Using Spreadsheets in the Science Classroom: an example from Chemistry

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INTRODUCTION

At heart, real understanding in science is essentially qualitative yet is often expressed in mathematical relations. Most advanced science students therefore spend a great deal of time and effort doing calculations. These calculations pose two kinds of demands:

- some of the mathematical models involved are complex and/or
- there is a need for repetitive analysis of large amounts of data

and both of these can serve to focus students' attention on mechanical mathematics at the expense of their understanding of the underlying scientific principles. Using Ogborn and Miller's phrase (Chapter 4) they reduce the level of cognitive 'chunking'. This a serious hindrance to students' learning and the need is for a tool or tools that can be used to raise the level of chunking so that pupils can focus on the underlying scientific concepts. Ideally such a system would be capable of being used by both pupils to model simple systems in which they can express their understanding of the science involved and by their teachers to construct more complex models for the pupils to explore. This chapter examines a variety of ways in which one tool, a spreadsheet, can be used to promote learning in an important concept area, that of chemical equilibrium.

WHY SPREADSHEETS?

Spreadsheets have a number of attributes which make them suitable for use as a computational tool in the school laboratory:

- They can be used to write both static and dynamic models and can therefore be employed in a wide variety of situations
- They possess (increasingly) well integrated graphing facilities (See Dreyfus & Feinstein 1991)
- They can be used in either of two complementary modes. In the first, students use the tool to express their own ideas, usually by testing a *variety of models* (of their own construction) using *fixed data*. while in the second, students explore models which express the thinking of others, usually by feeding *variable data* into a *fixed model*. The latter category commonly involves exploring the accepted scientific models although it also encompasses students exploring expressions of each others ideas. The differences between these modes of use are similar to the **expressive**/**exploratory** distinction described by Joan Bliss in Chapter 3. Bliss et al (1992a, 1992b), Kemmis et al (1977) and Schibeci (1989) provide further useful discussions of these ways of using models.
- They are existing well known software packages, capable of being used in many different conceptual areas across the school curriculum.
- They are becoming much more widely used by classroom teachers. Recently a number of articles have appeared in journals including those written for and by classroom teachers. They cover all branches of science and range from the substantial to the brief 'hints and tips' variety. (A selection of these articles are listed in the references.) Attempts have also been made to make the interface of a standard package (Excel) more 'user-friendly (Beare 1992).

Spreadsheets thus appear to meet the need for a powerful, flexible and widely available microworld within which students can interact with models to both express their own understanding of a situation and explore the meanings of others.

THE NATURE OF STUDENTS' DIFFICULTIES WITH EQUILIBRIUM

Chemical equilibrium is a core chemical concept, an understanding of which is essential for most qualitative and quantitative work in chemistry and thus its study forms a central part of advanced chemistry courses. These courses tend to stress the quantitative aspects of the topic - fulfilling the (necessary) function of teaching students to use the appropriate equations. Studying equilibrium therefore involves both difficult and/or repetitive calculations. In their different ways these provide barriers to conceptual understand. The topic thus provides a good focus for exploring the different kinds of barriers both these types of arithmetical demand pose to conceptual understanding.

It is also a conceptual area where previous work has shown that students have well structured 'alternative conceptions' which are highly resistant to change. Recent research (e.g. Hackling and Garnett 1985, Gorodetsky and Gussarky 1986, Maskill and Cachapuz 1989, Prout 1989) has reinforced the feeling, long held by teachers, that many pupils find the concept of chemical equilibrium difficult. In particular it has highlighted the way that students base their understandings of chemical equilibria on ideas and meanings associated with other, more everyday, concepts of equilibrium. They have a different qualitative understanding of 'the way things are' to the scientist.

One further difficulty is that chemical equilibrium is commonly portrayed using both static models - which work backward from laws to deduce concentrations, and dynamic models - which stress the process of movement towards equilibrium. Within this latter category there are both probabilistic models - representing the process at the level of individual molecules and deterministic models - based on rate laws. This plethora of conceptual approaches confuses many students who cannot see the links between them. However it provides an ideal forum for examining the ease with which students can move between different representations of the same system.

