Computer Simulations: Creating Opportunities for Science Writing

COMMUNICATION

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A computer simulation allowed second-year students to carry out a simulated investigation of factors affecting the rate of an enzyme-catalysed reaction and to write a report on this in the style of sections of a scientific paper.
The simulated investigation allowed students to generate data of sufficient quantity and quality to justify the requirement that their report should be in the style of a real paper.
Examination of the student reports reveals a number of weaknesses in the students' understanding of what makes for good professional writing.
We conclude that students need careful guidance if they are to get the maximum benefit from this opportunity.

Introduction

Most laboratory work carried out by chemistry students, at least during the first year of a degree course, consists of what Meester and Maskill[1] refer to as 'controlled' experiments which involve following recipes. There are many advantages in this approach. It allows the students to concentrate on laboratory technique[2], it maximises safety, and it helps to maximise not only the number of procedures which a student experiences, but also the number from which they obtain useful and interpretable results. This last point is crucial to the development of the student's confidence in a range of procedures.

The recipe approach has the disadvantage that it provides no opportunity for students to design investigations. It has been suggested that computer simulations can provide one way of filling this gap[3,4]. Of a number of computer simulations which we have written[4,5], enzymeLAB was specifically designed to enable students to design a simulated investigation of the characteristics of a newly isolated enzyme. This simulation allows students to study the effect of the key variables of pH, enzyme concentration, substrate concentration and inhibitor concentration on the rate of an enzyme-catalysed reaction. The speed with which data can be simulated by the computer means that an investigation which would take an experienced researcher many days to complete can be completed within two or three hours. The simulated experimental error is at a level which a competent experimentalist would expect.

A student report which included this large amount of raw data would create an unacceptable marking load on a conscientious tutor. We therefore made a virtue out of necessity by requiring students to summarise their data in the form of sections of a scientific paper.This preliminary account of our assessment of the outcome of the writing exercise leads us to conclude that the potential benefits to the students are considerable.We also suggest ways in which others wishing to adopt this or a similar exercise for their own students could avoid some of the shortcomings we identified.

The computer simulation

The simulation used for this work deals with the kinetics of an enzyme-catalysed reaction. The original version was created by Garratt and Groves[6], for use by second year students studying biochemistry. It has since been updated to a Windows version[7]. The program, known as enzymeLAB, provides each new user with different simulated but realistic characteristics of an enzyme which obeys Michaelis Menten kinetics, is sensitive to pH, and is inhibited by azide (widely used to prevent bacterial growth on columns). We are preparing a detailed paper describing our evaluation of this simulation as a tool for teaching experimental design and this will include details of the simulation package and the way we use it.

The program provides relevant information which a real experimenter would acquire during the purification of a new enzyme. This information includes:

- the range of reaction rates which can be satisfactorily determined by the assay system;
- the fact that the enzyme is inhibited by azide;
- the rate of reaction observed at pH 7 using 1 mg of enzyme and substrate at 20 mmol dm^{-3}.

The aims of the investigation are described to the student as follows:

'The questions you are likely to be asking yourself are:

i) what is the optimum pH for the enzyme?
ii) what effect does pH have on K_M and V_{max}?
iii) does azide inhibit substrate binding, the catalytic process, or both?
iv) what is the dissociation constant for the enzyme-azide complex?
v) how precise are your measurements of rates?

There is no single correct procedure to adopt to answer these questions and you must work out your own preferred strategy.'

The student task is focused by the requirement for a report which includes a summary, a results section, and a discussion section. Additional guidance given to the students is shown in Figure 1. No further formal guidance on report writing was provided specifically in conjunction with this exercise.

Figure 1: Instructions on the preparation of the enzymeLAB report.

You should present your results in the style of fragments of a paper from a scientific journal. If you are not sure what this means, look at a few papers in a journal like *Biochemical Journal, Journal of Biological Chemistry*, or *Biochimica Biophysica Acta.*

You should write the following sections:

Summary

This must consist of numbered statements giving your conclusions.

The first of these should be:

1. A new ... ase (ref. no ...), isolated from B. *yorkii* has been characterised.

Results

You may present your data in three figures or three tables or two of one and one of the other. No more than a total of three will be accepted. You may use up to three different symbols on any figure (e.g.●, ■, ◆) to represent different sets of data. All figures and tables must be numbered, have a short informative title and may have a brief legend.

You should write a brief description of your results which conveys useful information without the need to refer to the figures and tables.

Discussion

Write a concise paragraph about the effect of pH on the enzyme and another about the inhibition of the enzyme by azide. Each paragraph may include results of calculations and any interpretations of your data.

