Estimation – An Empowering Skill for Students in Chemistry and Chemical Engineering

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Abstract

Today's students are from the generation that has always used calculators to compute the answers to problems. This has rendered them with no means to estimate numerical answers and no way to recognize an unrealistic answer. Lower-level undergraduate students are able to overcome these deficiencies by means of training in piece-by-piece execution of a complex algebraic computation. By moving to fewer and fewer products and quotients in a single equation, an estimate of the final value of a complicated algebraic equation can be made readily; the students gain a sense of scale when they see that their estimates are within 10% of the exactly computed value. At first, students resist this training, claiming that they will always have a calculator at hand. This presentation addresses how to overcome student resistance and how to move step-wise through practice exercises to the goal of rapid and reliable estimation final values.

Introduction

As a rule, today's students have a poor sense of the expected size of a physical quantity, and they cannot tell if their computed value is realistic or preposterous. Students place great faith in the correctness of calculators, but they fail to acknowledge that they can make mistakes in typing numerical values or in entering mathematical operations. These factors together not only contribute to poorer grades on exams and problem sets in their coursework but also lead to embarrassing mistakes on group projects and in the professional workplace.

Wrong answers can be greatly reduced if the students 1) adopt the practice of presenting the solution to a problem in several reasonable steps and 2) learn to rapidly and reliably estimate the numerical value of each step until the final result is reached. While the first step may be assumed to be routinely practiced by most students, today's students tend to carry out the complete computation process on the calculator before writing down the final result (which is often wrong). Even when instructed to "show their work," they write down only one intermediate step, a practice that fails to allow them to check their work and that offers no insight to the instructor as to where the student went wrong. Even those students who have previously been taught to write out multiple explicit steps still may generate the wrong answer, because they are not able to estimate, and therefore are not able to check, the numerical values associated with each step.

Approach for the Teaching of Estimation

The present paper provides the details to an approach that has been observed to improve the students' ability to make computations correctly and also to enhance their confidence and speed in working problems. In learning this approach, the students are forced to observe more closely the sizes of the intermediate steps and of the final answers in various types of problems. While the approach presented here is based on personal observations, it was developed through trials with many students over several years of teaching in the physical sciences. Typically one class time (one hour) early in a course is devoted to this approach, which is composed of training in estimation skills and in step-by-step presentation of the computation. The number of steps required for adequate display of a computation is determined by the limitation that only a few (no more than 2 or 3) algebraic operations are allowed for each step. Below, we describe the approach explicitly in terms of five successive exercises. All of these exercises must be done without calculators. Calculators may be used, at the instructor's discretion, after each exercise for comparison of calculator values with estimated values.

The first exercise is for the purpose of overcoming the students' assumption of invincibility in making calculations. A good way to make them realize their vulnerability is to give them a nontrivial equation in class and to ask them all take out their calculators and compute the answer. A good example is the equation for enthalpy change for the process of heating a mole of copper at constant pressure from 500 K to 1000 K. The heat capacity coefficients and the formula are supplied:

$$\Delta H = \int_{500K}^{1000K} (30.29 - 10.71x10^{-3}T - 3.22x10^{5}T^{-2})dT$$

Typically 15 - 20 % of the students get answers that differ from the correct answer by significant amounts. The students have no trouble doing the integration; where they stumble is on the arithmetic operations required after plugging in the temperature limits. They are taken aback when they state their answers orally and there are so many different answers, some of them orders of magnitude different from others. This is enough to convince them that there is indeed a problem. After this, the students must work without calculators.

