AUTOMATIC 'BALANCING' OF CHEMICAL EQUATIONS

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Abstract—A computer program conceived as an aid to chemistry students is presented for the calculation of the stoichiometric coefficients of chemical equations. Once these coefficients are calculated, the entire corresponding chemical equation with the respective coefficients is shown on the screen. The program is run from an "Options Menu", so the user does not have to learn commands. To compute the stoichiometric coefficients of a given chemical equation, the user must enter, in the same order that he or she would usually do on paper with a pencil or pen all the chemical species involved in an equation. Then, the calculations to compute the coefficients are carried out and the solution is shown. The program accepts and solves problems with ion species. Among other questions, the program checks that formulation rules are not broken and that chemical elements, formulae and characters such as parentheses and subscripts are properly entered. Chemical formulae can be represented by means of special graphic characters or by means of normal text characters.

INTRODUCTION

One of the most frequent tasks, in both laboratory and chemistry class, is obtaining a set of stoichiometric coefficients to 'balance' a chemical equation. This task is a necessary first step towards solving most school problems. As has been pointed out, the expression "balancing a chemical equation" is a contradiction of terms (Missen & Smith, 1989). A chemical equation is fundamentally a conservation statement about atomic species and, thus, it should already be balanced. Missen and Smith advise the use of more precise language. Instead of 'balancing an equation' the expression 'writing an equation' ought to be used.

The problem of finding the proper stoichiometric coefficients for a chemical equation has originated considerable literature. On one hand, there are studies on the difficulties that students encounter in understanding stoichiometry (see, for example, Savoy, 1988) and then there are the many papers dealing with the problem of 'balancing' chemical equations.

Usually, students obtain coefficients by a trial and error method. This effort yields no profit and loses a lot of time. When a moderate number of chemical species (8 or more) are involved in a given skeletal equation, the task is nearly impossible to solve by trial and error. Thus, some special methods are necessary. Three main methods can be used which are: the oxidation-number method (Boikess & Edelson, 1978, pp. 492-497); the ion-electron method (Boikess & Edelson, 1978, pp. 492-497; Petrucci, 1972); and the matrix method (Smith & Missen, 1982, chap. 2; Blakley, 1982). Other methods can be found in the literature (Harjadi, 1986; Garcia 1987; Kolb, 1981; Ling, 1979, pp. 72-79).

Teaching and practicing the above methods takes time from learning other more important topics. Students learn to use these 'recipes' without fully comprehending the principles on which they are based. As a result, students use rules by rote and spend a lot of time patiently fighting through a lot of redox, acid-base, etc., reactions. Of course, students may become true experts in the art of writing chemical equations and computing the proper stoichiometric coefficients. As I have noted elsewhere, this is one of the most familiar 'initiation ceremonies' of any future chemist (Campanario & Ballesteros, 1991). Nevertheless, and in spite of formal chemistry teaching, these same students may harbor persistent and serious misconceptions about chemical equilibrium (Yarroch, 1985) or redox reactions (Bueso et al., 1988). The curriculum is not covered and no kind of general skill can be acquired by rote memorization and practice of calculation methods for obtaining stoichiometric coefficients without fully comprehending their bases and implications. However, as Blakley points out, the proper place for chemical reasoning is before and after the "equation balancing process" (sic), not during it (Blakley, 1982, p. 734).

Yarroch carried out an interesting study on this topic (Yarroch, 1985). Fourteen high school chemistry students from two different schools were interviewed in depth on how they wrote simple chemical equations (i.e. \( \text{N}_2 + \text{H}_2 = \text{NH}_3 \)). All students were able to write the equations successfully. However, seven students were not able to construct diagrams that were consistent with the equations. These students would typically represent three hydrogen molecules \((3\text{H}_2)\) as six linked 'H'. Coefficients and subscripts were described as number distinguished by their location.
in the equation. Both were said to give the same information, the number of atoms present. These students were also willing to change the subscripts while writing equations. The students produced the right answers to the chemistry problems without understanding much of the chemistry involved.

