The Goals of General Chemistry—
A SYMPOSIUM

Chemical Equation Balancing

A General Method which is Quick, Simple, and has Unexpected Applications

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Introduction.

Some skeletal chemical equations, such as

$$CO + CO_2 + H_2 = CH_4 + H_2O$$

are known to have a variety of truly distinct balancings, several of which describe various different chemical reactions which have been observed. For example the balancings

$$CO + 3H_2 \rightarrow CH_4 + H_2O$$
$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$
$$2CO + 2H_2 \rightarrow CH_4 + CO_2$$

of the aforementioned skeletal chemical equation are all known (*1*) to occur during the synthesis of methane at various temperatures between 280°C and 370°C in the presence of a nickel catalyst. We will say that such original skeletal chemical equations have a *many parameter family of balancings*. And we will show how to calculate the number n of parameters exactly. In the example above the number of parameters can be shown to be equal to 2. A few more of the infinitely many members of the 2 parameter family of balancings of the skeletal chemical equation above are

$$CO + CO_2 + 7H_2 = 2CH_4 + 3H_2O$$
$$2CO + CO_2 + 10H_2 = 3CH_4 + 4H_2O$$
$$CO + 2CO_2 + 11H_2 = 3CH_4 + 5H_2O$$
$$3CO + CO_2 + 13H_2 = 4CH_4 + 5H_2O$$

Other skeletal chemical equations, such as

$$CH_4 + O_2 = CO_2 + H_2O$$

are known to have an essentially unique balancing. That balancing is

$$CH_4 + 2O_2 = CO_2 + 2H_2O$$

It would be silly to regard other balancings, such as

$$2CH_4 + 4O_2 = 2CO_2 + 4H_2O$$

or

$$3CH_4 + 6O_2 = 3CO_2 + 6H_2O$$

or even

$$0CH_4 + 0O_2 = 0CO_2 + 0H_2O$$

as being essentially different from the first balancing. They just say that, if you put 2 or 3 or 0 times as much in, you get 2 or 3 or 0 times as much out. Such skeletal chemical equations are said to have a *one-parameter family of balancings*. This terminology is synonomous with *essentially unique balancing*.

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Still other skeletal chemical equations, such as

$$(NH_4)_2SO_4 = NH_4OH + SO_2$$

have no balancings at all, except the rather trivial-looking balancing

$$0(NH_4)_2SO_4 = 0NH_4OH + 0SO_2$$

This is a shorthand way of saying that no reaction whatever takes place if only some, or all, of the components appearing in the original skeletal chemical equation are allowed to take part. In this last case we say that the original skeletal chemical equation has a *zero-parameter family of balancings*. In other words, there is *no nontrivial balancing*.

Only the matrix method (described below) is powerful enough to balance the skeletal chemical equation

$$\begin{aligned} &H_2 + Ca(CN)_2 + NaAlF_4 + FeSO_4 + MgSiO_3 + KI \\ &\quad + H_3PO_4 + PbCrO_4 + BrCl + CF_2Cl_2 + SO_2 \\ &= PbBr_2 + CrCl_3 + MgCO_3 + KAl(OH)_4 + Fe(SCN)_3 \\ &\quad + PI_3 + Na_2SiO_3 + CaF_2 + H_2O \qquad (1) \end{aligned}$$

Moreover, if shown the balancing (which can *easily* be obtained by the matrix method)

$$\begin{aligned} &88H_2 + 15Ca(CN)_2 + 6NaAlF_4 + 10FeSO_4 + 3MgSiO_3 \\ &\quad + 6KI + 2H_3PO_4 + 6PbCrO_4 + 12BrCl + 3CF_2Cl_2 + 20SO_2 \\ &= 6PbBr_2 + 6CrCl_3 + 3MgCO_3 + 6KAl(OH)_4 + 10Fe(SCN)_3 \\ &\quad + 2PI_3 + 3Na_2SiO_3 + 15CaF_2 + 79H_2O \end{aligned}$$

nobody today has a method at his disposal, other than the matrix method, capable of saying whether it is the only balancing of the foregoing original skeletal chemical equation. The matrix method easily verifies that this is the only possible balancing, however, in the process of finding it.

Again, of course, we speak of a one-parameter family of balancings and we do not consider a balancing such as

$$\begin{aligned} &880H_2 + 150Ca(CN)_2 + 60NaAlF_4 + 100FeSO_4 + 30MgSiO_3 \\ &+ 60KI + 20H_3PO_4 + 60PbCrO_4 + 120BrCl + 30CF_2Cl_2 + 200SO_2 \\ &= 60PbBr_2 + 60CrCl_3 + 30MgCO_3 + 60KAl(OH)_4 \\ &+ 100Fe(SCN)_3 + 20PI_3 + 30Na_2SiO_3 + 150CaF_2 + 790H_2O \end{aligned}$$

to be essentially different from the first balancing. If you use ten times as much of each reactant, you will obviously get ten times as much of each product. The matrix method does more than balance the given skeletal equation. It shows that—if you choose any 19 or fewer of the 20 chemcial species above—it is impossible to find a balanced chemical equation *involving only those 19 or fewer chemical species*. The given list of 20 chemical species is all or nothing. If you want a reaction you do it the way the above balancing indicates, or not at all.

