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A Self-Directed Workshop for Developing Advanced Data Processing and Analysis Skills in Chemistry Using Microsoft Excel

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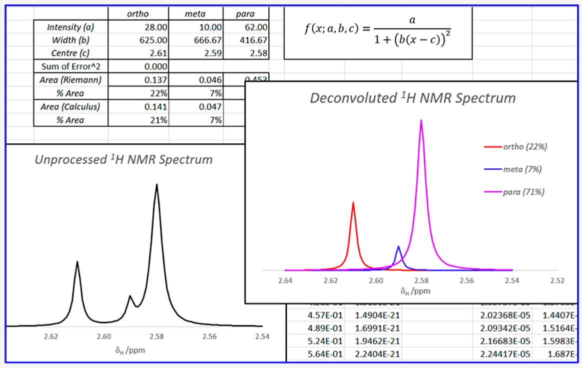
ABSTRACT: Data-handling, processing, and analysis skills are an integral part of a chemist's skill set and, more generally, are highly sought by employers. We report a self-directed workshop to develop and advance these key skills using the popular spreadsheet program Microsoft Excel. Making use of its accessible user interface, various contextualized problems relevant to chemistry are introduced, linking theory to practical applications and providing insight and understanding of processes that operate behind-the-scenes in many specialized data processing packages. The workshop has been delivered as a remote exercise for both our first and second year undergraduate cohorts (216 students completed). Students reported a positive impact from the workshop, including the development of a wide range of important skills, the utility for future practical work, and the effectiveness of communication remotely to address their issues.



KEYWORDS: *Second-Year Undergraduate, Upper-Division Undergraduate, Analytical Chemistry, Organic Chemistry, Physical Chemistry, Computer-Based Learning, Laboratory Computing/Interfacing, Mathematics/Symbolic Mathematics*

■ COVID-19 PANDEMIC CONSIDERATIONS

The worldwide COVID-19 pandemic is significantly changing the landscape for university teaching, including the delivery of practical teaching laboratories. This led us to initiate various projects, including developing the #DryLabs20 international network for practical laboratory considerations,[1] coding tasks,[2] and the use of simulations,[3] also reported in this special issue of the *Journal of Chemical Education*: "Insights Gained While Teaching Chemistry in the Time of COVID-19".

Recognizing the potential of resources that could be delivered online, we describe herein a self-directed workshop primarily focused on developing data-handling, processing, and analysis skills. The choice of Microsoft Excel software, available to all students undertaking the workshop and previously introduced through introductory workshops on-site, was paramount to ensure the practical remained accessible despite being delivered and assessed entirely online. Given the challenges of delivering material internationally, assistance was provided primarily through email. Chat and video calls were also scheduled for more extensive assistance using Microsoft Teams, including the use of screen-sharing for guidance through particular tasks.

■ INTRODUCTION

An integral part of studying any science is the handling, processing, and analysis of experimental data. The importance of data processing and statistical analyses is recognized as these are essential parts of approved and accredited degree programs, including both the American Chemical Society (ACS) and Royal Society of Chemistry (RSC).[4] Data processing skills are widely introduced as part of a broader practical program, alongside "hands-on" work in both synthetic and analytical skills.

It is widely recognized that the practical teaching laboratory is "a complex learning environment",[5] where a myriad of skills are introduced, including safe working practices, manual dexterity and practical technique, and the operation of various analytical instrumentation. Even at this stage, a significant cognitive demand is placed on the student, from assessment of raw data quality, to data processing and analysis, and finally to interpretation of results. The workshop targeted strengthening the skills that accompany practical experimental work and are essential as part of students' scientific development, namely, problem-solving, data handling, and analysis.

■ WHY MICROSOFT EXCEL?