Similar findings have been obtained by Lythcott (1990). This author completed a study on the relationship between chemical knowledge of high school chemistry students and problem-solving approaches. Students were taught to solve problems according to two different approaches. After instruction, students were asked individually to solve two simple problems. Students also had to draw simple drawings of the chemical reactions involved in the problems. After the problem solving task, students were interviewed. The results are quite pessimistic. Of the 13 students who produced correct or almost correct solutions, only two had a clear notion of the proportionality of coefficients and only five were able to draw the whole chemical equation adequately. As Lythcott points out, "much (of what we teach) is so mechanical that a student can follow the rules without ever really struggling after the chemical meanings" (Lythcott, 1990, p. 251).

I believe the program described here is a new approach to this situation. In the same way that modern calculators have removed logarithm tables (essential in the past for pH calculations) from classrooms, computers can be introduced into laboratory and classroom as a useful calculation tool. Devoting the student's learning time and energy understanding general principles and scientific theories is preferable to devoting it to carrying out overwhelming manipulations that contribute little to their scientific training. Nowadays few teachers would argue a need to teach students to handle logarithm tables, and yet, recipes for solving the problem of "chemical equation balancing" (sic) are still taught. This situation is similar to the problem of computing concentration of species in chemical equilibrium: students sometimes do not understand properly when some simplifications can be made and they use rote learning strategies for calculation. This problem can be overcome by using computer programs (Campanario & Ballesteros, 1990/91)

**PRINCIPLES**

A chemical equation is a conservation statement about atomic species and, sometimes, electric charges (Missen & Smith, 1989). In fact, electric charges can be considered as additional chemical elements. The problem of writing a chemical equation is mainly algebraic and can easily be solved by using the matrix method which is grounded in the mass and charge conservation principle [see Dugudgi & Ugi (1973) for a general overview of the algebraic models and matrices theory that can be used in many areas of Chemistry]. The idea of the matrix method is to turn

<table>
<thead>
<tr>
<th>Table 1. Matrix and set of linear equations corresponding to the skeletal equation Zn + NOJH = (NOI)Zn + H2O + N2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Stoichiometric coefficients are ( x_1, \ldots, x_n )</td>
</tr>
</tbody>
</table>
| \[
\begin{align*}
\text{Zn} + x_1 \text{NO}_2 \text{H} & = x_2 \text{(NOI)} \text{Zn} + x_3 \text{H}_2 \text{O} + x_4 \text{N}_2 = 0 \\
\text{Set of linear equations:} \\
\begin{bmatrix}
0 & 0 & 3 & -6 & -1 & 0 \\
1 & -1 & 0 & 0 & 0 & 0 \\
0 & -2 & 0 & 0 & 0 & 0 \\
0 & 3 & -6 & -1 & 0 & 0 \\
0 & 1 & 0 & 2 & 0 & 0 \\
\end{bmatrix} \\
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4 \\
x_5 \\
\end{bmatrix} = \begin{bmatrix} 0 \\
0 \\
0 \\
0 \\
0 \\
\end{bmatrix}
\end{align*}
\]
<table>
<thead>
<tr>
<th>Matrix:</th>
</tr>
</thead>
</table>
| \[
\begin{bmatrix}
\text{Zn} & \text{NO}_2 \text{H} & \text{(NOI)} \text{Zn} & \text{H}_2 \text{O} & \text{N}_2 \\
0 & 0 & 3 & -6 & -1 & 0 \\
1 & -1 & 0 & 0 & 0 & 0 \\
0 & -2 & 0 & 0 & 0 & 0 \\
0 & 3 & -6 & -1 & 0 & 0 \\
0 & 1 & 0 & 2 & 0 & 0 \\
\end{bmatrix}
\]
the sound on or off and choose the characters that will be used to represent the chemical formulas. To turn the sound on or off the user should choose the corresponding option in a menu. The user can choose the options by means of two menus. There are graphic characters (40 characters per line) and normal text characters (80 characters per line). For graphic characters the computer needs a CGA or VGA card. Properly positioned subscripts and superscripts are used with these graphic characters.