This paper gives a completely general solution to the chemical equation balancing problem. It is elementary in the sense that it uses only the rudiments of algebra, no higher mathematics, and no specifically chemical principles, other than conservation of atoms and charges. Though trivial in

small cases, it is hard to carry out by hand for big examples. The example in eqn. (1) was originally done by hand before computer programs had been written, but that was a tedious job. Finally, the matrix method is far faster than any other approach when implemented on a large computer. Many very large examples of skeletal chemical equations (including eqn. (1)) have been balanced on the computer. The run time (excluding a 1/2 second program compile time) has always been less than a second when no more than 20 kinds of molecules involving no more than 20 chemical elements are involved.

Using Matrices to Solve Mathematical Equations

Before balancing chemical equations we will have to solve some mathematical equations. This section is a review and upgrading of universally known high school mathematics techniques for solving systems of homogeneous linear equations. Many readers may want to skip this section on a first reading, and go immediately to the next section to get an idea of what the method of this paper can accomplish. With this in mind, readers can see the use of going through the three examples immediately below. The idea behind them is to use concrete instances of equations to show how the standard techniques for solving systems of homogeneous linear equations lead to the Gauss-Jordan (*2, 3*) method of row reducing a matrix to Hermite normal form (*4*). They also show how to use Hermite normal form to produce a standard vector space basis (*2, 3*) for the collection of all solutions of the system.

Example 1

Suppose somebody wants to solve the system

$$\begin{aligned} 2x + 2y + 4z \qquad\qquad &= 0 \\ z + a + b &= 0 \\ y \qquad + 2a + b &= 0 \end{aligned}$$

of three equations in five unknowns, x,y,z,a,b. He observes only one occurrence of x, which is a good sign. He can set out to remove y from the first equation by subtracting two copies of the third equation from it. This gives a new first equation of the form

$$2x \qquad + 4z - 4a - 2b = 0$$

Replacing the old first equation by the new first equation he gets the equivalent, but simpler looking, system

$$\begin{aligned} 2x \quad + 4z - 4a - 2b &= 0 \\ z + a + b &= 0 \\ y \qquad + 2a + b &= 0 \end{aligned}$$

Now x and y occur only once, which is good. To remove z from the first equation he can subtract four copies of the second equation from it. This yields the newer first equation

$$2x \qquad - 8a - 6b = 0$$

Putting the newer first equation in place of the new, he gets the equivalent, but even simpler looking, system

$$\begin{aligned} 2x \qquad - 8a - 6b &= 0 \\ z + a + b &= 0 \\ y \quad + 2a + b &= 0 \end{aligned}$$

Now the unknowns x, y, and z occur only once. At this point he can pay a little attention to appearances. If he replaces the newer first equation by half of itself, and interchanges the second and third equations he gets the equivalent, and simplest possible in appearance, system

$$\begin{aligned} x \qquad - 4a - 3b &= 0 \\ y \quad + 2a + b &= 0 \\ z + a + b &= 0 \end{aligned}$$

It can, of course, be written

$$\begin{aligned} x \quad &= 4a + 3b \\ y \quad &= -2a - b \\ z &= -a - b \end{aligned}$$

to emphasize the fact that, no matter what values the unknowns a and b take on, there is a corresponding solution list (x,y,z,a,b). If he lets $a = 1$ and $b = 0$ then the solution is

$$x = 4, \quad y = -2, \quad z = -1, \quad a = 1, \quad b = 0$$

If he lets $a = 0$ and $b = 1$ then the solution is

$$x = 3, \quad y = -1, \quad z = -1, \quad a = 0, \quad b = 1.$$

It is easy to see that these two assignments of values solve the original system of equations. These two solutions are basic. He has only two degrees of freedom, amounting to choice of a, followed by choice of b. Letting one be 0 and the other be 1 is the simplest way to choose. Nevertheless, there are many other solutions of the final system of equations. And, of course, the solutions of the final system are the same as the solutions of the original system. Example of other solutions are

$$\begin{array}{llllll} x = 30, & y = -10, & z = -10, & a = 0, & b = 10; & \text{or} \\ x = -2, & y = 0, & z = 1, & a = 1, & b = -2; & \text{or} \\ x = 5 & y = -3, & z = -1, & a = 2, & b = -1. & \end{array}$$

The infinitely many solutions in question form a plane (i.e., a two dimensional vector subspace) in the five-dimensional vector space consisting of all lists (x,y,z,a,b) of five real numbers.

Example 2

The variable symbols x, y, z, a and b are no help, really, and cannot be used by a computer. So let us redo the description of Example 1, using just numbers and arrays, so that it can be programmed on a computer. Start with the coefficient matrix

$$\Sigma = \begin{bmatrix} 2 & 2 & 4 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 2 & 1 \end{bmatrix}$$

of the original system of equations. The original system of homogeneous linear equations in Example 1 is the same as the matrix equation

$$\Sigma \begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix} = \begin{bmatrix} 2 & 2 & 4 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 2 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Let us now use matrix language to express the solution process we went through in Example 1. First replace ROW 1 of the matrix Σ by ROW 1 − 2(ROW 3) to get the matrix

$$\begin{bmatrix} 2 & 0 & 4 & -4 & -2 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 2 & 1 \end{bmatrix}$$

In this latter matrix, replace ROW 1 by ROW 1 − 4(ROW 2) to get the matrix

$$\begin{bmatrix} 2 & 0 & 0 & -8 & -6 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 2 & 1 \end{bmatrix}$$

Now, in the matrix immediately above, do two things. Replace ROW 1 by (1/2)(ROW 1), and interchange ROW 2 with ROW 3, to get

$$\Phi = \begin{bmatrix} 1 & 0 & 0 & -4 & -3 \\ 0 & 1 & 0 & 2 & 1 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix}$$

The matrix Φ has been gotten from the original matrix Σ by three kinds of operations:

1) Replace a row by a nonzero multiple of itself;
2) Replace a row by a nonzero multiple of itself plus a multiple of another row;
3) Interchange 2 rows.

