Learning Stoichiometry with Spreadsheet Simulations

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Abstract The pedagogical role of simulations in the teaching of chemistry is discussed here, along with the contribution made by simulations designed with spreadsheets, and the possibility of these being created by the students themselves. A sequence of activities is presented for use in the teaching of stoichiometry by means of simple spreadsheets that have the scroll bar incorporated as an interactive resource. Using this method as an alternative to routine ways of doing exercises, students will become more motivated and active, setting up numerical simulations and answering questions like "What happens if…?" Simultaneous visualization of initial and final experimental quantities, and of the stoichiometric relation, makes it possible to deal with students' alternative conceptions.

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1. Introduction

1.1. Simulations and the Teaching of Chemistry

The pedagogical role of animation and simulation in chemistry classes are well known [1]. Animation enables the different entities or components of a system to be visualised and put in motion. Simulations, on the other hand, open the activity up to the user, allowing control, interactivity, and feedback [2]. Control is understood as the extent to which the user can assign the initial parameters of the system and explore them as they please. Interactivity is the means by which the simulation provides the user with opportunities to influence the behaviour of the system in real time, while the simulation is running. Feedback refers to the information received by the user with regard to their interaction and their choices made while working with the simulation. Students therefore have greater control over their learning, as they can select the initial conditions, modify their implementation and receive feedback from the simulation.

According to Wieman et al. [3], the most effective simulations are those which: (a) represent the modelled systems faithfully, seeking to make visible the abstract or imperceptible structures and properties of the real system, (b) focus the user's attention both on basic scientific concepts and variables and key properties of the system being modelled, (c) offer a high level of interactivity, producing immediate responses to the user's actions, (d) present simple, intuitive controls that require little reading or analysis to understand how they work, and (e) are based on graphic design that is attractive to the student, inviting interaction and exploration.

Well-prepared simulations facilitate the development of a set of complex procedures and abilities that go beyond mastery of basic laboratory techniques, such as proposing hypotheses, designing experiments, controlling variables, making observations (on the screen), taking measurements (virtually), analysing results, making comparisons and reaching conclusions. They complement experimental work in an extraordinary way, generating great interest in students, partly because there is less likelihood of error in comparison with an experiment, and because correcting errors takes less time. Therefore, while the use of simulations does not replace working with real material in the laboratory, these two ways of working complement each other, enriching the processes of teaching and learning scientific subjects [4].

While using a computer simulation, meaningful learning is favoured as students have freedom to look for answers to their own questions about the system being studied, or to design their own strategies in order to respond to questions posed by the teacher [3].

These simulations recreate a situation or phenomenon by applying a mathematical model [5]. They are therefore algorithmic, given that they contain a structure with underlying rules, or algorithm [6]. The algorithms dictate how the simulation functions and determine its degree of suitability and precision. Simulations carried out with spreadsheets allow the visualisation and availability of the mathematical models they run. The spreadsheet is therefore a very powerful tool for simulating scientific processes [7], and chemistry in particular [8,9]. Furthermore, given that learning to use them is simple, they can be constructed by the students themselves.

1.2. Teaching Stoichiometry with Spreadsheets

Stoichiometry is one of the central concepts in chemistry, since it deals with the quantitative aspects of chemical reactions. The complexity of the subject often presents students with difficulties that go beyond mathematical complications (such as understanding proportionality) and alternative conceptions are often maintained even after teaching. This happens because stoichiometry deals with quantitative relationships in chemistry, constructed on a qualitative, conceptual base. Resolving stoichiometric situations requires understanding of concepts such as chemical reaction, reactant and product, chemical formula, chemical equation, subscript and stoichiometric coefficient.