Next an Options Menu comes up with the following options:

1. Write a Chemical Equation
2. Program Information
3. Show the Last Problem Solved
4. Program Exit

To choose any item the user should push the corresponding number key or use the arrow keys and the ENTER key. The following explains the menu.

Write a chemical equation

This choice permits the program to write a chemical equation from a problem without stoichiometric coefficients or a skeletal equation. A window appears in the upper part of the screen that shows the problem as the user keys it in. The program will also print the chemical equation in the same window once the problem has been solved. The user should type the skeletal equation into the computer just as if he or she were writing it down on paper [i.e. NO,H + Zn = NO,NH, + (NO&Zn + H?O)]. Upper case and lower case letters should be differentiated to prevent errors of interpretation (i.e. 'Co' is Cobalt and 'CO' is carbon monoxide). A warning signal always appears when a wrong or inexistant chemical symbol is keyed. For example if 'Ag' is typed instead of 'Ag' (silver), the first character, 'A' is accepted first, and the next letter, 'G' is considered. Since 'G' is an upper case, not a lower case letter, it can only be the first letter of a new chemical element. Taking this into account, the program goes back to the character 'A' to interpret it as a chemical element and searches its memory for the element that corresponds to 'A'. There is no such chemical symbol, so the computer prints a warning message and deletes 'A'.

The program can accept and solve problems with ion species. As has been noted, an electric charge in a skeletal equation can be considered another element. The sign of negative charge should be entered with the '-' key and the positive charge sign with the '+' key. However, these signs are correctly shown on the screen as '-' and '+'. Numerical superscripts can also be used. Numerical superscripts must always be followed by a plus sign, an equal sign or ENTER to close the input.

The numerical subscripts that give the number of atoms and the numerical superscripts that give the number of positive and negative charges are also entered on the keyboard without specially advising the program beforehand. Obviously, and in agreement with chemical nomenclature standards, subscripts and superscripts should be greater than 1 and agree with the chemical nomenclature standards (i.e. Cl, Na, and NO\textsuperscript{-1} are wrong). To facilitate precision it has also been established that subscripts and superscripts should be < 100 (i.e. CO\textsubscript{2}H\textsubscript{13} is wrong and the program will print a warning signal).

Some chemical formulas require parenthesis [i.e. (NH\textsubscript{4})\textsubscript{2}SO\textsubscript{4}] that can be entered in the computer when the user remembers that a parenthesis must always be followed by a subscript > 1 and < 100. For instance Fe(CN)\textsubscript{H}\textsubscript{4} could not be written because the parenthesis is not followed by a subscript > 1. In this case the correct entry for the compound is Fe(CNH). If the user tries to end a skeletal equation while a parenthesis is still open the machine will print a warning message. A parenthesis cannot be opened nor can an equal sign '+' be added while there is a pre-existing unclosed left parenthesis.

The maximum number of different chemical elements that can be used is 50. The maximum number of different species that can be used is 51 and 50 is the maximum number of equal or different elements that can be placed within a parenthesis. If these limits are passed, the program prints a warning.

The following are samples of proper skeletal equations for chemical equation writing:

\[ \text{Fe(CN)_{4}} + \text{SO}_{3}{\cdot}\text{H}_{2} + \text{H}_{2}\text{O} = \text{SO}_{2}\text{K}_{3} + \text{Fe}^{2+} \]

\[ \text{SO}_{4}\text{Fe} + (\text{NH}_{4})\text{SO}_{4} + \text{CO} \]

\[ \text{I}_{2}\text{Cr} + \text{Cl}_{2} + \text{NaOH} = \text{IO}_{4}\text{Na} + \text{CrO}_{4}\text{Na} + \text{Cl}_{2}\text{Na} + \text{H}_{2}\text{O} \]