This last matrix Φ is in Hermite normal (*4*) form (i.e., reduced row echelon form (*2, 3, 5*)). This means that

I. The first nonzero entry in any row is 1;
II. The first nonzero entry in a lower row is to the right of the first nonzero entry in an upper row; and

III. If the first nonzero entry in ROW i occurs in COLUMN j, then every other entry in COLUMN j is 0.

If Σ is an m by n matrix then a series of elementary row operations of types 1, 2, and 3 above will take Σ to an m by n matrix Φ in Hermite normal form. Φ is said to be row equivalent (*2, 3, 5*) to the original matrix Σ. Moreover, Φ is unique. Almost any book on linear algebra or matrix theory has a theoretical development of this material. There are several elementary texts (*2, 3*), widely used in college freshman courses, which contain a full treatment, replete with worked out examples, of Gauss-Jordan reduction to Hermite normal form.

But let us return to the matrix Σ and to its Hermite normal form, the matrix Φ. Since elementary row operations produced Φ from Σ it is well known (*2, 3, 5*) that

$$\Sigma\begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix} = \begin{bmatrix} 2 & 2 & 4 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 2 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \theta$$

if and only if

$$\Phi\begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & -4 & -3 \\ 0 & 1 & 0 & 2 & 1 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \theta$$

where we use θ for the column vector with all zero entries above. The columns of the Hermite normal form Φ which contain first nonzero entries of rows will be called slave columns. The rest will be called master columns. In this example, columns 1, 2 and 3 are slave columns (corresponding to the fact that the first three unknowns, x, y and z, in the solution of the original system of equations were "forced" to take on values determined by a "free" choice of a and b). The fourth and fifth columns of Φ are master columns (because the last two unknowns, a and b, were considered to be free to take on any value). Correspondingly the first three entries, x,y,z, of a solution vector

$$\begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix}$$

are called slave entries and the last 2 entries, a,b, are called master entries. There are thus two degrees of freedom in picking solutions to the original system of equations. Put another way, there is a 2 parameter family of solutions to the system. In geometric language we say that the solutions of the matrix equation above form a vector space. Its dimension is the number of columns of Φ minus the number of nonzero rows of Φ. In this case its dimension is $5 - 3 = 2$. The solutions thus form a plane through the origin of the 5 dimensional column-vector space. To describe this solution plane we first find 2 vectors which form a vector space basis (*2, 3, 4, 5*) for this solution space. In other words we want 2 solutions

$$\begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix} \text{ and } \begin{bmatrix} x^* \\ y^* \\ z^* \\ a^* \\ b^* \end{bmatrix}$$

with the property that every other solution is a linear combination (*2, 3*) of them, i.e., that it is of the form

$$\text{solution vector} = p\begin{bmatrix} x \\ y \\ z \\ a \\ b \end{bmatrix} + q\begin{bmatrix} x^* \\ y^* \\ z^* \\ a^* \\ b^* \end{bmatrix} = \begin{bmatrix} px + qx^* \\ py + qy^* \\ pz + qz^* \\ pa + qa^* \\ pb + qb^* \end{bmatrix}$$

for some choice of real numbers p and q. A standard, easy, informative way (*2, 3, 4, 5*) to pick a vector space basis vector is to let one master variable be 1, let all the other master variables be 0, and then find out what each slave variable must be to satisfy the matrix equation. Doing this with each master variable in turn provides the vector space basis. So let $a = 1$, $b = 0$. Since we must satisfy the equation

$$\begin{bmatrix} 1 & 0 & 0 & -4 & -3 \\ 0 & 1 & 0 & 2 & 1 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \theta$$

we know that

$$\begin{aligned} (1)(x) + (0)(y) + (0)(z) + (-4)(1) + (-3)(0) &= 0 \\ (0)(x) + (1)(y) + (0)(z) + \quad (2)(1) + \quad (1)(0) &= 0 \\ (0)(x) + (0)(y) + (1)(z) + \quad (1)(1) + \quad (0)(0) &= 0 \end{aligned}$$

and, hence, that

$$x = 4, \qquad y = -2, \qquad z = -1$$

for this first basis vector, which is therefore equal to

$$\alpha = \begin{bmatrix} 4 \\ -2 \\ -1 \\ 1 \\ 0 \end{bmatrix}$$

Next let $a = 0$, $b = 1$. Since we must have

$$\begin{bmatrix} 1 & 0 & 0 & -4 & -3 \\ 0 & 1 & 0 & 2 & 1 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \theta$$

we know that

$$\begin{aligned} (1)(x) + (0)(y) + (0)(z) + (-4)(0) + (-3)(1) &= 0 \\ (0)(x) + (1)(y) + (0)(z) + \quad (2)(0) + \quad (1)(1) &= 0 \\ (0)(x) + (0)(y) + (1)(z) + \quad (1)(0) + \quad (1)(1) &= 0 \end{aligned}$$

and, hence, that

$$x = 3, \qquad y = -1, \qquad z = -1$$

for this second basis vector, which is therefore equal to

$$\beta = \begin{bmatrix} 3 \\ -1 \\ -1 \\ 0 \\ 1 \end{bmatrix}$$

Examples of other solutions are found by building vectors of the form $p\alpha + q\beta$ for various choices of p and q. Three cases in point are