There is a variety of commercial programs available to handle and process data. Microsoft Excel is generally one of the most familiar data-handling programs available to most university-

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level students.[6] Its graphical user interface for data input and management, easily implementable calculations, and readily customizable graphics and reporting capabilities[7] make it accessible to students. By contrast, other specialist programs possess their own unique interfaces, can be less accessible (requiring institutional subscriptions or licenses), and may require a higher level of coding skills. Other programs may perform operations or analyses whose workings are invisible to the user (so-called "click-and-run" software), the opacity of which has been the subject of concern.[8]The versatility of Microsoft Excel offers an additional advantage for students' career prospects. Nationwide surveys of the recent job markets in the US and the UK identified "productivity software", including Microsoft Excel, as one of the most important skills sought by employers; in the UK, Microsoft Excel was ranked as the most requested "productivity software" skill.[9]

First year students undertaking the chemistry degree at the University of Oxford are introduced to Microsoft Excel and data analysis in a practical undertaken near the start of the first term ("Skills Practical S102: Data and Error Analysis"). This practical introduces students to data processing using various common operations within Microsoft Excel (including simple calculations using formulas and graphical presentation of data). The tasks culminate in the construction of a spreadsheet to perform linear regression for data acquired experimentally (calorimetric data from the dissolution of ammonium chloride in water), considering residuals, standard error, statistical confidence, and uncertainty in the gradient and intercept. These and related data processing tasks using Microsoft Excel have been reported in this *Journal*.[10] The workshop reported here was designed to follow from the practical S102, with students encouraged to refer to both manuals as appropriate.

By implementing the already familiar user interface of Microsoft Excel, we were able to introduce a variety of challenging chemistry-relevant scenarios covering data processing, introducing new concepts and operations, and also developing students' ideas and problem-solving skills.

■ MOTIVATION FOR FURTHER DEVELOPMENT

The practical component of our chemistry degree program features a two-part strategy using a "spiral" curriculum design, where key scientific skills are introduced in the first part of each year and revisited throughout the remainder of the year. Although data and error analysis is a recurrent theme in practicals throughout the course, performing these analyses was a particular weakness, both in terms of student confidence and from an assessment perspective. After completing one year of the course, only 61% of previous first year students (n = 50) indicated they were confident with performing data and error analysis, registering as one of the lowest-rated confidences for any skill in the first year practical course. This lack of competence/confidence in data manipulation can result in an extensive time being needed to complete postlaboratory tasks. As noted by DeKorver and Towns,[11] students often see undergraduate practicals as an exercise to be completed as quickly as possible. Thus, significant analysis time may adversely impact the perceived value of these tasks, the quality of the analysis, and the students' overall enjoyment of laboratory practice. Investment in strengthening these skills could therefore have a positive effect on both on students' engagement and overall scientific development.

In creating a workshop to develop further students' skills in processing and analyzing data, we chose to introduce new and interesting facets of analysis capabilities within Microsoft Excel, with a particular emphasis on answering problems relevant to chemistry. This workshop sought to tie in with a number of key objectives in our practical program:

(i) experience in processing imperfect data;
(ii) contextualization of data processing to real-life applications;
(iii) appreciation of how and why particular data are collected;
(iv) improvement of understanding of "back-end" operations that relate to processing data in specialist computer programs;
(v) development of students' organizational skills dealing with large data sets, and coding skills.

Aligning with our overall practical course strategy, a key pedagogical objective of the workshop was for students to gain an appreciation of the background analytical processes performed by software, often considered so-called "black-boxes". As noted by Taber,[12] "science is based on a dialectic between theory and empirical observation, [...] whereas the application of science just to achieve practical ends is something else—technology." By better informing our students of underlying principles, we provide means for the student to develop strategies to assess and interpret data, ultimately understanding how to solve potential problems that may arise.

■ STRUCTURE AND CONTENT

As mentioned above, this workshop builds upon concepts from our introductory course in Microsoft Excel. The focus of this further workshop relates to processing of information related to chemistry, generally performed by more tailored software programs, including the following:

- numerical integration under a curve,
- use of algorithms for optimization of parameters,
- nonlinear curve-fitting,
- deconvolution of overlapping signals using different model functions.

Students also gain experience in many other aspects of data manipulation, including mathematical/trigonometric, and logical and statistical functions. This workshop complements various reported works by Cooper on the use of Riemann summation in Microsoft Excel related to black-body radiation,[13] and Magalhães on applications of the Newton−Raphson algorithm.[14] The approach taken here joins together concepts of numerical integration, algorithms, and curve-fitting, culminating in determination of the relative proportions of species from overlapping signals in an NMR spectrum.