With the task defined, and after a formal class designed to help students to develop an effective strategy for carrying out their investigation, the students are allowed access to the computer.The software is available on networked computers in three classrooms across the campus, two of which are open 24 hours a day. Students are expected to spend about three hours working at the terminal. They have a free hand to choose conditions under which measurements of the rate of reaction are to be obtained. As already indicated, there are four variables: the pH of the assay system, the concentration of substrate (S) and inhibitor (I) in the assay system, and the volume of enzyme solution (of known concentration) to add to the assay system.

Having selected a set of variables, the student clicks the 'run experiment' button, and the computer calculates a value for the rate of reaction under these conditions. Before displaying the value, the computer adds a random error with a standard deviation of 5% of the calculated value. This ensures that displayed values of the rate (v) have a realistic experimental error.

Data can easily be transported to a spreadsheet of the student's choice, so that it can be manipulated and presented in graphical or tabular form.

The structure of the student report, given in Figure 1, is justified as follows:

An *Abstract* of numbered points is specified in order to encourage students to focus clearly on what they regard as the main conclusions of their study; only a few professional journals insist on this style of abstract, but in our view it is an appropriate one for this exercise.

Neither an '*Introduction*' nor a '*Methods*' section are required because this exercise does not provide a context in which students can realistically practice this important skill.

The *Results* section limits the number of graphs and tables to a maximum of three because the important information can be presented clearly and concisely in three graphs.

The *Discussion* section is intended to encourage the students to interpret their data constructively.

The student reports

This analysis is based on our evaluation of the 16 reports handed in for assessment by a cohort of biochemistry students who carried out this exercise in the summer term of their second year.

Student abstract

On the whole the students showed poor judgement both in selecting and expressing the information which they included in their abstracts.Two points which we would expect to find in an abstract are the fact that the enzyme obeys Michaelis Menten kinetics, and a value for the specific activity of the enzyme. Only two students mentioned the former, and one of these and one other gave a value for the specific activity. Six other students quoted values for V_{max}, and this could be regarded as a different word meaning specific activity. However, only three of these students specified that the value quoted had been obtained at the optimum pH, and none gave appropriate units.

Seven students made a clear statement about the effect of pH on K_M and V_{max}, and thirteen on the type of inhibition observed.

Many (but not all) students showed a lack of appreciation of appropriate language. Examples of specific sentences given are:

'The inhibitor (azide) does not work by binding to the substrate'.

cf 'Azide is a competitive inhibitor of this enzyme'.

'K_M and V_{max} were measured'. (No values were given.)

cf 'The enzyme has an optimum activity at pH 7 where K_M = 1.14 mM and V_{max} = 2.59 μmol min^{-1}'. (Note that this sentence is faulty in that it is meaningless to give a value for v_{max} without specifying the amount of enzyme used.)

Student results

One student offered as a table a list of all the data obtained. One would expect this in a laboratory notebook, but not in a paper.

Seven students chose to show the effect of pH on K_M and V_{max} as a table. Five submitted a graph of substrate concentration *vs* rate of reaction at three well chosen values of pH (Figure 2 is an example).Three submitted an equivalent graph, but first transformed the data to a linear form (1/S, vs 1/v, v vs v/S, etc.) (Figure 3 is an example).The effect of the inhibitor was shown as a graph by all students; ten submitted

Figure 2: Plot to illustrate the effect of pH on initial rate of reaction

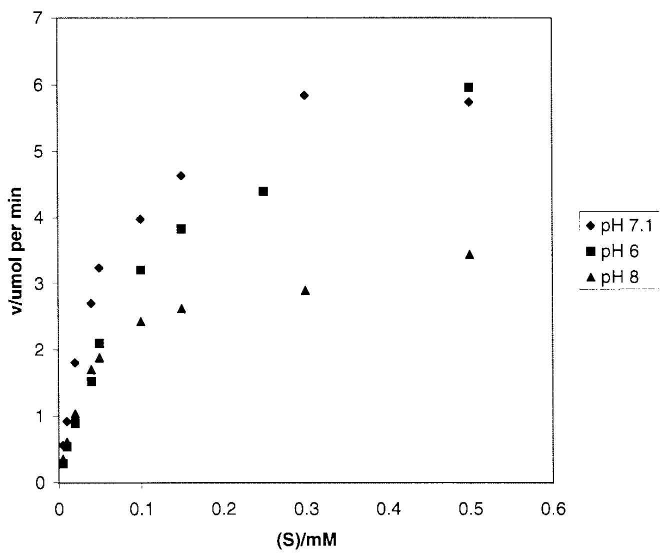
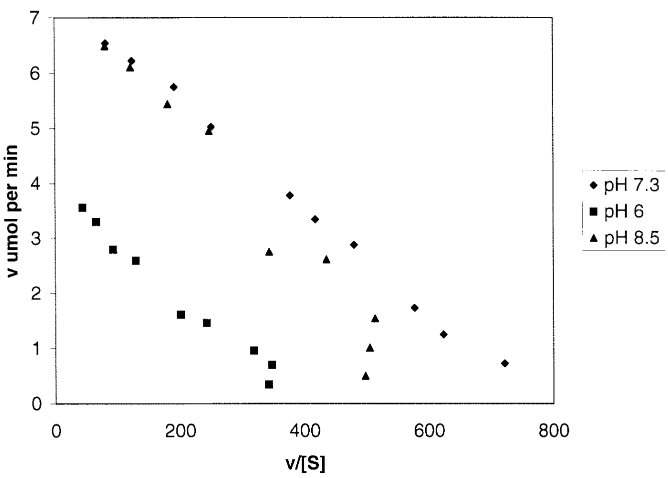