$$0\alpha + 10\beta = 0\begin{bmatrix} 4 \\ -2 \\ -1 \\ 1 \\ 0 \end{bmatrix} + 10\begin{bmatrix} 3 \\ -1 \\ -1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 30 \\ -10 \\ -10 \\ 0 \\ 10 \end{bmatrix}$$

$$1\alpha + (-2)\beta = 1\begin{bmatrix} 4 \\ -2 \\ -1 \\ 1 \\ 0 \end{bmatrix} + (-2)\begin{bmatrix} 3 \\ -1 \\ -1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -2 \\ 0 \\ 1 \\ 1 \\ -2 \end{bmatrix}$$

$$2\alpha + (-1)\beta = 2\begin{bmatrix} 4 \\ -2 \\ -1 \\ 1 \\ 0 \end{bmatrix} + (-1)\begin{bmatrix} 3 \\ -1 \\ -1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \\ -3 \\ -1 \\ 2 \\ -1 \end{bmatrix}$$

All these solutions are matrix descriptions of the solutions given at the end of Example 1. The general solution vector is, of course, of the form

$$p\alpha + q\beta = p\begin{bmatrix} 4 \\ -2 \\ -1 \\ 1 \\ 0 \end{bmatrix} + q\begin{bmatrix} 3 \\ -1 \\ -1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 4p + 3q \\ -2p - q \\ -p - q \\ p \\ q \end{bmatrix}$$

for any numbers p and q.

Example 3

Consider the system

$$\begin{aligned} 4w \qquad\quad + 2z &= 0 \\ w \quad + y \qquad &= 0 \\ 2x + 2y + z &= 0 \end{aligned}$$

which is the same as

$$\begin{bmatrix} 4 & 0 & 0 & 2 \\ 1 & 0 & 1 & 0 \\ 0 & 2 & 2 & 1 \end{bmatrix} \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \theta$$

The Gauss-Jordan reduction process (*2*, *3*) applied to

$$\Sigma = \begin{bmatrix} 4 & 0 & 0 & 2 \\ 1 & 0 & 1 & 0 \\ 0 & 2 & 2 & 1 \end{bmatrix}$$

subtracts four copies of ROW 2 from ROW 1 to get a new ROW 1 and, thus, a new matrix

$$\begin{bmatrix} 0 & 0 & -4 & 2 \\ 1 & 0 & 1 & 0 \\ 0 & 2 & 2 & 1 \end{bmatrix}$$

In this latter matrix, ROW 2 is replaced by ROW 1 plus 4 copies of ROW 2 to yield

$$\begin{bmatrix} 0 & 0 & -4 & 2 \\ 4 & 0 & 0 & 2 \\ 0 & 2 & 2 & 1 \end{bmatrix}$$

In this third matrix, ROW 3 is replaced by ROW 1 plus 2 copies of ROW 3 to produce

$$\begin{bmatrix} 0 & 0 & -4 & 2 \\ 4 & 0 & 0 & 2 \\ 0 & 4 & 0 & 4 \end{bmatrix}$$

Now that several columns have been pretty well emptied out, it is time to spruce things up a bit. This is done by multiplying ROW 1 by $-1/4$, ROW 2 by $1/4$, and ROW 3 by $1/4$. The resulting matrix is

$$\begin{bmatrix} 0 & 0 & 1 & -1/2 \\ 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

Interchanging ROW 1 and ROW 2 leads to

$$\begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 0 & 1 & -1/2 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

Now, upon interchanging ROW 2 and ROW 3, we obtain the Hermite normal form

$$\Phi = \begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & -1/2 \end{bmatrix}$$

Since Φ has 4 columns and 3 nonzero rows it is clear that the collection of all solutions λ of

$$\Phi\lambda = \Phi \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & -1/2 \end{bmatrix} \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \theta$$

is a one-dimensional vector subspace of the four-dimensional space consisting of all columns

$$\begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix}$$

of four real numbers. In other words, there is one degree of freedom in choosing solutions to the original system, i.e., there is a one-parameter family of solutions. In more geometric language, the solution set is a line containing the zero vector (again symbolized by θ)

$$\theta = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

A vector space basis for this 1 dimensional vector space consists of a single nonzero vector. Evidently w, x, and y are slave variables (since the first three columns of Φ are slave columns). So we consider the master variable z and let $z = 1$. To solve

$$\Sigma \begin{bmatrix} w \\ x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} 4 & 0 & 0 & 2 \\ 1 & 0 & 1 & 0 \\ 0 & 2 & 2 & 1 \end{bmatrix} \begin{bmatrix} w \\ x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \theta$$

is the same as to solve

$$\Phi \begin{bmatrix} w \\ x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & -1/2 \end{bmatrix} \begin{bmatrix} w \\ x \\ y \\ 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} = \theta$$

which means

$$\begin{aligned} (1)(w) + (0)(x) + (0)(y) + \quad (1/2)(1) &= 0 \\ (0)(w) + (1)(x) + (0)(y) + \qquad (1)(1) &= 0 \\ (0)(x) + (0)(x) + (1)(y) + (-1/2)(1) &= 0, \end{aligned}$$

and thus the vector

$$\alpha = \begin{bmatrix} -1/2 \\ -1 \\ 1/2 \\ 1 \end{bmatrix}$$

is a basis for the vector space of solutions of the original matrix equation. Other members of this vector space are -50α, 2.71α and, more generally,

$$z\alpha = z \begin{bmatrix} -1/2 \\ -1 \\ 1/2 \\ 1 \end{bmatrix} = \begin{bmatrix} -z/2 \\ -z \\ z/2 \\ z \end{bmatrix}$$

In other words (w,x,y,z) is a solution of the original system of linear equations if and only if

$$w = -z/2, \qquad x = -z, \qquad y = z/2$$

where z is any number.