The second exercise addresses the trouble the students have in computing quotients and products accurately when these quotients and products are not round numbers presented in an instantly comprehensible form. Therefore, the first exercise they are asked to do is to express a set of provided quotients as a larger number divided by a smaller number, where both numerator and denominator are multiplied by the appropriate powers of ten. This does not mean conversion to scientific notation -- rather, numerator and denominator must be converted to numbers that are readily divided mentally without mistake. It is important to recognize that students find it easy to do mental division when the numerator is larger than the denominator. Completely worked examples are shown in Figure 1 below.

a) $\frac{\mathbf{0.50}}{\mathbf{200}} = \frac{\mathbf{500}x\mathbf{10^{-3}}}{\mathbf{200}} = \mathbf{2.5}x\mathbf{10^{-3}}$;

b) $\frac{\mathbf{0.20}}{\mathbf{5}} = \frac{\mathbf{20}x\mathbf{10^{-2}}}{\mathbf{5}} = \mathbf{4}x\mathbf{10^{-2}}$;

c) $\frac{\mathbf{0.27}}{\mathbf{300}} = \frac{\mathbf{2700}x\mathbf{10^{-4}}}{\mathbf{300}} = \mathbf{9}x\mathbf{10^{-4}}$.

d) $\frac{\mathbf{1.08}}{\mathbf{120}} = \frac{\mathbf{108}x\mathbf{10^{-2}}}{\mathbf{12}x\mathbf{10^{1}}} = \mathbf{9}x\mathbf{10^{-3}}$

Figure 1. Examples of conversion of quotients to final values.

The instructor can show the students how to reduce one or two initial quotients to a final number, and then can give the students a longer list of initial expressions to work themselves. The extra time required to change the numerator and denominator to numbers multiplied by powers of ten is offset by the rapidity and confidence with which the students can carry out the division. After doing a half a page of this exercise, the students are proficient.

The third exercise is to have the students round the numerators and denominators of realistic quotients to ***simple*** numbers, use powers of ten to convert the numerator to a larger number than the denominator, and mentally compute the final answer. Examples are shown in Figure 2.

a) $\frac{\mathbf{0.52}}{\mathbf{210}} \approx \frac{\mathbf{0.50}}{\mathbf{200}} = \frac{\mathbf{500}x\mathbf{10^{-3}}}{\mathbf{200}} = \mathbf{2.5}x\mathbf{10^{-3}}$;

b) $\frac{\mathbf{0.283}}{\mathbf{323}} \approx \frac{\mathbf{0.27}}{\mathbf{300}} = \frac{\mathbf{2700}x\mathbf{10^{-4}}}{\mathbf{300}} = \mathbf{9}x\mathbf{10^{-4}}$.

c) $\frac{\mathbf{597}}{\mathbf{0.023}} \approx \frac{\mathbf{600}}{\mathbf{0.025}} = \frac{\mathbf{600}}{\mathbf{25}x\mathbf{10^{-3}}} = \frac{\mathbf{6 \cdot 100}}{\mathbf{25}x\mathbf{10^{-3}}} = \frac{\mathbf{6 \cdot 4}}{\mathbf{10^{-3}}} = \mathbf{24}x\mathbf{10^{3}}$

Figure 2. Examples of conversion of quotients to mentally operable expressions.

After the students have been shown once how to do this, they can tackle a half a page of initial expressions to do themselves. For the estimate to be as close as possible to the actual answer, an increase (or decrease) in the numerator should be paired with an increase (or decrease) in the denominator. Although the final answers to these quotients are estimates, typically they are well within 10% of the answer one would obtain with a calculator. After half a page of this type of exercise, the students are proficient.

The fourth exercise is more complex but is still not very time consuming. Students are given more complicated initial expressions and are asked to show their work in multiple steps. They are instructed to do no more than two arithmetic operations per step, where a step is understood to be the material between equal signs. Figure 3 below shows three examples, completely worked out in steps. The instructor might demonstrate by working out one initial expression to the final answer, but then the students should be given several different initial expressions and should develop the final answers themselves.

a) $$\frac{276}{6.02x10^{23}}\cdot\frac{8.134}{373}\approx\frac{300}{400}\cdot\frac{8}{6x10^{23}}=\frac{300}{400}\cdot\frac{4}{3x10^{23}}=\frac{3}{4}\cdot\frac{4}{3x10^{23}}=1x10^{-23}\ ,$$

b) $$\frac{3.68x10^{-3}}{298}\cdot\frac{0.08206}{7500}\approx\frac{4x10^{-3}}{3x10^{2}}\cdot\frac{8x10^{-2}}{7x10^{3}}=\frac{32x10^{-5}}{21x10^{5}}\approx\frac{30}{20}x10^{-10}=1.5x10^{-10}\ ,$$