Amongst the difficulties detected by didactic research into the learning of stoichiometry are the following:

- students confuse different chemical quantities (mole, concentration, mass, volume) involved in the resolution of problems [10]
- they do not conserve mass and atoms in a chemical reaction, or they encounter difficulties with the conservation of atoms and non-conservation of molecules in chemical change [11]
- they sustain that the limiting reactant in a chemical reaction is the substance with the lowest stoichiometric coefficient in the balanced chemical equation [12]
- they present incomplete understanding of the chemical equation and its relation with the empirical situation. Some students, given the initial composition of the system, are not able to determine the final state using the chemical equation [13]
- they assert that in order to produce a chemical change the reactants have to be in a particular proportion at the initial stage, (e.g., the proportion given by the stoichiometric coefficients) since they confuse the left side of the chemical equation with the initial state of the system [14].

With respect to the teaching of this topic, as with the teaching of many other concepts in chemistry, there would seem to be a degree of methodological monotony focused on the resolution of exercises with, generally, little experimental work or use of varied didactic resources. In order to generate a higher level of motivation on the part of students it has been proposed, for example, that stoichiometry problems be presented with substances from everyday life which students are familiar with [15], or the use of analogies [16].

In this article we present a simple method of resolving stoichiometry problems using a spreadsheet (e.g., Excel or Calc), which includes the scroll bar as an interactive resource.

Spreadsheets have great potential for the teaching of science, their first applications used in the teaching of chemistry having been recognised in the mid 80s [17]. Their availability, versatility, and usefulness when it comes to dealing with chemical data has been highlighted by many authors, such as Van Houten [18], Collins & Williams [19], and Zielinski & Swift [20]. For teaching purposes the following attributes of spreadsheets are significant: (a) they are easily learned and can be used immediately, (b) in many cases they can replace a programming language which is difficult to learn and (c) given their capacity for simulation, they enable students to answer questions such as "What if…?" In a previous article [21], the usefulness and versatility of spreadsheets was described for the verification and re-creation of previously designed simulations which can be found on internet.

The numerical simulations to be constructed are based on the ICF approach, which distinguishes the situations: Initial, Change and Final. This helps us to visualise the chemical composition at different stages of the reaction and differentiate this from the stoichiometric relationships (the proportions at which the species react). One proposal for using the scroll bar for chemical equilibrium with the ICE (Initial, Change and Equilibrium) approach is given in Raviolo [22].

The procedure developed allows students to deal with some of the difficulties they face, such as confusion between the stoichiometric coefficients and the quantities present in a reaction, given that they frequently: (a) consider that the substances are present in quantities which are equal to the coefficients, or (b) confer the significance of coefficients on the experimental quantities.

The sequence followed in this article, which increases gradually in complexity (in both chemical and computing terms), may be used as a methodological sequence to work on with pupils, at either high school or university level. Throughout, the formulation of questions on the part of the teacher is a key aspect; these questions should challenge the students and generate activities with the simulation.

2. Sequence of Activities

2.1. Stoichiometry with Number of Moles

This method is based on the stoichiometric relationships established between substances in a chemical reaction. Our starting point is the balanced chemical equation, for example, for the decomposition reaction of mercury oxide:

$$2HgO(s) \rightarrow 2Hg(l) + O_2(g)$$
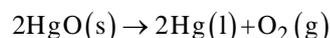
From this equation reasoning can take place, for example: for every two moles of mercury oxide which are decomposed, two moles of mercury and one mole of oxygen are formed; and according to a given generic quantity, x, of moles: for every 2x that the number of moles of mercury oxide decreases, the number of moles of mercury increases by 2x and the amount of oxygen increases by x.

It is convenient to express this reasoning using the ICF approach; for example, if at the start there are only four moles of oxide:

$$2HgO(s) \rightarrow 2Hg(l) + O_2(g)$$

	$2HgO(s)$	$2Hg(l)$	$O_2(g)$
Initial (mol):	4	0	0
Change (mol):	$-2x$	$+2x$	$+x$
Final (mol):	$4-2x$	$0+2x$	$0+x$

The equilibrium situation is not necessarily when the reaction is complete, since the quantities present can be determined at any time during the process.

The method of simulation proposed consists in assigning a range of possible values for x using the scroll bar on a spreadsheet, and determining the quantity of reactants and products at any time during the reaction, based on the stoichiometric relationships. A simulation is constructed as shown in Figure 1.