ADDRESSING THE STUDENTS' DIFFICULTIES

In this section I will list some of the main problems that students have in coming to a full understanding of chemical equilibrium and illustrate some of the ways in which spreadsheets can be used to address these difficulties.

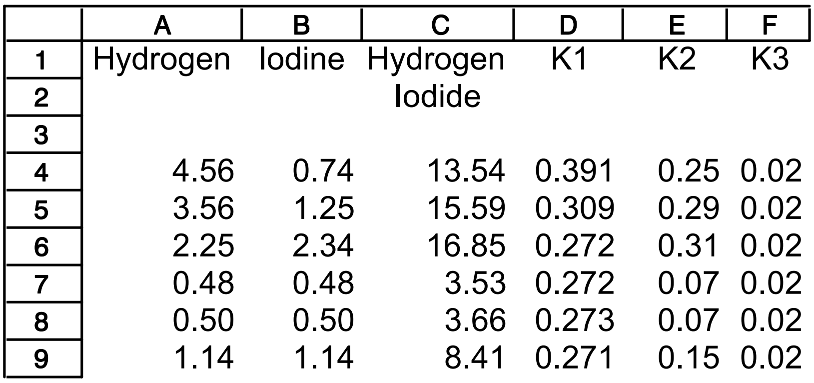
The ratio of equilibrium concentrations

Students often believe that at equilibrium the composition of the reacting species is equal to, or at least in the ratio of, the balanced chemical equation for the reaction. e.g. that for the reaction

$$2HI \qquad H_2 + I_2$$

the equilibrium concentrations of hydrogen, iodine and hydrogen iodide are in the ratio 1:1:2. This fits with an everyday notion of balance. As a result many students cannot accept (and therefore have difficulties with) the equilibrium law expression. One way of addressing these problems is to show that the general form of the equilibrium law 'works' in that it is applicable to a wide variety of reactions with many sets of equilibrium concentrations. Unfortunately the repetitive nature of the necessary calculations soon make them tedious as well as taking a great deal of time. This means that not only is the discussion usually limited to just one or two examples but that the range of alternative equilibrium law formulations which can be tested is also circumscribed. One solution to this problem is for a teacher to enter data sets of equilibrium concentrations on a worksheet and allow the pupils to write their own equilibrium law expressions and see the consequences. Knowing the balanced chemical equations the students are free to try any analytic relation they choose on one data set until they find one or ones that give constant values. They then try and generalise from this and apply their ideas to another data set. They then try and generalise from this and apply their ideas to another data set. In the example shown in figure 1, students are given sets of equilibrium concentrations for the hydrogen/ iodine/ hydrogen iodide system described above and asked to write different possible equilibrium law expressions. Typically they use equations such as those shown where

$K1=([H_2]+[I_2])/[HI]$ $K2=([H_2]*[I_2])/[HI]$ $K3=([H_2]*[I_2])/[HI]$^2



	A	B	C	D	E	F
1	Hydrogen	Iodine	Hydrogen	K1	K2	K3
2			Iodide			
3						
4	4.56	0.74	13.54	0.391	0.25	0.02
5	3.56	1.25	15.59	0.309	0.29	0.02
6	2.25	2.34	16.85	0.272	0.31	0.02
7	0.48	0.48	3.53	0.272	0.07	0.02
8	0.50	0.50	3.66	0.273	0.07	0.02
9	1.14	1.14	8.41	0.271	0.15	0.02

Figure 1. Possible Equilibrium Law expressions for the Hydrogen/Iodine/Hydrogen Iodide system