A major addition to the workshop is the use of the Solver add-in, a subprogram algorithm that significantly extends the capabilities of Microsoft Excel to solving problems. The Solver add-in enables determination of optimal parameters for multivariable problems (up to 200 parameters), including to find optimal parameters to fit functions. Nonlinear relationships are encountered across many scientific disciplines, including environmental science,[15] engineering and physics,[16] and Michaelis−Menten enzyme kinetics in biochemistry.[17] Examples of applications of nonlinear functions in chemistry relate to spectral simulation/deconvolution and chromatography.[18] The modeling of functions can then be extended to deconvolution of overlapping signals, scenarios widely encountered within spectroscopy (including UV−vis, infrared (IR), NMR spectroscopies), and chromatography (gas chromatography and HPLC). Separation (deconvolution) and identification of the individual components in these spectra poses a challenge, particularly to the uninitiated, particularly owing to the mixture of functions required to model accurately each signal type. UV−vis and NMR spectra can be modeled solely as Gaussian and Lorentzian functions, respectively, making them an ideal choice for the introduction to the technique aimed in this practical.[19] The method of curve deconvolution using Solver has been reported by Muelleman and Glaser in this *Journal*,[18a] with an emphasis on using Microsoft Excel's built-in normal distribution function and Solver for simulating complex IR and UV−vis spectra from academic research. This task was considered too complex for an introduction to the concepts of signal deconvolution, which we wanted to illustrate using simpler systems; additionally, we wished to reinforce students in the construction of formulas (including syntax) applicable to any model function. There are various algorithms within the Solver package to perform such parameter optimizations, with the generalized reduced gradient (GRG) algorithm being applied in this instance.[20] Using either minimization of the sum of the squared error (SSE) or maximization of the R^2 correlation index statistical parameter, the Solver algorithm optimizes the parameters of the model function to achieve best fit with the experimental data.

The process is contextualized by the use of data to answer scientific questions, including practical operational and synthetic considerations (see below). These questions were introduced to provide opportunities for students to construct links between data collection and analysis/interpretation, which is a key problem-solving skill applicable throughout their future scientific development.

Given the online delivery of this practical, the workshop was designed to be self-guided, using a Vygotsky scaffolding-style approach (Table 1).[21]

Students would work sequentially through the exercises, guided by the instruction manual. Upon completion of each task, the student's knowledge and understanding would be expanded, enabling them to complete subsequent tasks. The initial tasks would introduce new applications of Microsoft Excel in performing repetitive tasks, and to utilize the skills introduced from the earlier introduction to Microsoft Excel; students were expected to design the formulas to be applied, rather than being provided with specific instructive guidance. For the remainder of the tasks, students would then utilize the skills developed and used in previous tasks to complete the later questions. This removal of scaffolding was devised to develop students' study and problem-solving skills. Provision of support, primarily via email, also provided an unintentional opportunity for development of students' written communication skills, through the articulation of queries or issues encountered.

The first task (task 1) is a basic introduction to constructing formulas, recapping simple operations that are structured around determining roots of quadratic equations using the familiar quadratic formula. It also introduces the use of spreadsheets for variation of parameters, namely, the coefficients of x^2, x^1, and x^0. The next task (task 2) extends the concept of solving equations to the use of iterative numerical analysis, namely, determination of real roots of a (differentiable) polynomial function using the Newton−Raphson algorithm. This reinforces the use of general parameters, introduces students to the use of algorithms, and, crucially, demonstrates the need for good initial root approximations to enable rapid convergence. Task 3 introduces the concept of numerical integration using Riemann summation, namely, application of

