

DOCUMENT RESUME

ED 218 083

SE 037 854

AUTHOR Grimaldi, Ralph P.
 TITLE Balancing Chemical Reactions With Matrix Methods and Computer Assistance. Applications of Linear Algebra to Chemistry. Modules and Monographs in Undergraduate Mathematics and Its Applications Project. UMAP Unit 339.
 INSTITUTION Education Development Center, Inc., Newton, Mass.
 SPONS AGENCY National Science Foundation, Washington, D.C.
 PUB. DATE 80
 GRANT SED-76-19615-A02
 NOTE 26p.

EDRS PRICE MF01 Plus Postage. PC Not Available from EDRS.
 DESCRIPTORS Answer Keys; *Chemistry; *College Mathematics; *College Science; Computer Programs; Educational Technology; Higher Education; Instructional Materials; *Learning Modules; *Mathematical Applications; *Matrices; Problem Solving; Supplementary Reading Materials; Textbooks
 IDENTIFIERS *Linear Algebra

ABSTRACT This material was developed to provide an application of matrix mathematics in chemistry, and to show the concepts of linear independence and dependence in vector spaces of dimensions greater than three in a concrete setting. The techniques presented are not intended to be considered as replacements for such chemical methods as oxidation-reduction or the balancing of half-reactions. It is noted that it is possible to write down a chemical reaction that does not take place and still balance it by the matrix methods provided. Exercises and references are included to the problems supplied. (MP)

 * Reproductions supplied by EDRS are the best that can be made *
 * from the original document. *

ED218083

umap

UNIT 339

MODULES AND MONOGRAPHS IN UNDERGRADUATE MATHEMATICS AND ITS APPLICATIONS PROJECT

U.S. DEPARTMENT OF EDUCATION NATIONAL INSTITUTE OF EDUCATION EDUCATIONAL RESOURCES INFORMATION CENTER (ERIC)

This document has been reproduced as received from the person or organization originating it

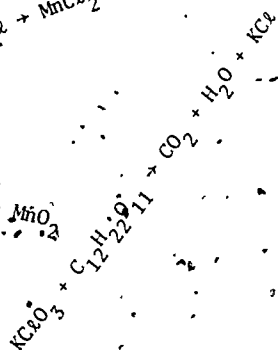
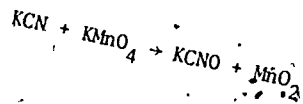
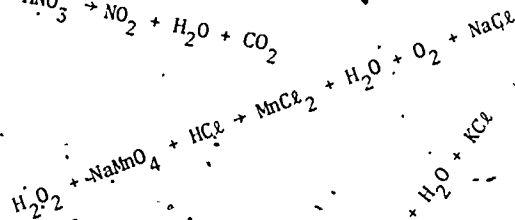
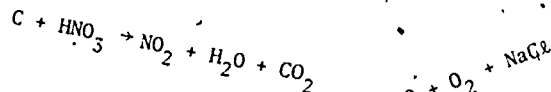
Minor changes have been made to improve reproduction quality

Points of view or opinions stated in this document do not necessarily represent official NIE position or policy

BALANCING CHEMICAL REACTIONS

WITH MATRIX METHODS AND COMPUTER ASSISTANCE

by Ralph P. Grimaldi



APPLICATIONS OF LINEAR ALGEBRA TO CHEMISTRY

edc/umap/55chapel st./newton.mass.02160

BALANCING CHEMICAL REACTIONS WITH MATRIX METHODS AND COMPUTER ASSISTANCE

by

Ralph P. Grimaldi Department of Mathematics Rose-Hulman Institute of Technology Terre Haute, IN 47803

TABLE OF CONTENTS

1. INTRODUCTION 1
2. BACKGROUND: MATHEMATICAL AND CHEMICAL 1
2.1 Vectors in Two and Three Dimensions 1
2.2 A Word About Chemical Elements 2
3. SOLVING LINEAR SYSTEMS: THE INVERSE MATRIX METHOD 3
4. BALANCING CHEMICAL REACTIONS 4
4.1 The Computer Supplies a Readily Recognizable Answer 4
4.2 The Computer Supplies an Answer Which Is Not Easily Recognized 9
4.3 Have We Only Dealt With Very Special Cases? 13
4.4 The Non-Unique Case 14
5. SUMMARY 17
6. EXERCISES 17
7. REFERENCES 18
8. ANSWERS TO EXERCISES 19

PERMISSION TO REPRODUCE THIS MATERIAL IN MICROFICHE ONLY HAS BEEN GRANTED BY

National Science Foundation

TO THE EDUCATIONAL RESOURCES INFORMATION CENTER (ERIC)



Intermodular Description Sheet: UMAP Unit 339

Title: BALANCING CHEMICAL REACTIONS WITH MATRIX METHODS AND COMPUTER ASSISTANCE

Author: Ralph P. Grimaldi
Department of Mathematics
Rose-Hulman Institute of Technology
Terre Haute, IN 47803

Review Stage/Date: III 4/14/86

Classification: APPL LIN ALG/CHEM

Prerequisite Skills:

1. Elementary matrix operations including the inverting of square matrices.
2. Some introductory chemistry on nomenclature and balancing chemistry equations.
3. Some knowledge of BASIC or BASIC PLUS would make comprehension of the module complete but is not totally necessary and depends on the individual instructor's intentions for the module's use.