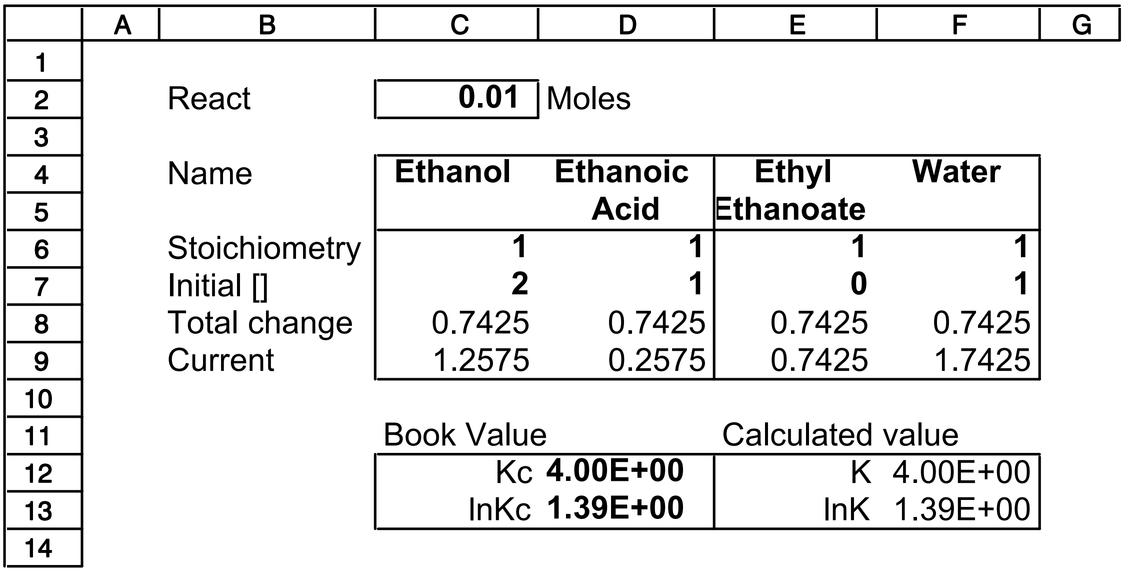
and can see by inspection that the last of these produces the most constant value. In this expressive example the students only write an equation once and then use a built in spreadsheet function to copy the formula into other cells. In this way they are free to concentrate on the models rather than the mathematics. The general nature of the relationship is then explored further by using other system - such as the Ethanol/ Ethanoic Acid/ Ethyl Ethanoate/ Water system (Brosnan 1989)

$$C_2H_5OH + CH_3COOH \qquad CH_3COOC_2H_5 + H_2O$$

where ‘common-sense’ suggests that the equilibrium concentration of all the species should be equal - but they are not.

The effect of changing concentrations on equilibrium

Another way of examining the non-equivalence of the equilibrium concentrations of reacting species is to use a spreadsheet to perform their ‘brute force’ calculation (Ogborn 1987, Brosnan 1990a). The student is free to choose any initial concentrations of the reacting species and then react or ‘unreact’ successive amounts of one species until the calculated equilibrium constant matches the book value. The worksheet uses the stoichiometry and amount it is told to react to calculate new concentrations and use these in turn to calculate an ‘equilibrium constant’. One particular use of this approach is to allow students to see the effect of adding more of one reagent, e.g. the example illustrated in figure 2 shows the effect on the reaction described above of starting with 2 moles of ethanol, one mole of Ethanoic acid and water and no ethyl ethanoate. The point here is to see how the pattern of equilibrium concentrations relates to the starting concentrations. In particular it can be used to show how unusual it is for the equilibrium concentrations to be in the same ration as illustrate that not only need the concentrations of species on any one side of the reaction need not equal - in fact it is unusual for them to be so.



	A	B	C	D	E	F	G
1							
2		React	**0.01**	Moles			
3							
4		Name	**Ethanol**	**Ethanoic**	**Ethyl**	**Water**	
5				**Acid**	**Ethanoate**		
6		Stoichiometry	**1**	**1**	**1**	**1**	
7		Initial []	**2**	**1**	**0**	**1**	
8		Total change	0.7425	0.7425	0.7425	0.7425	
9		Current	1.2575	0.2575	0.7425	1.7425	
10							
11			Book Value		Calculated value		
12			Kc	**4.00E+00**	K	4.00E+00	
13			lnKc	**1.39E+00**	lnK	1.39E+00	
14							

Figure 2. ‘Brute force’ calculation of equilibrium concentrations

The calculations involved in the examples above are simple but repetitive. However there are other systems, often those involving more than one competing equilibrium where the barrier to meaningful exploration is that the calculations are too difficult and the technique described above can be adapted for use with these systems also (Brosnan 1992a).