\[ \text{Ce}^{3+} + 1^{-} = \text{Ce}^{4+} + 1^{+} \]

\[ \text{Cr}_{2}\text{O}_{3} + \text{H}^{+} = \text{Cr}^{3+} + \text{H}_{2}\text{O} \]

\[ \text{ZnO}_{2}^{2-} + \text{H}_{2}\text{O} + \text{Hg} = \text{ZnHg} + \text{H}_{2}\text{O} \]

\[ \text{C}_{2}\text{H}_{5}\text{NH}_{3} + \text{Br}_{2} = \text{C}_{2}\text{H}_{5}\text{Br}_{2}\text{NH}_{3} + \text{Br}^{+} + \text{H}^{+} \]

When the user's input is too long and the first line is filled, the program starts another line in the window until a maximum of 4 lines is reached (see Figs 1 and 2). When this window is filled the program will open a new window. Thirty windows can be used.

(a) The ESCAPE key takes the computer off the skeletal equation and brings the menu back up on the screen.

(b) The help key '?' will tell the user which characters (first the upper case letters and second, the lower case letters for chemical element symbols, subscripts, signs, etc.) can be used at any one time, taking into account the preceding character. For example, a lower case
The next step is to compute the stoichiometric coefficients. This is done in two steps: first, a set of decimal coefficients is obtained with the Gauss–Jordan method of elimination. Next, a set of integer stoichiometric coefficients is obtained from the previous set of decimal coefficients. The set of final stoichiometric coefficients is obtained in such a way that coefficients are the smallest integers compatible with the set of linear equations. This is accomplished by dividing every decimal coefficient by the smallest one. Next, these new coefficients are multiplied by 1, 2, 3, ..., until a set of integer stoichiometric coefficients is obtained.

Normally the program will give the result of a calculation in a few seconds. However, on occasion, it may take longer, or the program may even have difficulty in solving the program. If this happens, the program will ask the user if he or she wants to continue the calculation. If the answer is affirmative, the correctly written chemical equation or a warning message will appear on the screen at the end of the program run. A sample is the following well-known problem (Blakley, 1967, p. 728):

\[ \text{H}_2 + \text{Ca(CN)}_2 + \text{NaAlF}_4 + \text{FeSO}_4 + \text{MgSiO}_3 + \text{IK} + \text{H}_2\text{PO}_4 + \text{PbCrO}_4 + \text{BrCl} + \text{CF}_2\text{Cl}_2 + \text{SO}_3 = \text{PbBr}_2 + \text{CrCl}_3 + \text{MgCO}_3 + \text{KAl(OH)}_4 + \text{Fe(SCN)}_3 + \text{PI}_2 + \text{Na}_2\text{SiO}_3 + \text{CaF}_2 + \text{H}_2\text{O} \]

The program takes about 40 s to calculate the corresponding chemical equation. By hand and, even with the help of some method, the same task is an overwhelming enterprise.

**Program information**

This option calls up information about program function onto the computer screen. The user is allowed to page both backwards and forwards through the screens. The user is also informed as to which page is currently displayed.

**Show the last problem solved**

This option calls up onto the screen the last chemical equation to have been calculated.

**Program exit**

This option allows the program to be abandoned and returns to DOS.

**SOME RECALCITRANT CASES**

This section explains why some problems cannot be solved. Sometimes it is impossible to find a solution because of formula or other entry errors. A warning message is printed in these cases and the skeletal equation is shown on the screen as given by the user. The program uses the Gauss–Jordan method of elimination. According to the general matrix theory, there are some situations that can be produced when
solving a given set of linear equations (Anton, 1977; Kolman, 1980). These problems can be detected by checking the determinant corresponding to the set of algebraic linear equations. Some error situations are the following.