Table 1. Skills, Aims, and Scaffolding of Tasks Covered

Task	Description	Skills Covered	Aim	Scaffolding
1	Solution of quadratic equations	Syntax, simple operations (indices, multiplication, multiple cells)	Recap basic use of Microsoft Excel	High
2	Determination of roots to polynomial function using the Newton−Raphson algorithm	Algorithms, initial guesses, convergence of outcomes	Introduce algorithms, encourage students to investigate effects of variation of initial guesses	High
3	Determination of area under a curve by Riemann summation (the "trapezoidal (trapezium) rule")	Data layout, setting up a cumulative counter, graphing function and integral	Introduce integration of peaks	High
4	Linearizable kinetics analysis	Recap of linear regression, linearization, statistical tests	Recap linear regression, identify that functions can be linearized	High
5	Reaction conversion	Nonlinear curve-fitting, confidence intervals	Nonlinear curve-fitting, statistical analysis of nonlinear functions (confidence intervals), introduction to using data to make predictions, evaluation of the model, introduction to Solver algorithm	Medium
6	Spectral deconvolution	Modeling and deconvolution of UV−vis spectra, judicious choice of initial parameter values	Application of the above techniques, analysis of the determined functions and relation to Beer−Lambert law	Low
7	Spectral deconvolution	Modeling and deconvolution of NMR spectra, judicious choice of initial parameter values	Application of above techniques, evaluation of model fit, relation to chemical theory	Low

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the trapezoidal (trapezium) rule (Figure 1). This concept is revisited in the final task (task 7).

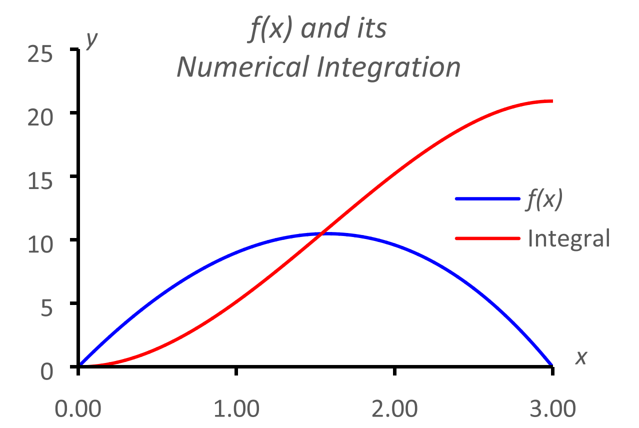

Figure 1. Illustrative example of the graphical output for the Riemann summation task.

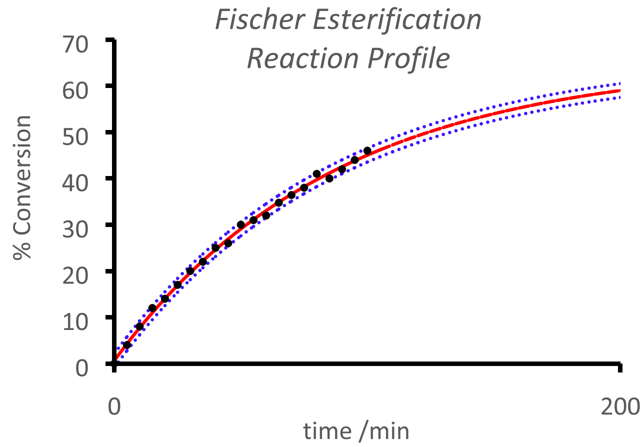

Figure 2. Illustrative submission for the reaction kinetics data analysis task (a Fischer esterification), with nonlinear fit, confidence interval, and forecasting of future reaction progression.

The final two tasks (tasks 6 and 7) required students to draw upon multiple concepts introduced earlier, with the ultimate objective of analyzing spectral data via deconvolution of overlapping signals. In order to reach this end goal, tasks 4 and 5 set out to contextualize how curve-fitting models operate. Task 4 refreshes students' understanding and application of linear regression, where the linearization of a nonlinear function (in this case, the analysis of exponential radionuclide decay) is highlighted and used to establish the half-life of fluorine-18.

In tasks 5−7, students are tasked to determine parameter values for model functions that provide reasonable approximations of the data. These approximations serve as the basis for the Solver algorithm to optimize fitting of the curve. The less scaffolded instructions for how to approach these problems formed a major part in the constructivist pedagogy, with the aim of developing a more systematic, methodical approach, rather than trial and error.[22] This hypothesis−evaluation−optimization process shares similarities to the problem-solving processes involved in experimental design, for example, determination of suitable solution concentration ranges for spectrophotometric analysis, where the judicious choice of parameters (e.g., concentration, wavelength range, and solvent) is important. In order to build up to signal deconvolution, nonlinear curve-fitting was introduced first, through modeling of a hypothetical reaction rate profile that cannot be linearized, namely, the Fischer esterification of benzoic acid with methanol (task 5, Figure 2). Questions were posed to the students to illustrate the important practical considerations when carrying out such a reaction, e.g., forecasting the conversion at particular time points, predicting the theoretical maximum conversion, and deciding upon a sufficient "end point" to the reaction.