A good example is the class of generalised acid/base equilibria. In these there are three competing equilibria - the dissociation of the acid, base and water:

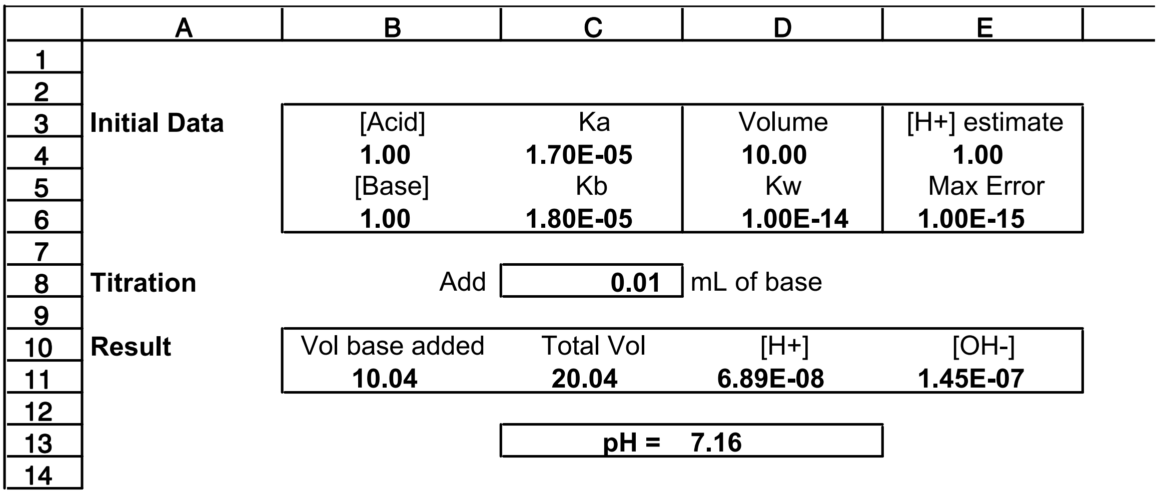
$HA(aq) \quad H^{+}(aq) + A^{-}(aq)$

$HB(aq) \quad H^{+}(aq) + B^{-}(aq)$

$H2O \quad H^{+}(aq) + OH^{-}(aq)$

(A and B are the acid and base respectively)

The pH curves of these systems are often obtained experimentally and comparing the results of direct experiment with those obtained from theoretical models is potentially of considerable interest. However while the chemical principles involved are relatively simple, determination of the pH is difficult since it requires solving a quartic equation in $H^{+}(aq)$. Figure 3 shows a worksheet devised to address this problem. In this example the user is free to set the initial concentrations of acids and bases of any strength and the concentration of $H^{+}(aq)$ is calculated by a function macro which uses the Newton-Raphson method iteratively to seek a chemically meaningful root. Using this worksheet students can ‘step through’ any acid-base reaction, see the effect of different acid and base concentrations and dissociation constants on the pH values during the titration and compare the results with those obtained by experiments on the system.