	A	B	C	D	E
1					
2		$2HgO(s) \rightarrow 2Hg(l) + O_2(g)$			
3					
4			x		
5			0.50		
6					
7			HgO	Hg	O_2
8		initial (mol)	**4.00**	**0.00**	**0.00**
9		change (mol)	(-2x)	(+2x)	(+x)
10		change (mol)	-1.00	1.00	0.50
11		final (mol)	3.00	1.00	0.50
12					
13		‹		›	
14			50		

Figure 1. Stoichiometric simulation with moles. The operations carried out are: cell C5: =C14/100, cell C10: =-2*C5, cell D10: =2*C5, cell E10: =1*C5, cell C11: =C8+C10, cell D11: =D8+D10, cell E11: =E8+E10

To insert the scroll bar into the 2010 version of the Microsoft Excel program, for example, click on Archive, Options, Quick Access Toolbar, Choose Commands from, Developer Tab, Insert Controls, Add, OK. Then in the Quick Access Toolbar, located in the upper right corner of the screen, you click Insert Controls, select the Scroll Bar and drag it with the mouse to the desired place.

Once the scroll bar has been inserted, Format Control can be opened on it, and Minimum value (0), Maximum value (200), Incremental change (1), and Cell link (C14) are completed (Figure 2).
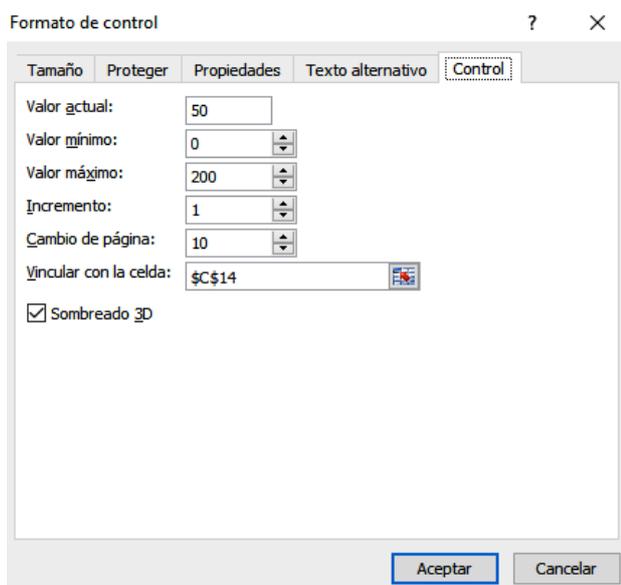
Figure 2. Dialogue box used to format the scroll bar

Given that decimal numbers cannot be inserted as the minimum value, in cell C5 the previous value is divided

by 100 and the result constitutes x. In this way, x can increase by 0.01, from 0 to 2. In other simulations, and in order to optimize results, it may be necessary to divide the value assigned by the scroll bar by a number different from 100, and perhaps modify the maximum value assigned.

In Figure 1 it can be seen that when the number assigned by the bar is 50, x = 0.50; one mole of oxide is broken down and the number of moles of the different species at that moment are 3.00, 1.00 and 0.50 respectively. Note that the maximum value assigned in the formatting of the scroll bar is 200, so that there will be no negative numbers and discussion of this aspect can thus be postponed for later, when the concepts of limiting and excess reactants can be developed.

Some possible questions to ask: How many moles of the products were produced when two moles of reactant were broken down? How many moles of oxygen were formed when 1.0 moles of mercury oxide remain? What are the maximum quantities of products that can be formed?

Once this simulation has been presented, or constructed together with the students, and after it has been applied to resolve different situations, the students can be asked to construct one for another chemical reaction, for example, for the synthesis of ammonia.