Output Skills:

1. To reinforce the abstract concept of linear independence by appealing to a concrete setting where the dimension exceeds 3.
2. To apply the inverse matrix method for solving linear systems to situations arising from chemical reactions.

MODULES AND MONOGRAPHS IN UNDERGRADUATE
MATHEMATICS AND ITS APPLICATIONS PROJECT (UMAP)

The goal of UMAP is to develop, through a community of users and developers, a system of instructional modules in undergraduate mathematics and its applications which may be used to supplement existing courses and from which complete courses may eventually be built.

The Project is guided by a National Steering Committee of mathematicians, scientists, and educators. UMAP is funded by a grant from the National Science Foundation to Education Development Center, Inc., a publicly supported, nonprofit corporation engaged in educational research in the U.S. and abroad.

PROJECT STAFF

Ross L. Finney	Director
Solomon Garfunkel	Consortium Director
Felicia DeMay	Associate Director
Barbara elczewski	Coordinator for Materials Production
Paula M. Santillo	Assistant to the Directors
Donna DiDua	Project Secretary
Janet Webber	Word Processor
Zachary Zeyitas	Staff Assistant

NATIONAL STEERING COMMITTEE

W. T. Martin (Chair)	M. I. T.
Steven J. Brams	New York University
Llayron Clarkson	Texas Southern University
Ernest J. Henley	University of Houston
William Hogan	Harvard University
Donald A. Larson	SUNY at Buffalo
William F. Lucas	Cornell University
R. Duncan Luce	Harvard University
George M. Miller	Nassau Community College
Frederick Mosteller	Harvard University
Walter E. Sears	University of Michigan Press
George Springer	Indiana University
Arnold A. Strassenburg	SUNY at Stony Brook
Alfred B. Willcox	Mathematical Association of America

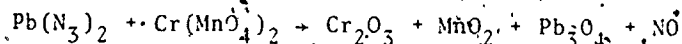
The Project would like to thank Andrew D. Jorgensen of Indiana State University, Evansville; Richard J. Allen of St. Olaf College, Northfield, Minnesota, and; Philip H. Anderson of Montclair State College, Upper Montclair, New Jersey, for their reviews, and all others who assisted in the production of this unit.

This material was prepared with the partial support of National Science Foundation Grant No. SED76-19615 A02. Recommendations expressed are those of the author and do not necessarily reflect the views of the NSF or the copyright holder.

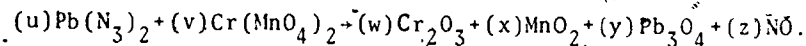
1. INTRODUCTION

This module was developed to provide an application of matrix mathematics in chemistry, and to show the concepts of linear independence and dependence in vector spaces of dimension greater than 3 in a concrete setting.

In balancing a chemical reaction such as



we seek positive integers u, v, w, x, y, z , which have no common divisor other than 1, so that



We say that the equation or reaction is *balanced* when the number of atoms of each chemical element involved is the same on each side of the reaction. For example, here, for the element Pb (lead), there are u atoms on the left side (the *reactant side*) of the reaction, and $3y$ atoms of Pb on the right side (the *product side*). The 3 in the term $3y$ comes from the fact that there are 3 atoms of Pb in each Pb_3O_4 molecule. For the reaction to be balanced we must have $u = 3y$. In the same way, we count the respective number of atoms on both sides of the reaction for the other chemical elements N, Cr, Mn, and O, and obtain a linear system of equations. The setting up of this system and its solution by matrix methods will be examined in detail in Section 4.1.

2. BACKGROUND: MATHEMATICAL AND CHEMICAL

2.1 Vectors in Two and Three Dimensions

Consider the operations of vector addition and scalar multiplication in the Euclidean plane, R^2 , where $(x, y) + (x', y') = (x + x', y + y')$ and $r(x, y) = (rx, ry)$ for any $(x, y), (x', y') \in R^2$, $r \in R$. Starting with the

vector $\vec{i} = (1, 0)$, and using only these operations, we can "build" or "construct" any vector in R^2 of the form $(r, 0)$, $r \in R$. However, to generate every vector (x, y) in R^2 we need an additional vector such as $\vec{j} = (0, 1)$, which is not a scalar multiple of \vec{i} . We cannot construct any vector with nonzero second component by applying our given operations only to $\vec{i} = (1, 0)$. For instance, it is impossible to express the vector $\vec{j} = (0, 1)$ as a sum of scalar multiples of $\vec{i} = (1, 0)$.