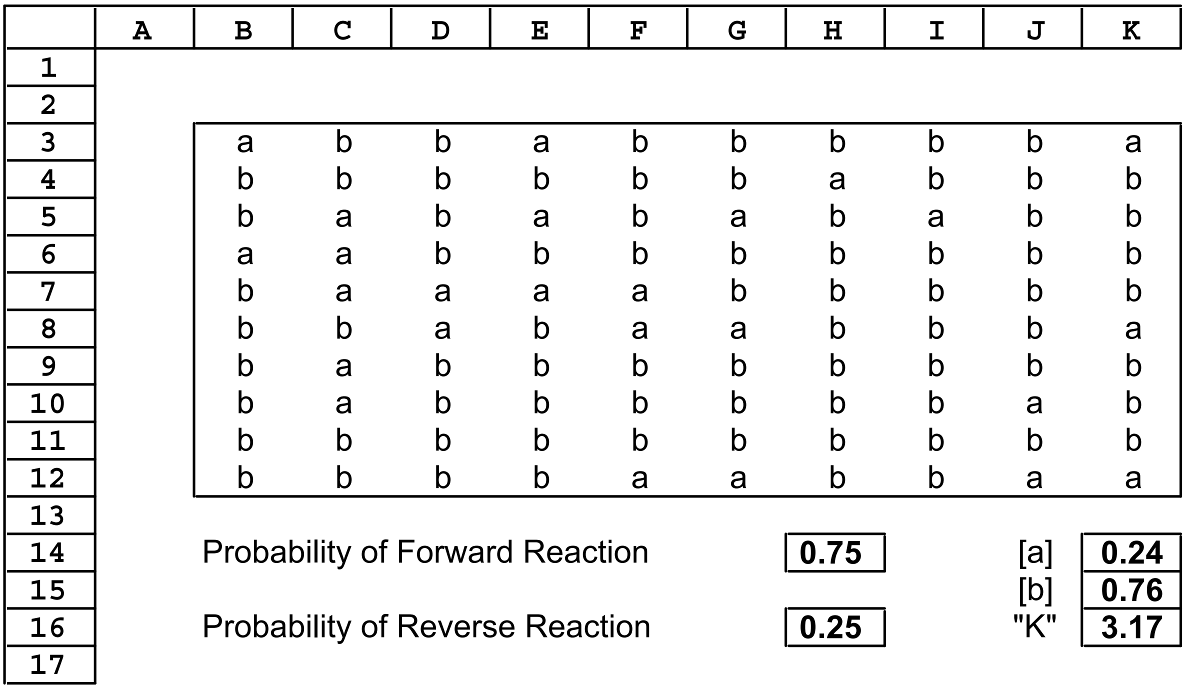


	A	B	C	D	E
1					
2					
3	**Initial Data**	[Acid]	Ka	Volume	[H+] estimate
4		**1.00**	**1.70E-05**	**10.00**	**1.00**
5		[Base]	Kb	Kw	Max Error
6		**1.00**	**1.80E-05**	**1.00E-14**	**1.00E-15**
7					
8	**Titration**	Add	**0.01**	mL of base	
9					
10	**Result**	Vol base added	Total Vol	[H+]	[OH-]
11		**10.04**	**20.04**	**6.89E-08**	**1.45E-07**
12					
13			**pH = 7.16**		
14					

Figure 3. A worksheet to calculate the pH of acid/base reactions

The dynamic and probabilistic nature of chemical equilibrium

A complementary approach to the same problem is to use a spreadsheet to model the dynamics of the movement of a chemical system towards equilibrium using a simple Monte-Carlo simulation of a system such as that between 'a' and 'b' shown in figure 4 (Brosnan 1992b).



	A	B	C	D	E	F	G	H	I	J	K
1											
2											
3		a	b	b	a	b	b	b	b	b	a
4		b	b	b	b	b	b	a	b	b	b
5		b	a	b	a	b	a	b	a	b	b
6		a	a	b	b	b	b	b	b	b	b
7		b	a	a	a	a	b	b	b	b	b
8		b	b	a	b	a	a	b	b	b	a
9		b	a	b	b	b	b	b	b	b	b
10		b	a	b	b	b	b	b	b	a	b
11		b	b	b	b	b	b	b	b	b	b
12		b	b	b	b	a	a	b	b	a	a
13											
14		Probability of Forward Reaction						**0.75**		[a]	**0.24**
15										[b]	**0.76**
16		Probability of Reverse Reaction						**0.25**		"K"	**3.17**
17											