c) $$3.22x10^{5}\left[\frac{1}{1000^{2}}-\frac{1}{500^{2}}\right]\approx 3x10^{5}\left[\frac{1}{(10x10^{2})^{2}}-\frac{1}{(5x10^{2})^{2}}\right]=$$
$$3x10^{5}\left[\frac{1}{100x10^{4}}-\frac{1}{25x10^{4}}\right]=3x10^{5}\left[\frac{100x10^{-2}}{100x10^{4}}-\frac{100x10^{-2}}{25x10^{4}}\right]=$$
$$3x10^{5}\left[1x10^{-6}-4x10^{-6}\right]=3x10^{5}\left[-3x10^{-6}\right]=-9x10^{-1}=-0.9.$$

Figure 3. Examples of more complicated expressions to be converted to a single numerical value.

The last expression in Figure 3 is an example of one that frequently gives the students trouble; they find it difficult to subtract two quotients correctly. Conversion of these quotients to those having larger digits in the numerator and smaller digits in the denominator improves the students' ability to correctly make the subtraction. Note that the powers of ten are the same for both terms in parentheses, i.e., both terms involved in the subtraction. Clearly, there is room for individual differences in rounding the numbers as well as in choosing which powers of ten to use. However, the use of multiple steps allows student, instructor, and colleagues to understand the process in an instant. The calculator values for the first, second, and third examples are 0.999 x 10^{-23}, 1.35 x 10^{-10}, and -0.966, respectively. The estimated values, shown in Figure 3, are all within 11% of the calculator values. Although the exercise shown above seems lengthy, it can be executed fairly quickly. In addition, the closeness of the estimate to correct calculator values boosts the students' confidence. It should be remembered that the simplification and estimation involved in obtaining a final answer obviate any emphasis on significant figures. After doing one page of this type of exercise, the students are proficient.

The fifth and final exercise is to estimate the final values for some typical physical science equations, given the constants and the values of the variables. This exercise, like the previous ones, must be done without a calculator. Three examples are given below.

a) Compute $\boldsymbol{P}$, the pressure of one mole of methane gas confined to a 250-mL volume. [1]

$$P = \frac{RT}{\overline{V}-b} - \frac{a}{\overline{V}^2} = \frac{\left(\frac{0.083415 L\cdot bar}{mol\cdot K}\right)(273.15K)}{\left(\frac{0.250L}{mol} - \frac{0.04307L}{mol}\right)} - \frac{\left(\frac{2.3026 L^2\cdot bar}{mol^2}\right)}{\left(\frac{0.250L}{mol}\right)^2}$$

$$= \frac{(0.080)(300)L\cdot bar}{(0.250-0.050)L} - \frac{2.50}{0.250^2}bar = \frac{(8.0x10^{-2})(300)bar}{0.20} - \frac{2500x10^{-3}bar}{(25x10^{-2})^2}$$

$$= \frac{2400x10^{-2}}{0.20} - \frac{2500x10^{-3}}{625x10^{-4}} = \frac{24}{2x10^{-1}} - \frac{100x10^3}{25x10^{-4}} = 12x10^1 - 4x10^1 = (120-40) = 80bar$$

The calculator yields 73.3 bar for this example, and the estimated value of 80 bar is within 10 % of the calculator value, an agreement that again enhances the students' confidence.

b) Use the generic empirical formula for heat capacity of copper[2] to compute ΔH for one mole of copper at constant (atmospheric) pressure for a temperature increase from 500 to 1000 K. [2]

$$\Delta H = \int_{500K}^{1000K} (30.29 - 10.71x10^{-3}T - 3.22x10^5 T^{-2})dT$$

$$= \left[(30.29)T - (10.71x10^{-3})\frac{T^2}{2} - (3.22x10^{5)}\frac{T^{-1}}{-1}\right]_{500}^{1000}$$

$$= 30[1000-500] - \frac{10x10^{-3}}{2}[1000^2 - 500^2] + 3x10^5\left[\frac{1}{1000} - \frac{1}{500}\right]$$