In like manner, starting with the vectors $\vec{i} = (1, 0, 0)$ and $\vec{j} = (0, 1, 0)$ in Euclidean space, R^3 , and using the standard operations of vector addition and scalar multiplication in R^3 , as we did in R^2 , we can form any vector in the xy -plane, that is, all vectors whose third component is 0. However, once again, to be able to construct every vector (x, y, z) of R^3 we need an additional vector whose third component is not zero. With $\vec{k} = (0, 0, 1)$, and \vec{i} and \vec{j} as above, we can form any vector in Euclidean space using vector addition and scalar multiplication. We could not have done this with just \vec{i} and \vec{j} , for it is impossible to "decompose" the vector \vec{k} into a linear combination, $r_1\vec{i} + r_2\vec{j}$, of the vectors \vec{i} and \vec{j} , with r_1 and $r_2 \in R$. We might also say that the vector \vec{k} is not dependent upon \vec{i} and \vec{j} or that the vectors \vec{i}, \vec{j} and \vec{k} are linearly independent.

2.2 A Word About Chemical Elements

In this section we shall see that the word "decompose" which appears in the last paragraph of Section 2.1 was specifically chosen for its suggestive value.

In the science of chemistry the term *pure substance* is used to describe any variety of matter which has a recognizably definite composition and possesses specific properties. The chemical reaction of *decomposition* is one in which such a pure substance breaks down to yield simpler forms of matter. Many of the substances known to

scientists do this, and release or absorb as much energy as 30,000 calories per gram in the process. (Processes that involve changes in the nucleus of a chemical element may result in even higher energy changes: This kind of reaction is termed *nuclear* rather than chemical.) Among all such pure substances, those that do not break-down at all within the energy range mentioned, or that give only one final product, as in the decomposition of ozone into oxygen, are called the *elements*. As of 1970 there were 105 known elements. (Element 105, Hahnium, chemically denoted Ha, was discovered in that year by the team of Ghiorso, Nurmia, Harris, K.A.Y. Eskola, and P.L. Eskola.) Elements are considered to be the chemical building blocks for forming all other substances; the smallest chemical unit of any such element being called an *atom*.

3. SOLVING LINEAR SYSTEMS: THE INVERSE MATRIX METHOD

One of the main topics covered in a first course in matrix algebra is the solution of a system of linear equations by way of techniques such as elementary row operations, Cramer's rule or the inverse matrix method. We shall find the inverse matrix method most suitable for our applications in Section 4.

The method can be described as follows: given a system of linear equations such as

$$a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1;$$

$$a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2;$$

$$a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3;$$

we can write this system in matrix form as

$$AX = B, \text{ where } A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, X = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

In elementary algebra, if a and b are real numbers, and $a \neq 0$, then the solution of the equation

$$ax = b$$

is

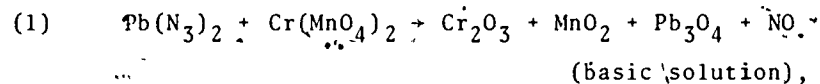
$$x = a^{-1}b.$$

We would like to expand this idea to the matrix equation $AX = B$, where A, B are matrices of real numbers, and be able to conclude that the solution is $X = A^{-1}B$. Here, however, we need more than just $A \neq 0$. We need $\det A \neq 0$, where $\det A$ is the determinant of the matrix A . One finds this to happen when the linear system is *independent*, that is, when none of the equations in the system can be obtained by combining multiples of some of the other equations.

4. BALANCING CHEMICAL REACTIONS

4.1 The Computer Supplies a Readily Recognizable Answer

Our first problem reads as follows: The reaction of lead (II) azide and chromium (II) permanganate in producing chromium (III) oxide, manganese (IV) dioxide, trilead tetroxide, and nitric oxide is given by the chemical equation



a reaction involving 3 oxidations and 1 reduction.

Before we tackle the problem of trying to balance this equation, let us reconsider the idea of linear independence of vectors in a chemical setting. Just as we could not create the vector $\vec{k} = (0,0,1)$ from the vectors $\vec{i} = (1,0,0)$, $\vec{j} = (0,1,0)$ in Section 2.1, in dealing with the above chemical equation, we know for instance, that we cannot create Pb from N and O or any other combination of elements from among N, O, Cr, Mn. This is inherent in the very nature of a chemical element, and we may thus view the elements involved in the chemical reaction as independent vectors in R^5 . We shall make the following atom assignments in solving the problem:

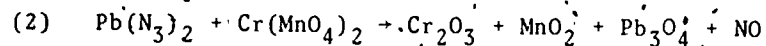
$$\text{Pb} = (1,0,0,0,0), \quad \text{Mn} = (0,0,0,1,0),$$

$$\text{N} = (0,1,0,0,0), \quad \text{O} = (0,0,0,0,1).$$

$$\text{Cr} = (0,0,1,0,0),$$

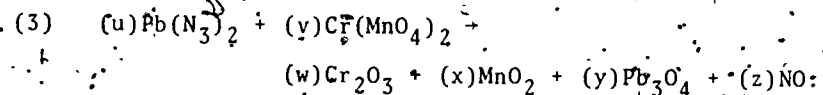
The basis for this idea can be found on pp. 26-27 of [2].

