A COMPUTER-BASED MATHEMATICS LABORATORY FOR UNDERGRADUATE CHEMISTRY STUDENTS: A PRELIMINARY EVALUATION REPORT

Phillip Kent,

Mathematics Department, Imperial College, London SW7; Ian Stevenson,

Mathematical Sciences, Institute of Education, London WCl.

This is a preliminary report from an evaluation of a first-year mathematics course for undergraduate chemists which is designed around a combination of motivatory lectures and assignments in a "mathematics laboratory", where students use the computer algebra package, Mathematica. A student questionnaire was administered and a half-dozen follow-up interviews were done. We report here on the findings from those, using summary data from the sample of 57 students, and a comparison of the interview data from two typical students (one with, and one without, A level mathematics).

Mathematics in the Chemistry course at Imperial College

The "mathematics laboratory" has been under development since 1994, and you can read about its earlier history in (Templer et aI, in press). We have been evaluating its latest version, which includes, for the first time this year, "chemical-mathematical" coursework assignments which require the students to think explicitly about how mathematics is used in chemistry to *model* chemical processes. The thinking behind this has been described by Ramsden & Templer (in press):

> We no longer see the relationship between the two subjects as strictly a matter of "learn the maths, then apply it to the science". We are trying to introduce mathematics as a natural, integral part of chemistry; *Mathematica's* power gives the students the opportunity to do this in an authentic, uncontrived way, with something of the flavour of real research.
>
> As one might expect students experience a mixture of emotions when presented with this sort of challenge. One of these is certainly shock. We have deliberately set out to stretch students, but not in a way that they would expect.
>
> Their anticipation is that they will learn the techniques and tricks which most perceive as being the proper realm of mathematical experience. Instead we present them with the sort of chemical problems found in research, and with the help of a powerful mathematical toolbox, ask them to investigate the chemistry using those tools.

That is not to say that they are not learning any mathematics, far from it. The problems are designed in such a way that they have to understand the mathematical processes that are being performed and the limitations that these may impart on their results.

In the evaluation, besides trying to assess pragmatically how well different elements of the course are working, we are trying to get a feel for how students are dealing with the triangle of relationships:

MATHEMATICAL KNOWLEDGE SCIENTIFIC KNOWLEDGE

COMPUTER MATHEMATICS SOFTWARE

Weare interested, among other things, in the nature and extent of the students' mathematical development, whilst working within a computational environment such as *Mathematica.* To that end, we present here some initial reflections on the questionnaire data, and interviews that we have conducted.

Backgrounds of the students

One can take it as read that all Imperial College chemistry students are highly qualified in terms of A level grades: 28-30 grade points is usual. What does matter, given the mathematical intensity of the first-year course, is the combination of subjects studied at A level. Out of the questionnaire sample of 57, 38 had single A level mathematics, 9 had double mathematics, and 10 no A level mathematics. Of those students who did not have A level mathematics, all 10 had Physics (at either an A or B grade), and 7 had Biology as their third A level; their GCSE results ranged from two starred A's to three B' s, and two students also had A-S Mathematics.

We were particularly interested in this non-A-Ievel group. They have the double challenge of using mathematics, which they are generally unfamiliar with, in the context of learning chemistry. The significance of having Physics A level is that some mathematics may be familiar from there. It is an open question as to whether students are able to either recognise their physics experience as "mathematics", or "transfer" their knowledge across subject boundaries.

A comparison of two students

To illustrate some of the issues associated with the non-A-Ievel group, we will compare two (male) students' responses to the experience of doing the assignment:

Student J. A levels: Chemistry, Biology, Physics; GCSE Maths. Has used graphical calculators a little in school, but computers not at all.

Student M. A levels: Chemistry, Physics, Maths, AS Further Maths (MEI modular courses).
Extensive use of graphical calculator, and some computer use (e.g. BASIC programming).

At the stage where we take up the story, the students had just completed a *Mathematica-based* assignment in which they had to fit curves, based on a quite complex sum-of-exponential-terms model, to a set of genuine experimental data.

The interview data concerns general mathematical background, general computing experience (both J and M have their own computers), overall experience with the mathematics course, and work on the chemical-mathematical assignment. We concentrate here on just three issues for purposes of comparison, which are relevant to the question of how J and M understood mathematics in a computational context related to chemistry: confidence and facility with qlathematics; intuitive knowledge; and learning.

Issue 1: Confidence and facility

J, the non-A-level student, suffers from a lack of confidence and facility in mathematics. But he reports that doing the assignment significantly boosted his confidence:

> I: What did you think when you were given [the assignment]?
>
> J: For quite a long time not knowing how to go about it. I started early planning to get it out of the way and ended up spending more time than most people doing it. It was quite straightforward at first, but as it became more complicated I seemed to stray off the path, where other people were finding more direct routes, I'd sort of wander about and find different methods ....It would have been more enjoyable with a bit more help on hand every so often, just to check, I spent a long time going down wrong paths, if I'd been steered more to the right direction I'd have had more fun doing it, done it much more quickly.
>
> I: Has having to try things out for yourself been a benefit, or a loss?
>
> J: It encouraged me not to give up too easily, which is what I tend to do when I see maths ... I didn't do maths, I can't do this-and don't really look at it, now I spend more time looking at it, think about what can I do.