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g).$$
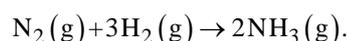
For greater visual impact the simulation shown can be extended further by the incorporation of a bar graph, which will be modified automatically as the scroll bar is moved. The quantities present at different moments of the reaction can be visualised by means of the bar graph. In Figure 3 the answer to the following question is given: What quantities are present when the amount of reactant is reduced by half?
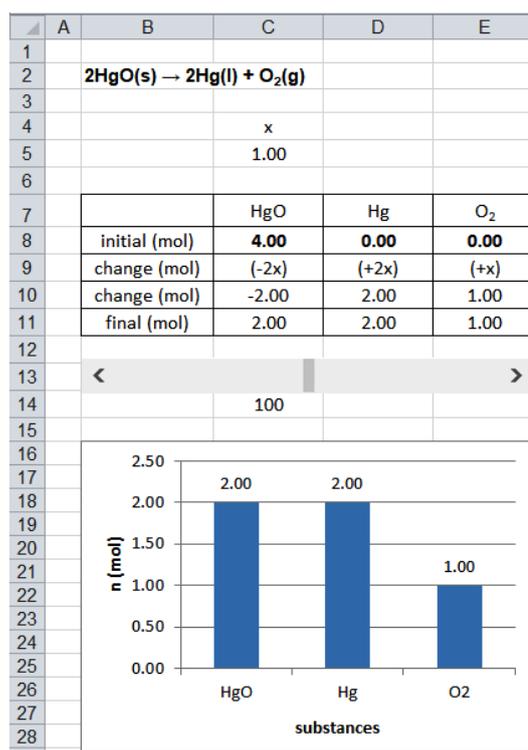
Figure 3. Stoichiometric simulation with moles and graphic representation

The simulation allows us to introduce the initial quantities of the three substances and calculate automatically the amounts present at any particular moment. In order to differentiate the "initial data" of these simulations from the other data, the initial experimental quantities are written in bold type.

Concerning the alternative conceptions mentioned previously, this is an opportune moment for teacher and pupils to discuss the numerical values the simulation enables us to individualise, and emphasize the differences between the initial number of moles, the stoichiometric coefficients and the final quantities. The teacher should highlight the fact that the stoichiometric coefficients of the reactants are not the initial quantities of the reaction, and that the reactant with the lowest stoichiometric coefficient is not necessarily the limiting reactant; the reaction will proceed even when the initial quantities in moles have lower values than the stoichiometric coefficients.

2.2. Stoichiometry with Volumes

The simulation shown in Figure 1 can be modified in such a way that it will automatically calculate the volume of oxygen obtained, and answer questions like: What volume of oxygen is obtained under standard conditions when two moles of mercury oxide are broken down? What volume will be obtained if the pressure of the system is 0.900 atm and the temperature 25.0 ℃?

Considering oxygen as an ideal gas, and applying the equation V= nRT/P, the answer to the first question is given in Figure 4, when the pressure is 1.00 atm and the temperature is 273 K.

	A	B	C	D	E
1					
2		$2HgO(s) \rightarrow 2Hg(l) + O_2(g)$			
3					
4			x		
5			1.00		
6					
7			HgO	Hg	O_2
8		initial (mol)	**4.00**	**0.00**	**0.00**
9		change (mol)	(-2x)	(+2x)	(+x)
10		change (mol)	-2.00	2.00	1.00
11		final (mol)	2.00	2.00	1.00
12					
13		‹		›	
14			100		
15					
16		R	T	P	Volume O_2
17		atm.L/K.mol	K	atm	L
18		**0.082**	**273**	**1.00**	22.4

Figure 4. Stoichiometric simulation with volume calculations. The operation cell E18: =E11*B18*C18/D18 is added

2.3. Stoichiometry with Masses

An application similar to the one in Figure 3 can be carried out with stoichiometric relationships in grams. Let us consider the reaction where water is formed from its elements, hydrogen and oxygen. The stoichiometric relationship tells us that 32 g of oxygen react with 4 g of hydrogen to obtain 36 g of water.