Outline of the Matrix Method for Balancing Chemical Equations

It is clear to anybody who thinks about the algebraic method (*6*, *7*) of balancing chemical equations that the problem is to solve a system of homogeneous linear equations. Various authors (*8–10*) have therefore pointed out that matrices are valuable tools for balancing chemical equations. They did not use all the most appropriate mathematical methods (especially module theory (*11*)) to analyze the solution, and gave short shrift to the question of what happens when the balancings of the original skeletal chemical equation make up a two (or more) parameter family. But they opened up interesting theoretical approaches and their work may be influential in the long run.

Example 4

The idea of the matrix method is to turn a skeletal chemical equation, such as

$$CH_4 + O_2 = CO_2 + H_2O$$

(or, if you prefer, to turn merely any list of chemical species, such as CO_2, CH_4, O_2, H_2O) into a matrix Σ. In this case the matrix is

$$\begin{array}{cc} & \begin{array}{cccc} CH_4 & O_2 & CO_2 & H_2O \end{array} \\ \Sigma = & \begin{bmatrix} 4 & 0 & 0 & 2 \\ 1 & 0 & 1 & 0 \\ 0 & 2 & 2 & 1 \end{bmatrix} \begin{array}{l} \text{hydrogen} \\ \text{carbon} \\ \text{oxygen} \end{array} \end{array}$$

It is obtained by entering the number of atoms of a given element e occuring in a given type of reagent molecule m into the matrix in the row corresponding to e and the column corresponding to m. Thus, reading down the first column of the matrix Σ above, we find that a single molecule of methane consists of:

4 atoms of hydrogen;
1 atom of carbon; and
0 atoms of oxygen.

We then use Gauss-Jordan elimination by row reduction to bring the original matrix Σ to Hermite (*4*) normal form Φ. Then we use standard techniques (*2–5*) to find a vector space basis for the collection of all column vectors λ such that $\Phi\lambda = \theta$ (where, as above, θ stands for the column vector with 0 in every entry). This collection is called the kernel (*3*) of Φ, or the null space (*4*) of Φ. For the matrix Σ above it follows from Example 3 above that

$$\Phi = \begin{bmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & -1/2 \end{bmatrix}$$

is the Hermite normal form of Σ. Balancings of the original skeletal chemical equation correspond to column vectors λ which Φ right annihilates, i.e., column vectors, such that the matrix product $\Phi\lambda$ is equal to the zero column vector θ. For example if

$$\lambda = \begin{bmatrix} -1 \\ -2 \\ 1 \\ 2 \end{bmatrix}$$

it is clear in this example that $\Sigma\lambda = \Phi\lambda = \theta$. Thus the kernel of Σ is equal to the kernel of Φ. The balancing corresponding to λ is

$$1CH_4 + 2O_2 = 1CO_2 + 2H_2O$$

obtained by attaching the successive entries of λ to the successive molecules which identified the columns of Σ, and then sorting the terms with positive coefficients onto one side of the equations and those with negative coefficients onto the other side (while stripping off their negative signs in the process). This is a one-parameter family of balancings because the kernel of Φ is a 1 dimensional vector space. This, in turn, is so (*3*) because Φ has 4 columns and 3 nonzero rows, and $4 - 3 = 1$. Balancings such as

$$3CH_4 + 6O_2 = 3CO_2 + 6H_2O$$

or

$$7CH_4 + 14O_2 = 7CO_2 + 14H_2O$$

$$\Phi = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

and observe that Φ has 3 columns and 3 nonzero rows. Since $3 - 3 = 0$ its kernel consists only of the zero vector θ, and there is only a zero-parameter family of balancings of any original skeletal equation such as

$$(NH_4)_2SO_4 + NH_4OH = SO_2$$

or

$$(NH_4)_2SO_4 = NH_4OH + SO_2$$

This means that the only balancing is the trivial balancing with all zero coefficients written down in the Introduction. In other words no reaction involving only those three chemical species can proceed. If you want some or all of them to take part you must either provide more reactants or accept more products (or both).

Example 6

Consider the problem of finding all reactions among hydrogen (H_2), carbon monoxide (CO), carbon dioxide (CO_2), methane (CH_4) and water (H_2O). We saw in Example 2 in the section on matrices that the matrix

$$\Sigma = \begin{array}{c} \begin{array}{ccccc} H_2 & H_2O & CH_4 & CO_2 & CO \end{array} \\ \begin{bmatrix} 2 & 2 & 4 & 0 & 0 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 2 & 1 \end{bmatrix} \end{array} \begin{array}{l} \\ \text{hydrogen} \\ \text{carbon} \\ \text{oxygen} \end{array}$$

has the Hermite normal form

$$\Phi = \begin{bmatrix} 1 & 0 & 0 & -4 & -3 \\ 0 & 1 & 0 & 2 & 1 \\ 0 & 0 & 1 & 1 & 1 \end{bmatrix}$$