Figure 3: Graph to show the effect of pH on Vmax and Km values



plots of untransformed data and six showed data transformed to give a linear plot. In our view the linear plot is, in both cases, the preferred way of presenting results because changes in slope and intercept are qualitatively immediately apparent to the eye and also because the graphs give a visual impression of the quality of the data from which the parameters K_M and V_{max} are determined. Tables are acceptable even though the implications of the tabulated values are less easy to comprehend at a glance; tables are probably the preferred way of presenting data if students wish to present more than three sets. A graph of the untransformed data is the worst option because it is almost impossible to compare quantitatively by eye the two key parameters to be determined from hyperbolic curves (see Figure 2) – namely the maximum rate and the concentrations giving the half-maximal rate.

Other criticisms could be made of the way lines were drawn (or sometimes not drawn) on graphs to indicate a relationship between *x* and *y*, and of the quality of legends. We make no comment on these aspects of report writing, since they probably do not differ from observations of reports on recipe labs.

Student discussion

This section showed the students' lack of experience with presentation and interpretation of data. It offered the opportunity to give a fairly detailed interpretation of the effect of pH on enzyme activity. The students were specifically asked to distinguish between an effect on K_M and V_{max}, and this can be interpreted as demonstrating an effect on substrate binding or on bond rearrangement (catalysis). Some tutors might hope that an estimate of the pK of the loss of activity might lead to a discussion of possible groups in the active site which might have such a pK. No students went into all these details.

The data obtained from using the inhibitor can be used to calculate a value for the dissociation constant for the enzyme inhibitor complete. Only three students took this step.

Student style

We noted many examples of unprofessional style and of the inclusion of inappropriate information. These illustrate the students' lack of experience with presentation of scientific data. Some examples are included in the section on Student Abstract. An example of a sentence which is both stylistically unprofessional and which was inappropriately placed in a Results section is

'In all the experiments it was decided that a volume of 10 μl of enzyme solution would produce sensible results'.

In many reports the working of unprofessional use of titles for figures needed improvement. For example, many students submitted titles such as those given in Figures 2 and 3, or

Fig 1: Graph to show the effect of pH on enzyme activity.

or

Fig 2: Plot to illustrate the effect of azide inhibitor on initial rate of reaction

cf Fig 1: pH profile of enzyme reference no. PR/86–340-100

Discussion

The characteristics of reports which we illustrated in the previous section have led us to three main conclusions. First, the experience of writing reports on laboratory work based on recipes is of only limited value in learning how to interpret and present data to a scientific reader. Second, computer simulations can provide data of a quantity and quality to create realistic exercises in writing a scientific paper. Third, students need careful guidance and feed-back if they are to take maximum advantage of the opportunity. Strictly speaking, our conclusions apply only to the small group of students in this study, but we believe they are more general.

We suggest two possible difficulties which students may have faced. First, few, if any of them, had significant experience of reading primary literature and it seems unlikely that many took up the suggestion (Figure 1) that they look at some journals. Second, they are heavily conditioned by their experience of writing reports on recipe-based laboratory work. The style and language they used suggested that most were concerned to describe what was important to them while they were collecting data. Insofar as they thought of their reader, they seemed to have in mind a tutor who was aware of the expected outcome of the investigation and not an independent scientist who was fresh to the work. In a sense the students were required to engage in a role-play, but the role was too unfamiliar for them to play effectively, and they were insufficiently engaged in the task they had been set.

Discussions with colleagues confirm our impression that many students have serious difficulties when they come to write reports or dissertations based on project work. Yet the writing of such reports is a key skill for professional scientists and is a useful model for many other forms of writing. It is therefore useful to provide more opportunities to practice this writing style than is given by a final year project report or literature review. As we show here, computer simulations of investigations can provide data of a quantity and quality to create realistic model data for presentation in the style of a professional paper. However, students will only obtain maximum advantage if they engage seriously in the role-play which is required. This requires that they understand both what the role is and why they will benefit from playing it. Furthermore, they need time for critical reflection on constructive feedback on their report.

Our analysis of this exercise will help us, and we hope others, to improve the quality of the guidance and feedback for students so that they can take better advantage of the experience of writing a report based on a simulated investigation.

EnzymeLAB and other computer-based simulations are available via the Internet[5].

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