The ICF approach is represented as follows:

$$O_2(g) + 2H_2(g) \rightarrow 2H_2O(l)$$

$$32g \qquad 4g \qquad 36g$$

$$\textit{Initial (mol):} \quad n_1 \qquad n_2 \qquad n_3$$

$$\textit{Change (mol):} \quad -x \qquad -2x \qquad +2x$$

$$\textit{Final(mol):} \quad n_1 - x \quad n_2 - 2x \quad n_3 + 2x$$

	A	B	C	D	E
1					
2		$O_2(g) + 2H_2(g) \rightarrow 2H_2O(l)$			
3					
4			x		
5			1.25		
6					
7			O_2	H_2	H_2O
8		molar mass(g/mol)	32	2	18
9		initial (g)	**40.00**	**30.00**	**0.00**
10		initial (mol)	1.25	15.00	0.00
11		change (mol)	(-x)	(-2x)	(+2x)
12		change (mol)	-1.25	-2.50	2.50
13		change (g)	-40.00	-5.00	45.00
14		final (mol)	0.00	12.50	2.50
15		final (g)	0.00	25.00	45.00
16			¡limiting!	excess	
17					
18		‹		›	
19			5000		
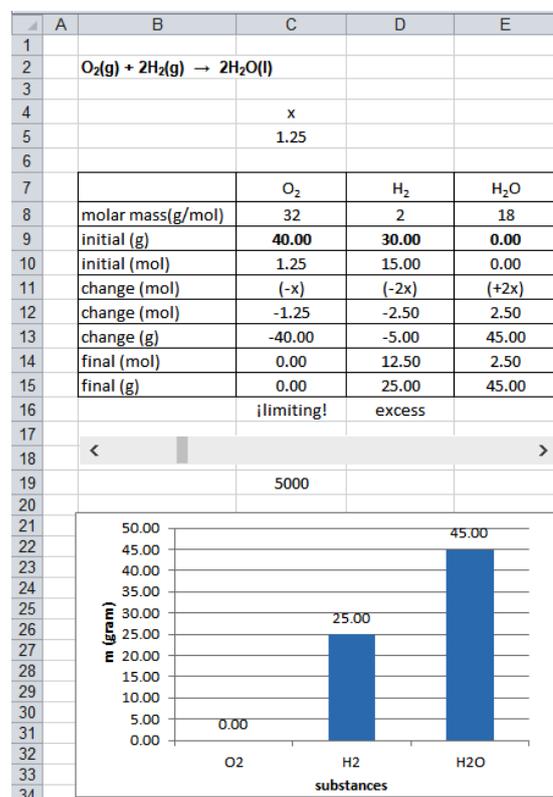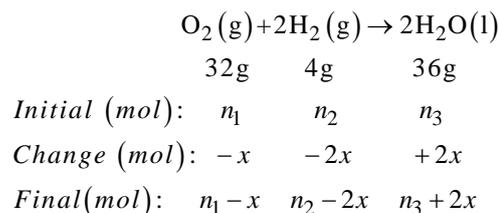
Figure 5. Stoichiometric simulation with masses. The operations carried out are: cell C5: =C19/4000, cell C10: = C9/C8, cell D10: =D9/D8, cell E10: =E9/E8, cell C12: = -C5, cell D12: =-2*C5, cell E12: =2*C5, cell C13: =C12*C8, cell D13: =D12*D8, cell E13: =E12*E8, cell C14: =C10+C12, cell D14: =D10+D12, cell E14: =E10+E12, cell C15: =C14*C8, cell D15: =D14*D8, cell E15: =E14*E8, cell C16: =IF((C15)<=0; "¡limiting!"; "excess"), cell D16: =IF((D15)<=0;"¡limiting!"; "excess")

The simulation in Figure 5 enables us to quickly answer questions of the following kind: How many grams of water are produced from 10.0 g oxygen and sufficient hydrogen? Which is the limiting reactant if an initial 40.0 g of oxygen is mixed with 30.0 g of hydrogen? How much excess reactant remains? What is the maximum amount of water (theoretical yield) that can be obtained? Figure 5 shows that when the final mass of oxygen is zero, the respective masses of hydrogen and water are 25.0 g and 45.0 g.