The concepts of fitting such functions with model parameters, akin to linear regression, were introduced using both the sum of the squared error (SSE) and R^2 correlation index as indicators of the goodness-of-fit. The concept of confidence interval in the model was presented according to the method of Brown, with parameters optimized using the Solver add-in.[23,24]

The final two tasks (tasks 6 and 7) progressed the use of nonlinear curve-fitting to scenarios where multiple functions must be simulated. Introducing Gaussian and Lorentzian functions, for the signals in UV−vis and NMR spectroscopy, respectively, the deconvolution of overlapping signals is required for determination of the proportions of the species in a mixture. For the UV−vis spectral deconvolution in task 6, determination of the relative concentrations is required, using the Beer−Lambert law relationship of absorbance intensity to concentration. Task 7 involves determining the proportions of a three-component system, namely, from the ^1H NMR spectrum of a mixture of regioisomers obtained from Friedel−Crafts acetylation of chlorobenzene (Figure 3). This final task requires the student to use multiple skills from the previous tasks, including determination of the parameters for each function and integration of the model functions using both Riemann summation (introduced in task 3) and calculus to obtain the relative proportions for each isomer. Students are invited to evaluate and compare the results and validity of the two integration methodologies, and consider experimental changes to improve peak separation.

■ DELIVERY AND EVALUATION

This workshop was introduced recently (April−June 2020) as a self-directed practical for first and second year students, and students were encouraged to contact the teaching laboratory staff by email with any queries or problems. To date, this optional practical has been completed by over 68% (n = 216) of the total cohort. Given our focus on skills development, we surveyed students following completion of the workshop (n = 48 for first year, n = 40 for second year) to examine

- which skills they identified as being developed,
- their assessment of the impact that the workshop had on developing of their identified skills.

Skills Identification

A close-text analysis of the responses (n = 222 identified skills) to the question "What skills do you think this workshop aims to develop? (List all that you feel are relevant)" indicated students were aware that the workshop served to develop a variety of skills (see Figure 4). Of all the students, 75% (n = 66) identified two or more skills being developed. Both year groups identified general proficiency with Microsoft Excel as the primary skill of the workshop (27% of all responses), with data analysis (14%), function modeling/curve-fitting (9%), and the use of algorithms (in many instances, specifically identifying the Solver add-in) (9%) being listed most often. Additional identified data-handling skills related to the layout of information/handling

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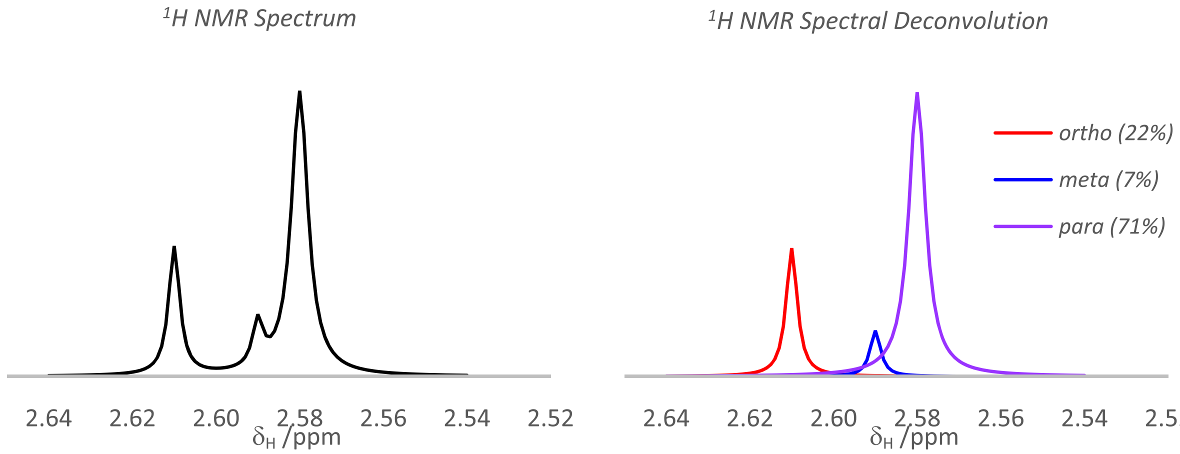