Figure 4. A simple Monte Carlo model of chemical equilibrium

When this worksheet is used, a macro selects a cell at random, and uses the set probability to decide whether to ‘react’ the contents of the cell - ‘beeping’ whenever the contents of a cell reacts. It keeps a running total of the numbers of each reacting species present and uses this to calculate an equilibrium constant. This example illustrates a number of important points, not just the non-equivalence of equilibrium concentrations:-

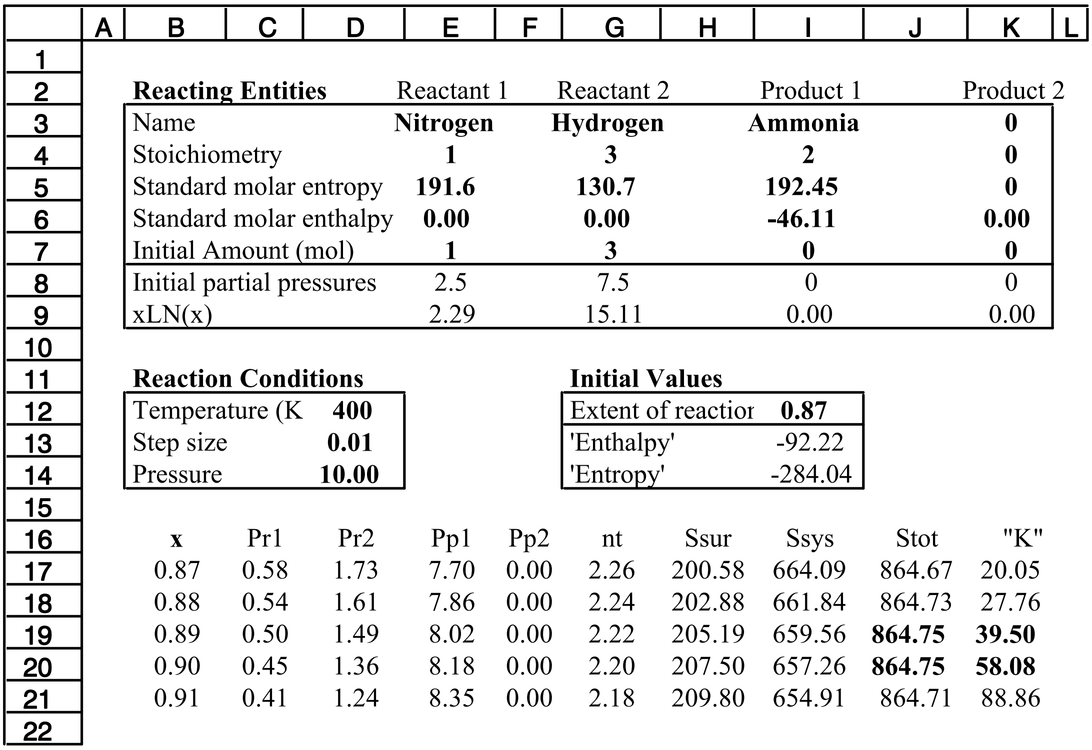
1. At equilibrium the concentration of each species (and hence the equilibrium constant) fluctuates only slightly but the two reactions are still proceeding - the beeping does not stop. The existence of this fluctuation is itself interesting, being a consequence of the non-deterministic nature of both the model and real chemical reactions. Boxes of different sizes can be used to see that as the size of the system increases the relative importance (although not the absolute size) of the fluctuations decreases. The amounts used in real reactions correspond to boxes about 10^13*10^13 so the effect of any fluctuation is usually undetectable!
2. The students can set the initial concentrations of each reactant and see that the equilibrium concentrations are independent of□these.
3. The students can also assign the probabilities of the forward and back reactions and see that although the **speed** of reaction (the frequency of the beeps) depends on their absolute values, the equilibrium concentrations (and hence the equilibrium constant) depend only on the **ratio** of their values. This can be used to explain the action of a catalyst - multiplying the probability of both reactions by a similar amount speeds up the reaction but as the ratio of the probabilities is still the same the equilibrium constant is unchanged.