Input error

This occurs when the right side does not contain the same elements as the left side. For example, the skeletal equation \( \text{Cl}^+ + \text{I}^- = \text{Cl}^- \text{I}^{-} \) is incorrect because the left side does not contain an element which appears on the right side.

Simultaneous adjustment of all elements is impossible

This occurs in some inputs like the following: \( \text{SeO}_2 + \text{H}_2 = \text{SeO}_2 \text{H} \). It is impossible to give coefficients that will simultaneously adjust the elements Se and O. The program can obtain a set of equations, but they will be mutually incompatible. The only solution is the trivial-looking ‘0’ for all the stoichiometric coefficients.

The number of chemical compounds is greater by one than the number of chemical elements

There is an infinite number of arbitrary solutions and no single method can find all of them. A system of compatible, but indeterminate, equations is reached. For example consider the input:

\[
\text{CO} + \text{CO}_2 + \text{H}_2 = \text{CH}_4 + \text{H}_2\text{O}
\]

This skeletal equation can be completed with an infinite number of coefficient sets, all of which are arbitrary. Two possible solutions are:

\[
\begin{align*}
\text{CO} + \text{CO}_2 + 7\text{H}_2 & = 2\text{CH}_4 + 3\text{H}_2\text{O} \\
2\text{CO} + \text{CO}_2 + 10\text{H}_2 & = 3\text{CH}_4 + 4\text{H}_2\text{O}
\end{align*}
\]

All of the above and more chemical equations are correct. This case is different from the ‘normal’ chemical equations that can also have infinite solutions, but in which all the possible sets of stoichiometric coefficients are multiples of a set of minimum coefficients. This is not true of the kind of problems considered in this section.

Chemical compounds are repeated

On some occasions, when a given compound is repeated (i.e. \( \text{H}_2\text{O} + \text{H}_2\text{O} + \ldots \)) it may be impossible to find a solution for reasons that are analogous to the above case. This does not always happen when chemical compounds are repeated, but only when a set of linear algebraic equations is reached that is both compatible and indeterminate.

The molecular formula for a compound is a multiple of the molecular formula of another compound

Sometimes, some of the molecules are multiples of the same formula of another molecule in the skeletal equations (i.e. \( \text{C}_8\text{H}_8\text{O}_4 = \text{C}_6\text{H}_6\text{O}_3 + \text{C}_2\text{H}_2\text{O} + \text{C}_4\text{H}_4\text{O}_2 \)). When this happens it may be impossible to find a non-arbitrary solution to the problem for the same reasons as above.

Other reasons

When the skeletal equation entered is too complicated (but not necessarily too long) or when the hypothetical solution is formed by very large coefficients that are not whole multiples of any number between 1 and 100 it may be impossible for the program to find a solution. It may also happen that negative coefficients are obtained (i.e. \( \text{H}_2\text{O} + \text{O}_2 = \text{H}_2\text{O} \)). If this happens in some chemical equations that the user is trying to solve and if the program does not receive more information it is possible that there is not method that will solve the problem. The author welcomes any suggestion on this particular.

CONCLUSIONS

Given the simplicity of the program, it is quite possible that the user can use it correctly by simply following the instructions as they appear on the screen. The matrix method is not used to extol the use of algebra and computers at the expense of knowing “chemistry” (Missen & Smith, 1989, p. 218). For a relatively simple system, this approach can be counter productive and when this is true the inspection method is not to be ignored. However, the possibility of automatically writing chemical equations is very attractive in the laboratory or when the goal of some problem is not to generate a chemical equation or the proper coefficients. Examples of the above are chemical equilibrium problems, redox equations, organic chemistry problems, equations with ion species, and so on. In addition, interdisciplinary aspects of teaching chemistry by using computers and algebra, can be stressed. The time saved from the mechanical exercises of balancing chemical equations can be devoted to other more creative and interesting tasks that lead to a better understanding of both the principles and laws of chemistry on the part of the student.

Program availability—A copy of the program can be secured by sending a disk to the author.

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