Figure 3. Illustrative spectral deconvolution of Lorentzian line-shapes for ^{1}H NMR spectroscopic analysis. Both Riemann summation and calculus were used to determine the proportions of the species in the ^{1}H NMR spectrum of a hypothetical Friedel−Crafts acylation of chlorobenzene affording *o*-, *m*-, and *p*-chloroacetophenones.

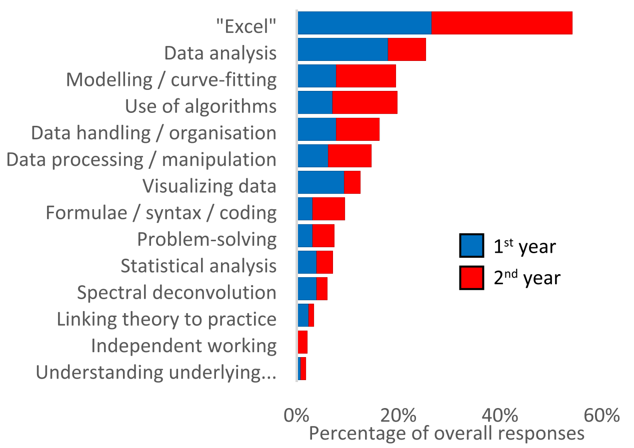

Figure 4. Skills identified by students as being developed in the workshop.

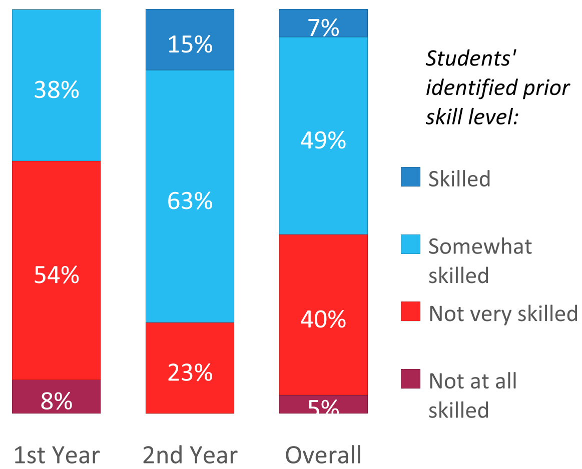

Figure 5. Self-identification of preworkshop skill level using Microsoft Excel (four-point scale).

large sets of data (8%), data processing (7%), and visualization of data (7%). More general transferable skills identified included rudimentary programming/construction of formulas (5%) and problem-solving (4%). Some students identified links and applicability of the skills to coding/programming, indicating these students recognized the transferability of the skills (see Supporting Information for full details of the responses).

Impact on Skills

We sought to evaluate the impact of the workshop, using reflective questions of both pre- and postperformance on a four- or five-point Likert scale, respectively (Figures 5 and 6, see Supporting Information for more details):

1. "How would you have described your Microsoft Excel skills prior to this workshop?"
2. "How do you consider your Microsoft Excel skills have changed after completing this workshop?"

Confirming our earlier survey findings, first year students registered a relatively low general proficiency using Microsoft Excel (Figure 5): 62% of the first year students indicated being "not very skilled" or "not skilled at all" with using Microsoft Excel; by contrast, only 23% of second year students indicated being "not very skilled," with no students responding as "not skilled at all". This suggests that the spiral curriculum approach appears to be an effective mechanism for improving students' proficiency with Microsoft Excel. Nonetheless, a significant proportion of the second year cohort still identified as "not very skilled", indicating the need to develop these skills further.

The results for the second question (Figure 6) indicated that the workshop had a positive impact on the majority of students' skills using Microsoft Excel. No student in either year group registered the workshop as having a negative impact on their skill level. Pleasingly, more than 40% of each year group registered their skill level as "significantly improved", alongside more than 57% registering as "slightly improved". Those who registered "no change" in skill level (3% of only second year students) had identified as being either "skilled" or "somewhat skilled" prior to completing the workshop. Of those who identified as "not at all skilled" or "not very skilled" prior to completing the workshop, the majority of each year group (>55%) identified as "significantly improved" postcompletion.