Since it has five columns and three nonzero rows, and $5 - 3 = 2$, it has a two-dimensional kernel. In other words, there is a two-parameter family of balancings of the skeletal chemical equation

$$H_2 + H_2O = CO + CO_2 + CH_4$$

Six of the infinitely many column vectors λ belonging to this two-dimensional kernel are

$$\alpha = \begin{bmatrix} 1 \\ -1 \\ 0 \\ 1 \\ -1 \end{bmatrix}, \quad \beta = \begin{bmatrix} 3 \\ -1 \\ -1 \\ 0 \\ 1 \end{bmatrix}, \quad \gamma = \begin{bmatrix} 4 \\ -2 \\ -1 \\ 1 \\ 0 \end{bmatrix}, \quad \delta = \begin{bmatrix} 2 \\ 0 \\ -1 \\ -1 \\ 2 \end{bmatrix}, \quad \epsilon = \begin{bmatrix} 0 \\ 2 \\ -1 \\ -3 \\ 4 \end{bmatrix}, \quad \eta = \begin{bmatrix} 5 \\ -3 \\ -1 \\ 2 \\ -1 \end{bmatrix}$$

merely repeat the first balancing on a larger scale, and so we regard them as not essentially different from it. In vector space terms, the first balancing shown is a vector space basis of the one-dimensional vector space of all balancings. It is, in fact, a module basis (*11*) of the kernel of Φ. In other words, every balancing of the equation can be gotten from λ by multiplying it through by a whole number (i.e., an integer).

Example 5

What reactions involving only ammonium sulfate ($(NH_4)_2SO_4$), ammonium hydroxide (NH_4OH) and sulfur dioxide (SO_2) are possible? To ask the question is to form the matrix

$$\Sigma = \begin{array}{c} \begin{array}{ccc} (NH_4)_2SO_4 & NH_4OH & SO_2 \end{array} \\ \begin{bmatrix} 8 & 5 & 0 \\ 2 & 1 & 0 \\ 4 & 1 & 2 \\ 1 & 0 & 1 \end{bmatrix} \end{array} \begin{array}{l} \\ \text{hydrogen} \\ \text{nitrogen} \\ \text{oxygen} \\ \text{sulfur} \end{array}$$

To answer the question is to produce the Hermite normal form Φ of the matrix Σ,

Evidently they correspond, respectively, to the balancings

$$\begin{array}{rcll} H_2 + CO_2 & = H_2O & + \ CO & (\alpha) \\ 3H_2 + CO & = H_2O & + \ CH_4 & (\beta) \\ 4H_2 + CO_2 & = 2H_2O & + \ CH_4 & (\gamma) \\ 2H_2 + 2CO & = CO_2 & + \ CH_4 & (\delta) \\ 2H_2O + 4CO & = 3CO_2 & + \ CH_4 & (\epsilon) \\ 5H_2 + 2CO_2 & = 3H_2O & + \ CO + CH_4 & (\eta) \end{array}$$

The second, third, and fourth (β, γ and δ) were discussed at the beginning of this paper. Any pair of these six vectors are a vector space basis for the two-dimensional kernel of Σ (which is the same as the kernel of Φ). However, while the vector space bases $\{\alpha,\beta\}$, $\{\alpha,\gamma\}$, $\{\alpha,\delta\}$, $\{\beta,\gamma\}$ and $\{\beta,\delta\}$ of the kernel of Σ are module bases (*11*) for the kernel of Σ, the vector space basis $\{\gamma,\delta\}$ of the kernel of Σ is not a module basis for the kernel of Σ. To make this clearer we note that it is easy to verify the vector equalities

$$\begin{aligned} 1\alpha + 1\beta &= \gamma \\ (-1)\alpha + 1\beta &= \delta \\ (-3)\alpha + 1\beta &= \epsilon \end{aligned}$$

$$
\begin{aligned}
2\alpha + 1\beta &= \eta \\
(-1)\alpha + 1\gamma &= \beta \\
(-2)\alpha + 1\gamma &= \delta \\
(-4)\alpha + 1\gamma &= \epsilon \\
1\alpha + 1\gamma &= \eta
\end{aligned}
$$

All coefficients above are whole numbers (integers). On the other hand

$$
\begin{aligned}
(1/2)\gamma + (-1/2)\delta &= \alpha \\
(1/2)\gamma + \quad (1/2)\delta &= \beta \\
(-1)\gamma + \qquad 2\delta &= \epsilon \\
(3/2)\gamma + (-1/2)\delta &= \eta
\end{aligned}
$$

In other words, every vector τ which belongs to the kernel of Φ—and which has only integer entries—can be written in the form

$$x\alpha + y\beta = \tau$$

where the weights (numerical coefficients) x and y of the vectors α and β are integers. Similarly $\{\alpha,\gamma\}$, $\{\alpha,\delta\}$, $\{\beta,\gamma\}$, $\{\beta,\delta\}$. However, it is sometimes (not always) necessary to use fractional weights v,w in order to write

$$\tau = v\gamma + w\delta$$

as a linear combination of the vectors γ and δ.

Example 7

Suppose a chemist knows only that bradykinin ($C_{50}H_{73}N_{15}O_{11}$) does not contain any amino acids (*12*) other than arginine ($C_6H_{14}N_4O_2$), glycine ($C_2H_5NO_2$), phenylalanine ($C_9H_{11}NO_2$), proline ($C_5H_9NO_2$), and serine ($C_3H_7NO_3$). If he wants to know whether it has any cyclic peptide bonds, he forms the matrix

$$
\begin{array}{cccccccc}
 & C_2H_5NO_2 & H_2O & C_3H_7NO_3 & C_6H_{14}N_4O_2 & C_5H_9NO_2 & C_9H_{11}NO_2 & C_{50}H_{73}N_{15}O_{11} \\
\Sigma = & \left[\begin{array}{c}2\\5\\1\\2\end{array}\right. & \begin{array}{c}0\\2\\0\\1\end{array} & \begin{array}{c}3\\7\\1\\3\end{array} & \begin{array}{c}6\\14\\4\\2\end{array} & \begin{array}{c}5\\9\\1\\2\end{array} & \begin{array}{c}9\\11\\1\\2\end{array} & \left.\begin{array}{c}50\\73\\15\\11\end{array}\right] \begin{array}{l}\text{carbon}\\\text{hydrogen}\\\text{nitrogen}\\\text{oxygen}\end{array}
\end{array}
$$