To balance the equation,



(basic solution),

we must find integers u, v, w, x, y, z , with no common integer divisors other than ± 1 , so that



Using the vector assignments above, we replace the chemical equation (3) by the vector equation

$$(4) \quad u(1,6,0,0,0) + v(0,0,1,2,8) = w(0,0,2,0,3) +$$

$$x(0,0,0,1,2) + y(3,0,0,0,4) + z(0,1,0,0,1),$$

where, for example, $(1,6,0,0,0)$ represents the lead (II) azide molecule, $\text{Pb}(\text{N}_3)_2$, since it is made up of 1 atom of Pb and 6 atoms of N, and using vector addition and scalar multiplication $(1,6,0,0,0) = 1(1,0,0,0,0) + 6(0,1,0,0,0)$.

Since vectors are equal only when all corresponding components are equal, by equating the first through fifth components in equation (4) we get the following system of 5 equations in 6 unknowns,

$$(5) \quad \begin{aligned} u + 0v &= 0w + 0x + 3y + 0z \\ 6u + 0v &= 0w + 0x + 0y + z \\ 0u + v &= 2w + 0x + 0y + 0z \\ 0u + 2v &= 0w + x + 0y + 0z \\ 0u + 8v &= 3w + 2x + 4y + z \end{aligned}$$

or,

$$(6) \quad \begin{aligned} 0v + 0w + 0x + 3y + 0z &= u \\ 0v + 0w + 0x + 0y + z &= 6u \\ -v + 2w + 0x + 0y + 0z &= 0u \\ -2v + 0w + x + 0y + 0z &= 0u \\ -8v + 3w + 2x + 4y + z &= 0u \end{aligned}$$

There are infinitely many solutions of this system. But from a chemical viewpoint this is in keeping with our experience, for if we have one solution that balances the chemical equation (3), any positive integer multiple of it yields another solution. Also, before proceeding, it should be pointed out that the techniques developed here work for our chemical reactions because they are electrically balanced.

Since we are not interested in the general solution, let us find the unique solution corresponding to $u = 1$. In matrix notation this will take the following form

$$(7) \quad \begin{bmatrix} 0 & 0 & 0 & 3 & 0 \\ -0 & 0 & 0 & 0 & 1 \\ -1 & 2 & 0 & 0 & 0 \\ -2 & 0 & 1 & 0 & 0 \\ -8 & 3 & 2 & 4 & 1 \end{bmatrix} \begin{bmatrix} v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 \\ 6 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

so that

$$(8) \begin{bmatrix} v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ -1 & 2 & 0 & 0 & 0 \\ -2 & 0 & 1 & 0 & 0 \\ -8 & 3 & 2 & 4 & 1 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 6 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The solution is immediate once we get the inverse of the given 5×5 matrix. Now although one can find an inverse for a square matrix A , where $\det A \neq 0$, by such methods as elementary row operations as found in Chapter 1 of [1], or by use of the adjoint as described in Chapter 2 of [1]; it is at this point that we shall use some computer assistance via the following BASIC-PLUS program:

```
10 REM THIS PROGRAM IS USED IN BALANCING CHEMICAL EQUATIONS
20 DIM A(5,5),B(5,1),I(5,5),S(5,1)
30 MAT READ A,B
40 MAT I = INV(A)
50 MAT S = I*B
60 DATA 0,0,0,3,0
70 DATA 0,0,0,0,1
80 DATA -1,2,0,0,0
90 DATA -2,0,1,0,0
100 DATA -8,3,2,4,1
110 DATA 1,6,0,0,0
120 PRINT "V=";S(1,1),"W=";S(2,1),"X=";S(3,1),"Y=";S(4,1),
    "Z=";S(5,1)
130 STOP
140 INPUT "K = "; K
150 DIM T(5,1)
160 MAT T = (K)*S
170 PRINT "U=";K,"V=";T(1,1),"W=";T(2,1),"X=";T(3,1),
    "Y=";T(4,1)
180 PRINT "Z=";T(5,1)
190 END
```

Ready

```
RUNNH
V= 2.93333 W= 1.46667 X= 5.86667 Y= .333333 Z= 6
Stop at line 130
```

Ready

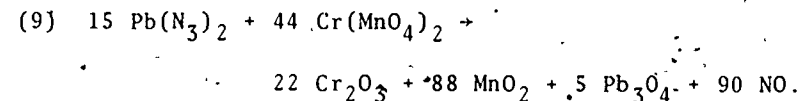
This program uses matrix operations that are available in BASIC or BASIC-PLUS. An excellent explanation of these computer matrix operations can be found in Chapter 10 of [4]. (The program here and all others found in this module were run at the Rose-Hulman Institute of Technology on a DEC PDP-11/70 using the RSTS version 7 operating system.)

At this point we must be prepared to recognize 0.03333 as $1/30$ and 0.06667 as $2/30$. So to express the answers in integer form we shall perform the scalar multiplication at line 160 by inputting the value of K at line 140 as 30, the least common denominator for all fractions involved. Upon typing CONT we get the following output.