Value of the Workshop

We also surveyed students on their perceived value of the workshop, mapped against the skills that they identified as being developed. A four-point Likert scale was used to qualify responses (first year n = 48, second year n = 40). All students within both year groups registered the workshop as being

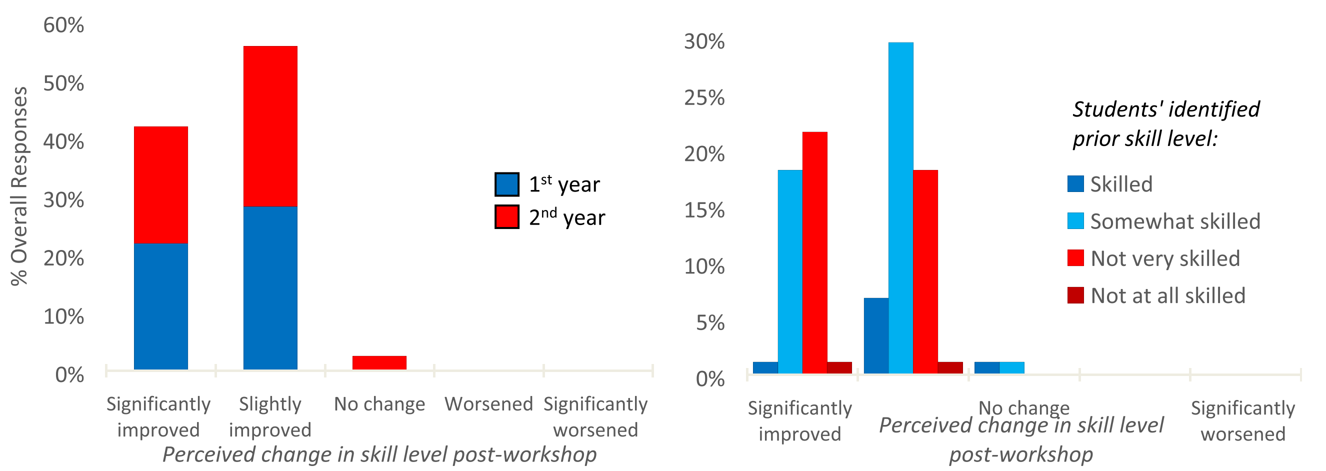

Figure 6. Change to perceived skills level postcompletion of the workshop. Left: By year group. Right: By prior skill level (as identified by the student).

"useful" or "very useful" (Figure 7), with second year students in particular perceiving the workshop as the latter (60%). Open

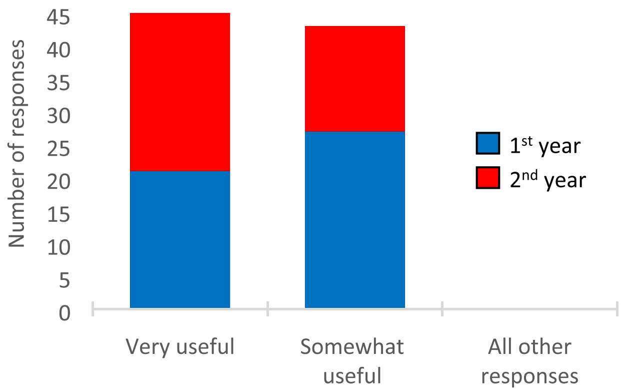

Figure 7. Student responses to the usefulness of the workshop in developing their identified skills.

comments from the survey indicated that students generally enjoyed completing the workshop, and they could appreciate the application of the skills to data analysis in the laboratory. Example students responses were the following: "I find this really helpful! It allows me to link back to the previous lab based practicals and understand why sometimes we see convoluted peaks, and how we can interpret and process them"; "Helpful lab both in terms of new content and refreshing already known skills". Some students commented on the repetitive nature of the latter tasks, but appreciated the impact the workshop had on skill development: "The workshop became very monotonous. However, it did improve my Excel skills significantly."

