machine errors and recursive calculation increased emphasis on the midpoint rule and the consideration of Romberg integration and the classical Filon integration a modified treatment of prediction correction methods and the addition of Hamming s method and numerous other important topics In addition reference lists have been expanded and updated and more than 150 new problems have been added Widely considered the classic book in the field Hildebrand s Introduction to Numerical Analysis is aimed at advanced undergraduate and graduate students or the general reader in search of a strong clear introduction to the theory and analysis of numbers

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