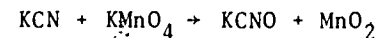
```
CONT
K = ? 30
U= 30 V= 88 W= 44 X= 176 Y= 10
Z= 180
```

Ready

Dividing each coefficient by 2 we find the equation balanced as follows:



In some balancing problems, it is possible to reduce the number of independent vectors involved if we can find a radical that does not break down in the reaction. The CN in the reaction



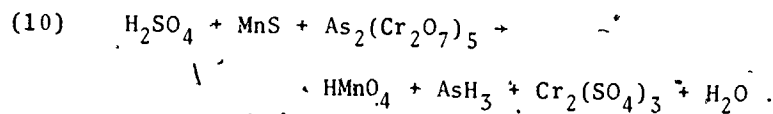
is a case in point. Instead of assigning a 5-dimensional vector to each of K, C, N, Mn, and O to balance this equation, we may assign a 4-dimensional vector to each of K, CN, Mn, and O. This simplifies the problem.

4.2 The Computer Supplies an Answer Which Is Not Easily Recognized

If we compare the 5×5 coefficient matrix in Equation (7) with the equations in (6), we see that the columns of the matrix are the vector representations of the molecules other than the first reactant. The minus signs occur in the columns for the other reactants. The product molecules have all positive components in their respective columns. The 5×1 column matrix of constants in (7) results from the vector representation of the first reactant, $\text{Pb}(\text{N}_3)_2$.

We shall now consider a second problem which will give us an opportunity to extend our use of matrix operations in BASIC-PLUS to the MAT INPUT statement and will employ the transpose of a matrix. This particular problem will provide us with techniques to consider when the output does not yield decimals whose equivalent fractions are as obvious as in the first problem we considered. In addition, the program below is more general and can be used in balancing other electrically balanced chemical equations.

Here we shall consider the chemical reaction



(This involves 2 oxidations and 2 reductions.)

We assign the following vectors to the atoms:

$$\text{H} = (1, 0, 0, 0, 0, 0), \quad \text{Mn} = (0, 0, 0, 1, 0, 0),$$

$$\text{S} = (0, 1, 0, 0, 0, 0), \quad \text{As} = (0, 0, 0, 0, 1, 0),$$

$$\text{O} = (0, 0, 1, 0, 0, 0), \quad \text{Cr} = (0, 0, 0, 0, 0, 1).$$

To balance the chemical reaction (10) we need to find integers t, u, v, w, x, y, z , as in Section 4.1, so that

$$(11) \quad t(2, 1, 4, 0, 0, 0) + u(0, 1, 0, 1, 0, 0) + v(0, 0, 35, 0, 2, 10) = \\ w(1, 0, 4, 1, 0, 0) + x(3, 0, 0, 0, 1, 0) + \\ y(0, 3, 12, 0, 0, 2) + z(2, 0, 1, 0, 0, 0)$$

Letting $t = 1$, we can write the vector equation (11) in the equivalent matrix form $AX = B$:

$$(12) \quad \begin{bmatrix} 0 & 0 & 1 & 3 & 0 & 2 \\ -1 & 0 & 0 & 0 & 3 & 0 \\ 0 & -35 & 4 & 0 & 12 & 1 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -2 & 0 & 1 & 0 & 0 \\ 0 & -10 & 0 & 0 & 2 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ 4 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Accordingly, the solution for the vector equation when $t = 1$ is given by

$$(13) \quad \begin{bmatrix} u \\ v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 3 & 0 & 2 \\ -1 & 0 & 0 & 0 & 3 & 0 \\ 0 & -35 & 4 & 0 & 12 & 1 \\ -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & -2 & 0 & 1 & 0 & 0 \\ 0 & -10 & 0 & 0 & 2 & 0 \end{bmatrix}^{-1} \begin{bmatrix} 2 \\ 1 \\ 4 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

Once again we shall turn to the computer for assistance in solving the matrix equation. Here, however, our program is somewhat different from that used in Section 4.1. It involves the transpose of a matrix, that is, the matrix that results from a given matrix by interchanging its rows and columns. (For more on the transpose of a matrix see pp. 67-68 of [1].)


```

10 REM THIS PROGRAM IS USED IN BALANCING CHEMICAL REACTIONS
20 REM N IS THE NUMBER OF DISTINCT ATOMS OR RADICALS INVOLVED
30 DIM A(20,20), B(20,1), I(20,20), J(20,20), S(20,1)
40 INPUT "N="; N
50 MAT INPUT A(N,N)
60 MAT INPUT B(N,1)
70 MAT I = TRN(A)
80 MAT J = INV(I)
90 MAT S = J*B
100 MAT PRINT S
110 END

```

Ready

At line 50 of this program we input the columns of the 6×6 matrix A of Equation (12). We start with $(0, -1, 0, -1, 0, 0)$, the negative of the vector representation of the second reactant MnS , and continue until we finish with the vector $(2, 0, 1, 0, 0, 0)$ for the last product H_2O . At line 60 we input the vector representation, $(2, 1, 4, 0, 0, 0)$, of the reactant H_2SO_4 . (The input is provided at the keyboard like the usual INPUT statement. A question mark appears when the computer is ready to receive the data. Upon typing in the value of N and hitting the RETURN key, the line feed key can be used if we wish to type the vector representations on successive lines, as shown in the rows following the inputting of the value of N. We then hit RETURN after typing in the last row vector.)

Lines 30, 40, 50, 60 constitute a redimensioning of the original matrices A and B. This allows the program to be flexible in its application to any electrically balanced equation that involves 20 or fewer atoms or radicals.