and finds its Hermite normal form Φ by row reduction. In fact it is not hard to verify that

$$
3\Phi = \begin{bmatrix}
3 & 0 & 0 & 0 & -18 & -36 & -123 \\
0 & 3 & 0 & 0 & -1 & -9 & -45 \\
0 & 0 & 3 & 0 & 13 & 27 & 96 \\
0 & 0 & 0 & 3 & 2 & 3 & 18
\end{bmatrix}
$$

Since Φ has seven columns, and four nonzero rows, and since $7 - 4 = 3$, he knows that there is a three-parameter family of balancings of the skeletal chemical equation

$$
\begin{aligned}
H_2O = C_2H_5NO_2 + C_3H_7NO_3 + C_5H_9NO_2 + C_6H_{14}N_4O_2 \\
+ C_9H_{11}NO_2 + C_{50}C_{73}N_{15}O_{11}
\end{aligned}
$$

As it stands this equation is chemically absurd. But the matrix method automatically sorts terms onto the proper sides and deletes terms which should not appear. The standard methods presented in the previous section proceed from Φ to the following vector space basis of the kernel of Σ (i.e., the collection of all balancings of the original skeletal chemical equation):

$$
\alpha = \begin{bmatrix} 18 \\ 1 \\ -13 \\ -2 \\ 3 \\ 0 \\ 0 \end{bmatrix}, \quad
\beta = \begin{bmatrix} 12 \\ 3 \\ -9 \\ -1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \quad
\gamma = \begin{bmatrix} 41 \\ 15 \\ -32 \\ -6 \\ 0 \\ 0 \\ 1 \end{bmatrix}
$$

The vector space basis $\{\alpha,\beta,\gamma\}$ of the kernel of Σ is, in fact, a module basis (*11*). None of the members of the basis $\{\alpha,\beta,\gamma\}$ correspond to a hydrolysis of bradykinin. In other words, the three corresponding balancings

$$
\begin{aligned}
18C_2H_5NO_2 + H_2O + 3C_5H_9NO_2 &= 13C_3H_7NO_3 + 2C_6H_{14}N_4O_2 \quad (\alpha) \\
12C_2H_5NO_2 + 3H_2O + C_9H_{11}NO_2 &= 9C_3H_7NO_3 + C_6H_{14}N_4O_2 \quad (\beta) \\
41C_2H_5NO_2 + 15H_2O + C_{50}H_{73}N_{15}O_{11} &= 32C_3H_7NO_3 \\
&\quad + 6C_6H_{14}N_4O_2 \quad (\gamma)
\end{aligned}
$$

do not isolate one bradykinin molecule and a few water molecules on one side of the equation and keep all five kinds of amino acid molecules on the other side.

The chemist wants to know all hydrolyses in the kernel of Σ. In other words, he wants to know all lists (a,b,c) of numbers such that the linear combination

$$\omega = a\alpha + b\beta + c\gamma$$

is a hydrolysis. Here he plays his hole care, the fact that $\{\alpha,\beta,\gamma\}$ is a module basis. It enables him to ignore fractional coefficients and concentrate exclusively on integer values of a, b and c. In other words the seventh entry of ω must be -1. Its second entry must be a negative (or at least nonpositive) integer. These two conditions get one bradykinin molecule and an as yet unknown number of water molecules on the side specified by negative signs. The other five entries of ω must be positive (or at least nonnegative) integers to get the amino acids onto the opposite side. He thus has the following seven conditions

$$
\begin{aligned}
18a + 12b + 41c &\geq 0 \\
a + \ 3b + 15c &\leq 0 \\
-13a - \ 9b - 32c &\geq 0 \\
-2a - \ b - \ 6c &\geq 0 \\
3a \qquad\qquad &\geq 0 \\
b \qquad &\geq 0 \\
c &= -1.
\end{aligned}
$$

When he simplifies them by plugging in -1 for c, he gets the following six inequalities

$$
\begin{aligned}
18a + 12b &\geq 41 \\
-a - \ 3b &\geq -15 \\
-13a - \ 9b &\geq -32 \\
-2a - \ b &\geq -6 \\
a &\geq 0 \\
b &\geq 0.
\end{aligned}
$$

They readily yield two further inequalities

$$-13a \geq -32, \quad \text{and} \quad -9b \geq -32$$

from which it is obvious that

$$-a \geq -2, \quad \text{and} \quad -b \geq -3$$

(since a and b must be integers). It is now easy to check all twelve integer lists (a,b,c) such that

$$0 \leq a \leq 2, \quad \text{and} \quad 0 \leq b \leq 3, \quad \text{and } c = -1$$

against the original seven conditions and verify that only the list

$$(a,b,c) = (1,2,-1)$$

satisfies all seven of them. Because he has the power of a module basis (*11*) at his disposal, not just that of a vector space basis, he is thus assured that $\omega = 1\alpha + 2\beta - 1\gamma$ is the only possible hydrolysis balancing of the original skeletal chemical equation. In other words the hydrolysis

$$
\begin{aligned}
C_2H_5NO_2 + C_3H_7NO_3 + 2C_6H_{14}N_4O_2 + 3C_5H_9NO_2 \\
+ 2C_9H_{11}NO_2 = 8H_2O + C_{50}H_{73}N_{15}O_{11}
\end{aligned}
$$

of bradykinin is unique. This is, of course, the empirically discovered relationship (*12*). Since the balancing above involves nine amino acid molecules and only eight water molecules it is clear that no cyclic peptide bond is present. Note, finally, that the initial assumption was only that no amino acids other than arginine, glycine, phenylalanine, proline, and serine were present in bradykinin. No one of the five was actually assumed to be present. But the analysis above proved that all were, in fact, present.