Student Enquiries

As this practical was self-led with enquiries sent primarily via email, we envisioned this could potentially present a barrier to some students contacting staff for assistance. The feedback to this different style of assistance to the conventional in-person approach was varied; a number of students commented that the email correspondence was very effective and responses were generally fast, while others felt it was less effective because of potentially long response times and not being able to convey their problem clearly. From those that submitted enquiries (26% of all students, $n = 57$), email correspondence generally demonstrated good written communication skills; problems were clearly and concisely articulated and specific issues identified. There were some distinctions in articulation here when compared with communications about our Mathematica practicals, where a significant number of students indicated struggling to explain their issues in written form.[2] Mapping the enquiries to the skills from the workshop (Figure 8) shows that

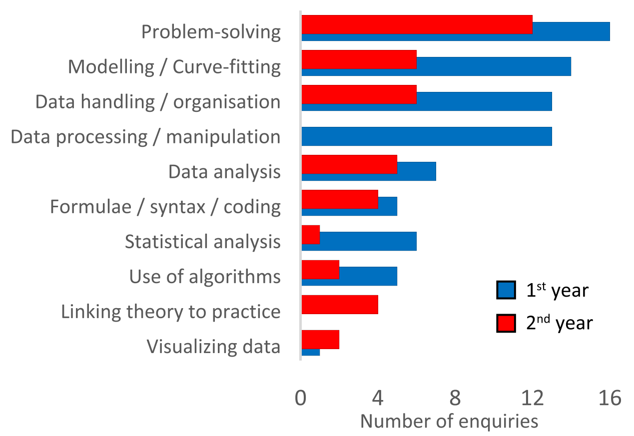

Figure 8. Categorization of student enquiries according to skill topic.

the predominant issues related to problem-solving and curve-fitting (issues that often went hand-in-hand). A number of students found using Solver challenging, with the algorithm failing to minimize the SSE or terminating prematurely if a parameter for the model function equaled zero. Students were aware that they should impose constraints for parameters but, interestingly, were less considerate of the nuanced difference between "greater than or equal to" and "greater than" when setting constraints. Solver only allows "greater than or equal to" (not "strictly greater than"), so students would input parameter constraints of ≥ 0. This often resulted in the algorithm terminating if the model involved a multiplication or division by that parameter equaling zero. When this was pointed out to students, they all recognized a workaround of imposing a constraint of a small value greater than zero, e.g., $\geq 1^{-20}$.

The majority of enquiries were related to problem-solving in the latter two tasks: in particular, identifying good initial estimates of parameters before applying the Solver algorithm. Students with only one year's experience of the chemistry course found these latter tasks particularly challenging, whereas the second year students appeared more comfortable. Enquiries and

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comments suggested that finding suitable initial values was troublesome, and a source of frustration. With little guidance to suggest values for each parameter, students that had issues here appeared to evaluate a somewhat random approach when trialing values, rather than assessing the impact of systematic variation of a single parameter. It is worth noting that, particularly for the final two tasks, students would evaluate a wide range of values >1 for the parameters, but often neglected values in the range 0−1 unless prompted. This was surprising, given that, for the first curve-fitting task (task 5), students were able to identify a parameter value for k within this range $0 < k < 1$ with relative ease.

■ CONCLUSION

We report an extensive workshop on developing higher-level data-handling, processing, and analysis skills that can be successfully implemented as a self-led exercise, deliverable remotely. The workshop provides an accessible introduction to various problems encountered surrounding practical chemistry, including fitting functions and spectral deconvolution. The contextualized nature of the problems relevant to practical chemistry, coupled with the problem-solving aspects in the later tasks, appeared to resonate with students from their feedback. Students recognized that various skills were being developed, as well as recognizing the value of the workshop in developing these skills. Crucially, an appreciable increase in perceived skills was shared across both year groups.

■ ASSOCIATED CONTENT

SI Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00732.

- Workshop manual for PCs (PDF, DOCX)
- Workshop manual for Macs (PDF, DOCX)
- Survey data (XLSX)
- Unprocessed spreadsheet data (XLSX)

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Notes

The authors declare no competing financial interest.

Fully processed spreadsheet data (XLSX), including formulas and visualization of data, and notes for instructors (DOCX) available from instructor upon request.

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