Upon typing RUNNH and inputting the value of N and the vector components for the reactants and products, the program yields the following results:

```

RUNNH
N =? 6
? 0,-1,0,-1,0,0
? 0,0,-35,0,-2,-10
? 1,0,4,1,0,0
? 3,0,0,0,1,0
? 0,3,12,0,0,2
? 2,0,1,0,0,0
? 2,1,4,0,0,0
.308725
.872483E-1
.308725
.174497
.436242
.583893

```

Ready

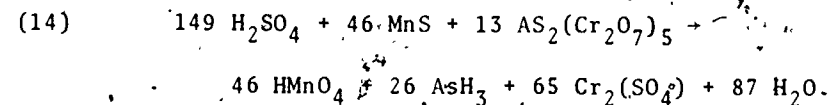
From the printout here we see that for $t = 1$, we obtain $u = .308725$, $v = .0872483$, $w = .308725$, $x = .174497$, $y = .436242$, $z = .583893$, which unfortunately are not readily recognizable as any specific "easy" fractions. However, if we divide each variable by the smallest value, namely $.0872483$ (since in chemical reactions we are primarily concerned with the ratios of compounds), we get a second solution where

$$\begin{aligned}
 t &= 11.46154, & x &= 2.00000, \\
 u = w &= 3.53846, & y &= 5.00000, \\
 v &= 1, & z &= 6.69231,
 \end{aligned}$$

to five decimal places.

Now considering all the fractional parts, we find that $0.53846 - 0.46154 = 0.07692$ is the smallest difference and that $(0.07692)^{-1} = 13.00052$, so $0.07692 \approx 1/13$. Then $0.46154 \approx 6/13$, and $0.69231 \approx 9/13$.

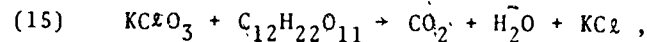
So multiplying our solution through by 13, we find the reaction balanced as follows:



4.3 Have We Only Dealt With Very Special Cases?

You may have noticed in reading Sections 4.1 and 4.2 that, to set up the matrix equations used there, both chemical reactions discussed were of the type where the total number of reactants and products exceeded the number of atoms and radicals involved by exactly 1. The number of radicals and atoms controls the number of linear equations involved, while the number m of reactants and products controls the number of unknowns. One need not look very far to find a chemical reaction where $n \neq m + 1$. In this section we shall deal with the case where $n = m$.

To balance the chemical reaction,



we make the following vector assignments for atoms and radicals:

$$\text{K} = (1, 0, 0, 0, 0), \quad \text{C} = (0, 0, 0, 1, 0),$$

$$\text{Cl} = (0, 1, 0, 0, 0), \quad \text{H} = (0, 0, 0, 0, 1).$$

$$\text{O} = (0, 0, 1, 0, 0),$$

We rewrite the chemical reaction as a vector equation and seek positive integers u, v, w, x, y with no common integer factor greater than 1 so that

$$(16) \quad u(1, 1, 3, 0, 0) + v(0, 0, 11, 12, 22) = w(0, 0, 2, 1, 0) + x(0, 0, 1, 0, 2) + y(1, 1, 0, 0, 0).$$

Setting $u = 1$ we would like to use the program of Section 4.2, but we do not have the necessary number, 6, of reactants and products. However, if we examine the actual linear system of equations,

$$(17) \quad \begin{aligned} 1 &= 0v + 0w + 0x + y, \\ 1 &= 0v + 0w + 0x + y, \\ 3 &= -11v + 2w + x + 0y, \\ 0 &= -12v + w + 0x + 0y, \\ 0 &= -22v + 0w + 2x + 0y. \end{aligned}$$

before going to the computer program, we see that the system is dependent. The first two equations are identical.

Here we can readily recognize an independent system, however. It consists of the four different equations in (17), and we shall apply our computer program to this 4×4 system. (If this were not the case we could apply the program of Section 4.2 to different combinations of 4 equations selected from the 5 until we have found an independent set of 4 equations which would yield a unique solution for the given system of all 5 equations.)

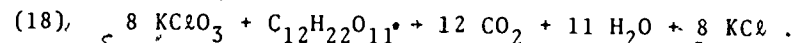
```
RUNNH  
N=? 4  
? 0,-11,-12,-22  
? 0,2,1,0  
? 0,1,0,2  
? 1,0,0,0  
? 1,3,0,0  
.125  
1.5  
1.375  
1
```

Ready

From the printout we see that for $u = 1$, we have

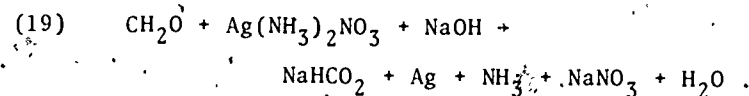
$$v = 0.125, \quad w = 1.5, \quad x = 1.375, \quad y = 1.$$

Since $0.125 = 1/8$, we can multiply all the values by 8 to balance the reaction as



4.4 The Non-Unique Case

For our final application we shall examine a chemical reaction where the total number m of products and reactants exceeds $n + 1$, where n is the number of distinct atoms and radicals involved. The reaction reads as follows:



With the following vector assignments,

$$C = (1, 0, 0, 0, 0, 0), \quad Ag = (0, 0, 0, 1, 0, 0),$$

$$H = (0, 1, 0, 0, 0, 0), \quad N = (0, 0, 0, 0, 1, 0),$$

$$O = (0, 0, 1, 0, 0, 0), \quad Na = (0, 0, 0, 0, 0, 1),$$

we seek positive integers s, t, u, v, w, x, y, z , with no common prime factor, so that

$$(20) \quad s(1, 2, 1, 0, 0, 0) + t(0, 6, 3, 1, 3, 0) + u(0, 1, 1, 0, 0, 1) \\ = v(1, 1, 2, 0, 0, 1) + w(0, 0, 0, 1, 0, 0) + x(0, 3, 0, 0, 1, 0) \\ + y(0, 0, 3, 0, 1, 1) + z(0, 2, 1, 0, 0, 0)$$

However, unlike our previous examples Equation (20) leads to a system of 6 linear equations in 8 unknowns, which we write in matrix form as

$$(21) \quad \begin{bmatrix} 1 \\ 2 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} s + \begin{bmatrix} 0 \\ 6 \\ 3 \\ 1 \\ 3 \\ 0 \end{bmatrix} t = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & -3 & 0 & 2 \\ -1 & 2 & 0 & 0 & 3 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ -1 & 1 & 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \\ x \\ y \\ z \end{bmatrix}$$

The system (21) has an infinite number of solutions, determined by the two parameters s and t . If we rewrite (21) as

$$\begin{bmatrix} u \\ v \\ w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 3 & 0 & 2 \\ -1 & 2 & 0 & 0 & 3 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ -1 & 1 & 0 & 0 & 1 & 0 \end{bmatrix}^{-1} \begin{bmatrix} 1 \\ 2 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} s + \begin{bmatrix} 0 \\ 6 \\ 3 \\ 1 \\ 3 \\ 0 \end{bmatrix} t$$

we can still use the program of Section 4.2 to assist us, but we need to use it twice. We use it once to compute the product of the inverse matrix with the column vector that precedes s , and again to compute the product of the inverse matrix with the column vector that precedes t .

RUNNH

N =? 6
? 0, -1, -1, 0, 0, -1
? 1, 1, 2, 0, 0, 1
? 0, 0, 0, 1, 0, 0
? 0, 3, 0, 0, 1, 0
? 0, 0, 3, 0, 1, 1
? 0, 2, 1, 0, 0, 0
? 1, 2, 1, 0, 0, 0
.75
1
0
0
.25
-.25
.5

Ready

RUNNM

N =? 6
? 0, -1, -1, 0, 0, -1
? 1, 1, 2, 0, 0, 1
? 0, 0, 0, 1, 0, 0
? 0, 3, 0, 0, 1, 0
? 0, 0, 3, 0, 1, 1
? 0, 2, 1, 0, 0, 0
? 0, 6, 3, 1, 3, 0
1.125
0
1
1.875
1.125
.75

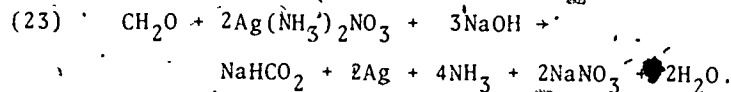
Ready

With these results we see that

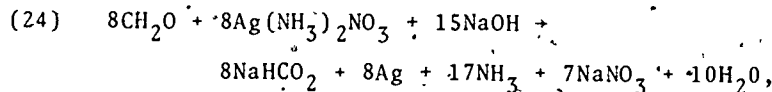
$$u = 0.75s + 1.125t, \quad x = 0.25s + 1.875t, \\ v = s, \quad y = -0.25s + 1.125t, \\ w = t, \quad z = 0.5s + 0.75t,$$

so that with s a positive integer multiple of 4 and t a positive integer multiple of 8 we can get an integer solution balancing the reaction. It is now possible, however, for two solutions to exist that are not multiples of each other, in contrast to what we found in our previous problems.

With $s = 4$ and $t = 8$ we can balance the reaction as



However, if we choose $s = t = 8$, the balanced reaction reads as



which is not a multiple of the solution in (23). This comes about because there are 2 independent chemical reactions taking place here.

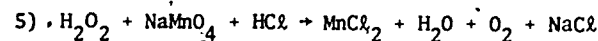
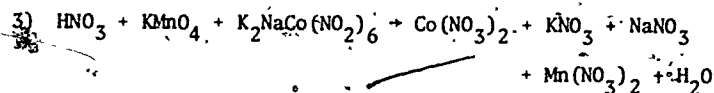
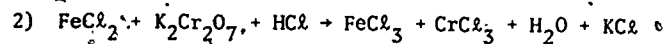
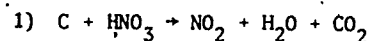
5. SUMMARY

Although this module was developed to provide some applications of matrix mathematics, these techniques are not to be considered as replacements for such chemical methods as oxidation-reduction, or the balancing of half-reactions where one learns a great deal about why and how reactions do or do not take place, in addition to how to balance them. For the chemical methods also enable one to learn a substantial amount about the properties of chemical elements. It is possible to write down a chemical reaction that does not take place and still balance it by the matrix techniques presented here! In addition, it must be pointed out again that all reactions considered in this module are electrically balanced.