Example 8

Somebody who knows that gramicidin-S ($C_{60}H_{92}N_{12}O_{10}$) contains no amino acids (*12*) other than leucine ($C_6H_{13}NO_2$), ornithine ($C_5H_{12}N_2O_2$), phenylalanine ($C_9H_{11}NO_2$), proline ($C_5H_9NO_2$) and valine ($C_5H_{11}NO_2$) can go quickly from

$$\Sigma = \begin{array}{c} \begin{array}{ccccccc} C_5H_9NO_2 & C_5H_{11}NO_2 & C_6H_{13}NO_2 & C_9H_{11}NO_2 & C_5H_{12}N_2O_2 & C_{60}H_{92}N_{12}O_{10} & H_2O \end{array} \\ \begin{bmatrix} 5 & 5 & 6 & 9 & 5 & 60 & 0 \\ 9 & 11 & 13 & 11 & 12 & 92 & 2 \\ 1 & 1 & 1 & 1 & 2 & 12 & 0 \\ 2 & 2 & 2 & 2 & 2 & 10 & 1 \end{bmatrix} \begin{array}{l} \text{carbon} \\ \text{hydrogen} \\ \text{nitrogen} \\ \text{oxygen} \end{array} \\ \begin{array}{ccccccc} \text{PRO} & \text{VAL} & \text{LEU} & \text{PHE} & \text{ORN} & \text{PROTEIN} & \text{WATER} \end{array} \end{array}$$

to

$$2\Phi = \begin{bmatrix} 2 & 0 & 0 & 8 & 0 & 40 & -2 \\ 0 & 2 & 0 & -14 & 0 & -114 & 9 \\ 0 & 0 & 2 & 8 & 0 & 70 & -5 \\ 0 & 0 & 0 & 0 & 2 & 14 & -1 \end{bmatrix}$$

to the module basis

$$\epsilon = \begin{bmatrix} 4 \\ -7 \\ 4 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad \zeta = \begin{bmatrix} 20 \\ -57 \\ 35 \\ 0 \\ 7 \\ -1 \\ 0 \end{bmatrix}, \quad \eta = \begin{bmatrix} 2 \\ -9 \\ 5 \\ 0 \\ 1 \\ 0 \\ 2 \end{bmatrix}$$

Thus, there is a three-parameter family of solutions to this equation balancing problem. A manipulation of inequalities analogous to the one in Example 7 then leads to only four possible hydrolysis balancing vectors

$$\alpha = \begin{bmatrix} 6 \\ 6 \\ 0 \\ 0 \\ 0 \\ -1 \\ -14 \end{bmatrix}, \quad \beta = \begin{bmatrix} 4 \\ 4 \\ 1 \\ 1 \\ 1 \\ -1 \\ -12 \end{bmatrix}, \quad \gamma = \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \\ 2 \\ -1 \\ -10 \end{bmatrix}, \quad \delta = \begin{bmatrix} 0 \\ 0 \\ 3 \\ 3 \\ 3 \\ -1 \\ -8 \end{bmatrix}$$

Counting water molecules and amino acid molecules, we see that α corresponds to three cyclic peptide bonds, β to 2, γ to 1 and δ to none. No leucine, ornithine or phenylalanine occurs in α. No proline or valine occurs in δ. The empirically observed (*12*) hydrolysis of gramicidin-S is γ. In other words, there are four possible solutions to our constrained problem. The only one so far observed in nature is the one corresponding to γ, namely

$$2C_5H_9NO_2 + 2C_5H_{11}NO_2 + 2C_6H_{13}NO_2 + 2C_9H_{11}NO_2 + 2C_5H_{12}N_2O_2 = C_{60}H_{92}N_{12}O_{10} + 10H_2O.$$

Summary

The matrix method (*8–10*) is all there is to chemical equation balancing, whether the chemical species involved are molecules or ions (or some of each). It is, in fact, all there is to a more general problem. If somebody has a list of chemical species and wants to know the collection (be it void or nonvoid) of all possible chemical reactions among them—but not involving any other chemical species as either reactants or products—the matrix method quickly (less than one second run time of an already compiled FORTRAN program on a large mainframe) and cheaply (a few 1982 dimes) gives the complete answer. Virtually every unconstrained chemical equation balancing problem which has ever been posed to date is mathematically trivial, although it is now possible to formulate nontrivial unconstrained equation balancing problems (i.e., problems involving very large numbers of chemical species). It has, of course, always been a nontrivial matter to find all suitably constrained solutions—such as all hydrolysis balancings—of a balancing problem. A computer program to do this should be available next year.

The proper place for chemical reasoning is before the equation balancing process and after it, not during it. Beforehand, chemical insight can be used to come up with a good list of chemical species to examine with a view to what reactions have the entries on the list as reactants or products. Afterwards, if a two or more parameter family of balancings is found, it then is necessary to decide which balancing provides—or which few balancings provide—an appropriate description of the reaction which takes place under the given conditions of temperature, pressure, incident and excident radiation, catalysts, etc.

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