The differing ways temperature and pressure/concentration affect equilibrium concentrations.

All the research evidence stresses that many students have great difficulty in predicting the way an equilibrium mixture will alter when the conditions change. One major reason for this has already been highlighted, i.e. the visualising of the system as being composed of two independent sides each of which can be separately varied. It may be important that some of the examples used in school text books to explain the differences between chemical and physical equilibrium reinforce the ‘two side’ view. A common example is to use a person walking up an escalator as an example of dynamic equilibrium. However the speed of either the person or the escalator may be changed without directly affecting that of the other whereas in a chemical system a change in any one component necessarily affects all the others.

Rules for deciding what happens when the temperature and/or pressure vary are usually learnt by rote without any real understanding of why they operate in the way that they do. As a result the rules are often misapplied or confused. For these reasons there is a pressing need to try and develop in pupils an understanding of the basis of the commonly used rules of thumb - such as Le Chatelier’s Principle. Such understanding requires an appreciation of the entropy concept and this can rapidly become very mathematical. Figure 5 (derived from Brosnan 1990b) show one approach to easing this problem. The model allows the calculation of the entropy change and ‘equilibrium constant’ in any homogenous reaction at any extent of reaction. In this model all the important variables - stoichiometry, standard enthalpy and entropy values, pressure/concentration, initial concentrations and temperature - can be set be the user, allowing their differing effect on both the equilibrium constant and the equilibrium composition to be seen. Using this approach the differing ways in which pressure and temperature affect equilibrium concentrations can easily be seen. In particular it can be observed that only the temperature has an effect on the equilibrium constant.

This final, exploratory, model seems far removed from the simplicity of the expressive ‘calculator replacement’ use of a spreadsheet discussed earlier and indeed its purpose is quite different. Rather than replacing boring or repetitive calculations its object is to remove mathematics from an area where its intricacy is often beyond the students (although of course the equations can be as hidden or open as the teacher desires). Instead of becoming trapped in mysterious equations, playing with the models like these can lead to fruitful discussions of why the effects obtained should occur, with attention focused on the shape and direction of the change rather than the precise numerical result. It is by providing this qualitative 'feel' that the computational tool is aiding the development of the students' chemical understanding.



Reacting Entities	Reactant 1	Reactant 2	Product 1	Product 2
Name	**Nitrogen**	**Hydrogen**	**Ammonia**	**0**
Stoichiometry	**1**	**3**	**2**	**0**
Standard molar entropy	**191.6**	**130.7**	**192.45**	**0**
Standard molar enthalpy	**0.00**	**0.00**	**-46.11**	**0.00**
Initial Amount (mol)	**1**	**3**	**0**	**0**
Initial partial pressures	2.5	7.5	0	0
xLN(x)	2.29	15.11	0.00	0.00

Reaction Conditions	
Temperature (K	**400**
Step size	**0.01**
Pressure	**10.00**

Initial Values	
Extent of reactior	**0.87**
'Enthalpy'	-92.22
'Entropy'	-284.04

x	Pr1	Pr2	Pp1	Pp2	nt	Ssur	Ssys	Stot	"K"
0.87	0.58	1.73	7.70	0.00	2.26	200.58	664.09	864.67	20.05
0.88	0.54	1.61	7.86	0.00	2.24	202.88	661.84	864.73	27.76
0.89	0.50	1.49	8.02	0.00	2.22	205.19	659.56	**864.75**	**39.50**
0.90	0.45	1.36	8.18	0.00	2.20	207.50	657.26	**864.75**	**58.08**
0.91	0.41	1.24	8.35	0.00	2.18	209.80	654.91	864.71	88.86

Figure 5. Worksheet to calculate entropy changes at different extents of reaction.

CONCLUSION

The examples briefly described above cover a range of conceptual, arithmetic and programming difficulties and are intended to illustrate some of the variety of ways spreadsheets can be used to address the variety of mathematical problems faced by students of science. The key point is that the computational tool is being used to allow students to see the quantitative consequences of differing qualitative conceptions. The apparently paradoxical conclusion of this is that a computational tool's most important attribute may be the help it gives in changing qualitative understandings.