Considering the example of Section 4.2, one can also see that the techniques are theoretically sound but with computer assistance one can get into some difficulty with round-off errors when larger matrices are inverted by the computer. Balancing chemical reactions without computer assistance but with the aid of generalized inverses of matrices is discussed by E.V. Krishnamurthy in [3].

6. EXERCISES

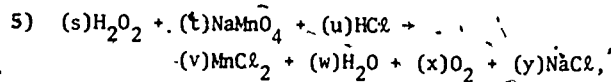
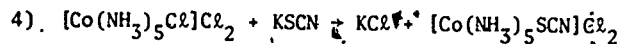
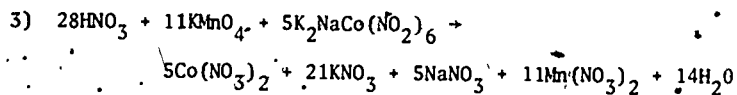
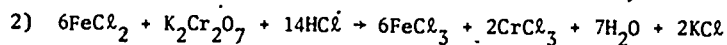
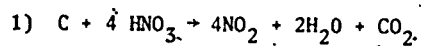
Balance the following chemical reactions:



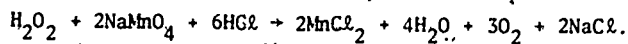
7. REFERENCES

- [1]. Anton, Howard. Elementary Linear Algebra, second edition. John Wiley & Sons, Inc., New York, 1977.
- [2]. Fletcher, T.J. Linear Algebra Through Its Applications. Van Nostrand Reinhold Company, London, 1972.
- [3]. Krishnamurthy, E.V. Generalized Matrix Inverse Approach for Automatic Balancing of Chemical Equations. International Journal of Mathematical Education in Science and Technology, 1978, Vol. 9, No. 3, pp. 323-328.
- [4]. Presley, Bruce, et al. A Guide to Programming in BASIC-PLUS. The Lawrenceville School, Lawrenceville, New Jersey, 1976.

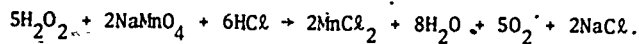
8. ANSWERS TO EXERCISES



where $(u, v, w, x, y) = s(0, 0, 1, 0.5, 0) + t(3, 1, 1.5, 1.25, 1)$. For
 $s = 2, t = 4$, the reaction is balanced as



With $s = 10$ and $t = 4$ the reaction can be balanced as



STUDENT FORM 1

Request for Help

Return to:
EDC/UMAP
55 Chapel St.
Newton, MA 02160

Student: If you have trouble with a specific part of this unit, please fill out this form and take it to your instructor for assistance. The information you give will help the author to revise the unit.

Your Name _____

Unit No. _____

Page _____

Upper

Middle

Lower

OR

Section _____

Paragraph _____

OR

Model Exam Problem No. _____

Text Problem No. _____

Description of Difficulty: (Please be specific)

Instructor: Please indicate your resolution of the difficulty in this box.

Corrected errors in materials. List corrections here:

Gave student better explanation, example, or procedure than in unit. Give brief outline of your addition here:

Assisted student in acquiring general learning and problem-solving skills (not using examples from this unit.)

25

Instructor's Signature _____

Please use reverse if necessary.

STUDENT FORM 2
Unit Questionnaire

Return to:
EDC/UMAP
55 Chapel St.
Newton, MA 02160

Name _____ Unit No. _____ Date _____

Institution _____ Course No. _____

Check the choice for each question that comes closest to your personal opinion.

1. How useful was the amount of detail in the unit?

- Not enough detail to understand the unit
 Unit would have been clearer with more detail
 Appropriate amount of detail
 Unit was occasionally too detailed, but this was not distracting
 Too much detail; I was often distracted

2. How helpful were the problem answers?

- Sample solutions were too brief; I could not do the intermediate steps
 Sufficient information was given to solve the problems
 Sample solutions were too detailed; I didn't need them

3. Except for fulfilling the prerequisites, how much did you use other sources (for example, instructor, friends, or other books) in order to understand the unit?

A Lot Somewhat A Little Not at all

4. How long was this unit in comparison to the amount of time you generally spend on a lesson (lecture and homework assignment) in a typical math or science course?

Much Longer Somewhat Longer About the Same Somewhat Shorter Much Shorter

5. Were any of the following parts of the unit confusing or distracting? (Check as many as apply.)

- Prerequisites
 Statement of skills and concepts (objectives)
 Paragraph headings
 Examples
 Special Assistance Supplement (if present)
 Other, please explain _____

6. Were any of the following parts of the unit particularly helpful? (Check as many as apply.)

- Prerequisites
 Statement of skills and concepts (objectives)
 Examples
 Problems
 Paragraph headings
 Table of Contents
 Special Assistance Supplement (if present)
 Other, please explain _____

Please describe anything in the unit that you did not particularly like.

Please describe anything that you found particularly helpful. (Please use the back of this sheet if you need more space.)