This simulation has been extended using IF function, so that messages appear (which mention the results obtained in neighbouring cells), such as: "limiting", "excess". In this way, when the mass of one of the reactants is zero (or has a negative value), the label automatically changes from "excess" to "limiting".

What happens if the initial quantity of hydrogen is 60 g? On introducing this value as initial data, it can be seen that when the reaction is complete, the same amount of water is obtained, and an excess mass of 55 g reactant remains.

To answer the question: How many grams of oxygen are necessary for the total amount of hydrogen to react? all that needs to be done is change the quantity of hydrogen to zero and the cell representing the final mass of oxygen will read "-200" g. In order to interpret this value, teacher and students should discuss the significance given to these negative quantities: "the amount that is lacking".

The simulation shown in Figure 5 establishes the correspondence between moles and grams in the three situations: initial, change and equilibrium. This simulation can be simplified by expressing the quantities only in grams (Figure 6). The user can choose between these two options, or an intermediate one.

Figure 6. Simplified stoichiometric simulation with masses. The operations carried out are: cell C5: =C15/4000, cell C10: -C5*C8, cell D10: =-2*C5*D8, cell E10: =2*C5*E8, cell C11: =C9+C10, cell D11: =D9+D10, cell E11: =E9+E10

As a practice activity, students can be asked to modify the first spreadsheet to represent the decomposition of 500 g of mercury oxide.

Finally, with the addition of two more cells this simulation can also include the calculation of percentage yield, one cell showing the theoretical yield (as a starting point) and the other with the calculation of actual percentage yield. This will provide the answer to the question: What is the percentage yield in the reaction of 40 g of oxygen and 30 grams of hydrogen if 42 g of water was produced?

2.4. Stoichiometry with Concentrations

At a later stage, stoichiometric problems with solutions can be tackled; for example, to answer questions like: How many moles of salt are obtained from the neutralisation of 200 mL of 2.00 M sodium hydroxide with 150 mL of 2.00 M sulphuric acid? Which is the limiting reactant and which the excess reactant? The answers to these questions can be obtained from the simulation with the scroll bar shown in Figure 7.

The simulation proposed allows us to determine the composition of the system in a case where a certain amount of salt is found in the initial situation.

Figure 7. Simulation of stoichiometry with concentrations. The operations carried out are: cell C5: =C18/200, cell C10: =C9*C8, cell D10: =D9*D8, cell E10: =E9*E8, cell C12: =-2*C5, cell D12: =-C5, cell E12: =C5, cell C13: =C10+C12, cell D13: =D10+D12, cell E13: =E10+E12, cell C14: =IF((C13)<=0; "¡limiting!"; "excess"), cell D14: =IF((D13)<=0; "¡limiting!"; "excess")

3. Conclusions

A different way has been presented here of addressing and resolving chemistry problems using the scroll bar in the context of a spreadsheet. The result is a dynamic, versatile simulation with a clear visual aid that enables students to formulate and answer questions such as, "What would happen if…?".

This proposal emphasises the conceptual aspects of stoichiometry over and above the routine calculations of numerical exercises. Using the stoichiometric relationships established between substances (reactants and products), students construct a numerical simulation that allows them to determine the composition of the system as the reaction progresses, starting from the initial condition.

The ICF approach (Initial, Change and Final) has enormous conceptual relevance, since it facilitates identification of the composition of a system at different moments of the reaction, revealing the difference between this and the stoichiometric relationship. The teacher can guide questions in such a way as to identify the presence of difficulties or alternative conceptions as mentioned in the introduction.

One advantage of these simulations is that they can be created by the students themselves with very little guidance from the teacher. The spreadsheet constitutes a powerful tool which is readily available, can be learned quickly and used immediately. The learning acquired related to use of the simulation programme can be transferred to other chemistry topics, to other school subjects and to daily life.

The Excel file with the simulations presented in this article can be requested from the author by e-mail.

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