In contrast, student M, with double A-level maths and a strong programming background, describes doing the assignment in very different language:

> I: How did you decide to go about doing the task?
>
> M: In the same [question] sheet there was an example, showing how to get data in and how to play with it, so I followed that to start with, drew a graph ... first I had to remove the background

count ["zero error"] which meant identifying which points were the background, finding the average of them and then subtracting that from all the data values ... then I had to turn the list of voltages, one-axis data ... the intervals between each reading were actually 467, so you had to thread together a second set of data, the values for the time.

Issue 2: Explicit and implicit knowledge, "intuition"

There is more commonality between the students on this issue:

I: Did [doing the assignment] in any way improve your understanding of the underlying chemistry? Did you make use of chemical understanding?

J: A bit of both I think ... the knowledge of what was happening in the reaction would have suggested to me, even if I hadn't seen the data, that it would have been exponential. Seeing the data and working with it helped to visualise better and understand what was going on in more detaiL .. I don't know which influenced which more.

Similarly, for M the process was helped by his own experience with chemistry and mathematics:

I: What was the process for fitting to the data?

M: Partly thinking about, this is a biological experiment, what is there a faint chance of it actually doing?

I: So you had in mind first of all the chemical processes?

M: Urn, chemical things don't tend to do curves to the power five, anything like that. I:

How did you know that?

M: Just sort of an intuition, I'd never come across something like this before.

I: But you had the sense that the reaction you were looking at had to have certain characteristics? M: Yes,

either it was going to be linear, or some sort of quadratic, or something to do with exponentials.

I: Where did that come from, that intuition?

M: Mostly previous experience with experiments, since I've been doing chemistry really .... The maths helps as well, you just generally get more of an idea.

Issue 3: "What do you think you've learnt?"

I: Having done the assignment, what have been the gains for you, in terms of understanding the chemistry or the mathematics, if there were any?

J: Certainly I've learnt to use the program much better, the different commands, the shortcuts, so the next project should be quicker. ... " I don't think I've learnt really any chemistry, I've learnt more about this particular reaction I suppose .... The maths has improved in this particular area, the understanding of the shapes of the equations, which is one of the things that I lack, [it gave] lots of practice in seeing what the graph would look like without having to plot it, that's helped.

1's response here is typical of most of the interview group, in saying that he doesn't feel that he's learnt any mathematics or chemistry except "in this particular area". This seems to us a key point for investigating our triangle of relationships: that understanding. the relationship between knowledge domains is precisely about establishing connections in a sequence of "particular areas". M seems to express a sense of this, with his talk of "experience":

I: What do you feel you've learnt using Mathematica, after all of this?

M: You wouldn't be able to do this kind of analysis on a real data set without Mathematica, as an exercise you'd be restricted to a simple experiment with 10 or 20 data points, do things by hand.

I: In terms of mathematics, did you learn anything new?

M: Not so much learnt, you get more experience, a better feel about how to make things fit, it'll be useful to use Mathematica now to do this kind of fitting, which I couldn't have done before.

Conclusions

At a superficial level it seems obvious that not having a background in formal mathematics, such as that given at A-level, made a difference to students' understanding of the assignment. Students without such a background may be forced to develop the capacities of perseverance, reflection, and self-guided instruction, focussed on a specific problem, that their more mathematically knowledgeable fellows may not be called on to use. In fact, through this harder work, our Chemistry colleagues have reported over the years that the non-A-level students often get ahead of the majority of their fellows, in developing good mathematical ways of working in the scientific context, *because* they are not able to coast along on the back of previous mathematical experience. These evaluation findings have important curriculum implications, in that these issues are of central concern to our colleagues in the Chemistry Department, given their aim of producing graduates who

S

are mathematically-equipped to begin doing chemical research-which, in fact, is the first destination of about 50% of the graduates.

The task that the students were given was principally about curve-fitting, and made relatively few demands on their chemical knowledge. However, as the Issue 3 extracts suggest, the nature and extent of the students' mathematical development is closely tied to the specificities of the context in which they meet the mathematics. This has important implications for mathematics education, since it raises issues in an "academic" setting that compare with our colleagues' work at the Institute of Education on mathematics in "vocational" situations (such as banking and nursing: Pozzi et aI, in press).

We have now completed an extended "maths lab" observation of three pairs of students as they worked on another chemical-mathematical assignment (a simple Newtonian mechanical simulation of ionic interactions); plus, all these students were interviewed again. In analysing the full data set, we will again be looking for data about the triangle of relationships (mathematical knowledgechemical knowledge-mathematics software), and the interaction of explicit and implicit knowledge, and the use of, and development of, "intuition". This analysis, we hope, will provide the basis for more substantial evaluation studies in subsequent years.

References

Pozzi, S., Noss, R. and Hoyles, C. (in press). "Tools in practice, mathematics in use". To appear in *Educational Studies in Mathematics.*

Ramsden, P. and Templer, R. (in press). "A new approach to mathematical training for chemists". To appear in *Education in Chemistry.*

Templer, R., Klug, D., Gould, I., Kent, P., Ramsden, P. and James, M. (in press). "Mathematics laboratories for science undergraduates". To appear in *Rethinking the Mathematics Curriculum,* edited by C. Hoyles, C. Morgan and G. Woodhouse. London: Falmer Press.