REFERENCES

Beare R. (1992) 'Software tools in the science classroom' *Journal of Computer Assisted Learning*, Vol. 8, No. 4.

Bliss J., Ogborn J., Boohan R., Briggs J., Brosnan T., Brough D., Mellar H., Miller., Nash C., Rogers C., Sakondis B., (1992a) 'Reasoning Supported by Computational Tools', *Computers in Education* Vol. 18, No. 1-3, pp 1-9, reprinted in Kibby M. R., Hartley J. R. (Eds) (1992) *Computer Assisted Learning* Pergamon Press.

Bliss J., Ogborn J., Boohan R., Briggs J., Brosnan T., Brough D., Mellar H., Miller., Nash C., Rogers C., Sakondis B., (1992b) ‘’, (*Tools for Exploratory Learning: End of Award Report.* Summary Report and six Technical Reports). London: University of London.

Brosnan T. (1989) ‘Teaching Chemistry using Spreadsheets 1: Equilibrium Thermodynamics’, *School Science Review*, Vol 70, No 252.

Brosnan T. (1990a) ‘Calculating Entropy Changes at Different Extents of Reaction’, *Journal of Chemical Education*, Vol 67, No 2.

Brosnan T. (1990b) ‘Using Spreadsheets in the Teaching of Chemistry 2: More ideas and some limitations’, *School Science Review*, Vol 71, No 256.

Brosnan T. (1992a) ‘Spreadsheets - of swans and swimming’ *Education in Chemistry* Vol. 29, No. 1.

Brosnan T. (1992b) ‘A Probabilistic Model of Chemical Equilibrium’, *School Science Review*, Vol 74, No 266.

Castledine R. (1991) ‘Spreadsheets in Chemistry Lessons’, *School Science Review*, Vol 72, No 260.

Dreyfus A. and Feinstein B. (1991) ‘*The spreadsheet as a “language” to enhance graphing skills*’. Paper presented at the 16th ATEE Annual Conference, Amsterdam, September 1991.

Elliot C. (1988) ‘Spreadsheets in science teaching’, *School Science Review*, Vol 70, No 251.

Goodfellow T. (1990) ‘Spreadsheets: powerful tools in science education’, *School Science Review*, Vol 71, No 257.

Gorodetsky M. and Gussarsky E. (1986) ‘Misconceptualization of the Chemical Equilibrium Concept as Revealed by Different Evaluation Methods’, *European Journal of Science Education*, Vol 8, No 4.

Graham I. (1987) ‘The application of spreadsheets to data analysis in biology’, *Journal of Biological Education*, Vol. 21, No. 1

Hackling M. and Garnett P. (1985) ‘Misconceptions of Chemical Equilibrium’, *European Journal of Science Education* Vol 7, No 2.

Kemmis S., Atkin R. and Wright E. (1977) ‘*How do Students Learn? Working Papers on Computer-Assisted Learning*’, (Occasional Publications No. 5). Norwich: University of East Anglia.

Leharne S. and Metcalfe E. (1989) ‘The Joy of Spreadsheets’ *Education in Chemistry* Vol. 26, No. 5.

Maskill R. and Cachapuz A. (1989) ‘Learning about the Chemistry Topic of Equilibrium’, *International Journal of Science Education,* Vol. 11, No. 1.

Ogborn J. (1987) ‘Computational Modelling in Science’, in *Trends in Computer Assisted Education*, Lewis R. and Tagg E.D. (eds) Blackwell Scientific.

Schibeci R. (1989) ‘Computers in the Chemistry Classroom’, *Education in Chemistry*, Vol. 26, No 1.

Stevens J. (1991) ‘Chemical Equilibrium - a spreadsheet’, *School Science Review*, Vol 73, No 263.

Stokes B. (1984 et seq) ‘*Revised Nuffield ‘A’ Level Chemistry*’, Longman