$$= 30[500] - 5x10^{-3}[100x10^4 - 25x10^4] + 3x10^5\left[\frac{1}{10x10^2} - \frac{1}{5x10^2}\right]$$

$$= 15000 - 5x10^{-3}[75x10^4] + 3x10^5\left[0.1x10^{-2} - 0.2x10^{-2}\right]$$

$$= 15000 - 375x10^1 + 3x10^5(-0.1x10^{-2}) = 15000 - 3750 - 0.3x10^3$$

$$= 15000 - 3750 - 300 = 15000 - 4050 = 10950J = 10.9kJ$$

The final value is positive, as it should be for the enthalpy change of a system to which heat is added. The last line allows the students to see that the leading term in the equation is the dominant one and that the second and third terms are relatively small and serve as refinements on the value of the dominant term. Had they not written out the solution step-by-step, they would not be able to gain this insight. The estimated answer of 10.9 kJ is within 1 % of the calculator answer of 10.8 kJ.

c) Use the generic empirical formula for heat capacity of calcium titanate[2] ($CaTiO_3$) to compute **Δ*H*** for one mole of $CaCO_3$ at constant (atmospheric) pressure for a temperature increase from 298 to 1000 K.

$$\Delta H = \int_{298K}^{1000K} (127.49 + 5.69x10^{-3}T - 27.99x10^{5}T^{-2})dT$$

$$= \left[(127.49)T + (5.69x10^{-3})\frac{T^2}{2} - (27.99x10^{5)}\frac{T^{-1}}{-1} \right]_{298}^{1000}$$

$$\approx 130[1000 - 300] + \frac{6x10^{-3}}{2}[1000^2 - 300^2] + 30x10^5 \left[\frac{1}{1000} - \frac{1}{300} \right]$$

$$= 130[700] + 3x10^{-3}[100x10^4 - 9x10^4] + 30x10^5 \left[\frac{1}{1x10^3} - \frac{1}{0.3x10^2} \right]$$

$$= 91000 + 3x10^{-3}[91x10^4] + 30x10^5 \left[1x10^{-3} - 3.33x10^{-3} \right]$$

$$= 91000 + 273x10^1 + 30x10^5(-2.33x10^{-3}) = 91000 + 2730 - 30x10^5(-2.33x10^{-3})$$

$$= 91000 + 2730 - 69.9x10^2 \approx 93730 - 7000 = 86730J = 87kJ$$

This estimated value is less than 5 % different from the calculated value of 85 kJ. When the students get to the point where they estimate, without calculators, the final values for realistic physical science equations, they are ready to do problems on an exam without calculators. For such an exam, this instructor counts their answers correct if the final values are within 15% of the value correctly obtained by computer or calculator. Students taking this type of exam typically do well and do not require extra time.

The approach described in the present paper was introduced a few years ago by the author because of the many errors made by students in their computations, on exams, on in-class problems, and on student projects. The described approach has greatly improved the performance of the students in these tasks. In addition to better performance on exams and better technical communication, undergraduate and graduate students who have been taught to practice estimation and step-by-step display of calculations save time and avoid mistakes by actively using this approach to check computed values needed in their research activities. An anecdote that illustrates an unexpected benefit of estimation and step-by-step display was related by a student who forgot to take her calculator to an exam in a course where estimation and step-by-step display was not the practice. She used the approach presented in the present paper and was given credit for correct answers by an impressed instructor.

Conclusions

The approach described in this paper leads to achievement of good estimating skills in college students in a minimum of time. They employ these skills to check their calculator work on exams, in problem sets and in class projects. In addition, they become committed to the practice of writing the solutions to problems in multiple steps, each of which can be checked readily by estimation, whether during an exam, during classroom projects, or by the instructor during grading. Students in classes in which estimation has been practiced typically get better grades on exam problems than students in classes where estimation was not introduced.

References

1. Donald A. McQuarrie and John D. Simon, *Physical Chemistry: A Molecular Approach*, University Science Books, Herndon, VA, 1997.

2. David R. Gaskell and David E. Laughlin, *Introduction to the Thermodynamics of Materials*, 3rd^{h} edition, Taylor & Francis, Washington, DC, 1984.