

## PQcalc, an Online Calculator for Science Learners

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## S Supporting Information

**ABSTRACT:** PQcalc is an online calculator designed to support students in college-level science classes. Unlike a pocket calculator, PQcalc allows students to set up problems within the calculator just as one would on paper. This includes using proper units and naming quantities strategically in a way that helps finding the solution. Results of calculations come with units of measurement and are given with a reasonable number of significant figures. The features of PQcalc were chosen to allow learners to spend more time on scientific reasoning while figuring out and communicating well-annotated, structured, and mathematically correct solutions to quantitative problems.

**KEYWORDS:** First-Year Undergraduate/General, Computer-Based Learning, Problem Solving/Decision Making, Mathematics/Symbolic Mathematics



1. Set up a problem
2. Solve it and press "go"
3. See the work and the results

$$m_{\text{oildrop}} = 0.413 \text{ g}$$

$$d_{\text{oil}} = 0.734 \frac{\text{g}}{\text{mL}}$$

$$\begin{aligned} V_{\text{oildrop}} &= \frac{m_{\text{oildrop}}}{d_{\text{oil}}} \\ &= \frac{0.413 \text{ g}}{0.734 \frac{\text{g}}{\text{mL}}} \\ &= 0.563 \text{ mL} \end{aligned}$$

Developing scientific reasoning skills is at the core of college-level science courses and programs. Students practice quantitative reasoning by solving problems and analyzing data measured in the lab. This requires not only content knowledge but also mathematical skills to calculate with physical quantities and their units. Nowadays, the required arithmetic steps are typically done with a pocket calculator. Because pocket calculators deal with pure numbers only, the problem solving process is separated into a content-rich mode where students figure out the path to the solution on paper, and a content-free mode where students manipulate nameless and unitless numbers on their calculator. Using calculators too early in the process and placing too large an emphasis on the algorithmic aspects distracts from the essence of problem solving.<sup>1</sup> Not returning to the content-rich mode after arriving at a numerical answer misses an opportunity to check and interpret results.<sup>2</sup> Thus, although suited to expert problem solvers, calculators may distract rather than help students learning science. The online calculator PQcalc described here, however, was designed specifically to support science learners by allowing students to integrate context and meaning into their calculations.

## ■ STEPS IN PROBLEM SOLVING

Solving a problem using PQcalc consists of three steps (Figure 1). First, you set up the problem by entering all the known quantities, including their name, value, and unit. Second, you yourself need to solve the problem, enter the formula prescribing how to calculate the unknown from the quantities already defined, and press "go". The calculator will proceed to do the arithmetic. Third, you will see the steps of the calculation and the arithmetically correct result (including units

1. Problem representation	{	<pre>&gt;&gt;&gt;&gt; m_oildrop = 0.413 g m_oildrop = 0.413 g &gt;&gt;&gt;&gt; d_oil = 0.734 g/mL d_oil = 0.734 g/mL &gt;&gt;&gt;&gt; V_oildrop = m_oildrop / d_oil V_oildrop = m_oildrop / d_oil = 0.413 g / 0.734 g/mL = 0.563 mL</pre>
2. Solution		
3. Work & result		

**Figure 1.** Solving a question with PQcalc in three steps: "What is the volume of 0.413 g of oil if the density of oil is 0.734 g/mL?" User input is shown in typewriter font following the ">>>" prompt.

and showing an appropriate number of significant figures), allowing you to interpret the result and to verify that your path to the solution is sound.

## Setting up the Problem

Expert problem solvers spend substantial effort on representing a problem before proceeding with calculations.<sup>3</sup> PQcalc nudges students to do the same by requiring that all known quantities be named and entered with units before a calculation is performed. Names can be complex, including subscripts, chemical formulas, and a wide range of symbols, but are simple and fast to enter, as the examples in Figures 1–3 show. PQcalc is aware of significant figures. For example, 2.00, 2.0, and 2. mol, have 3, 2, and 1 significant figures, respectively, whereas 2

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>>>> n[C3H8] = 34.9 mmol
nC3H8 = 34.9 mmol
>>>> # Need balanced equation to calculate _n[CO2]
Need balanced equation to calculate nCO2
>>>> #[C3H8 + 5O2 -> 3CO2 + 4H2O]
C3H8 + 5 O2 → 3 CO2 + 4 H2O
>>>> n[CO2] = 3 * n[C3H8]
nCO2 = 3 · nC3H8
      = 3 · 34.9 mmol
      = 104.7 mmol

```

**Figure 2.** PQcalc allows the use of chemistry markup in calculations (black) and in annotations (blue). User input is shown in typewriter font after the “>>>” prompt.

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ΔrG° = -R · T · ln(Keq)
      = -8.314  $\frac{\text{J}}{\text{K mol}}$  · 298.0 K · ln(2.54 × 106)
      = -2477.57  $\frac{\text{J}}{\text{mol}}$  · 14.7477
      = -3.654 × 104  $\frac{\text{J}}{\text{mol}}$ 
>>>> ΔrG° using kJ
ΔrG° = -3.654 × 104  $\frac{\text{J}}{\text{mol}}$ 
      = -36.54  $\frac{\text{kJ}}{\text{mol}}$ 

```

**Figure 3.** PQcalc shows stepwise calculation and allows switching units of results with a simple command. Note the use of Unicode characters in the example input after the “>>>” prompt to refer to the standard Gibbs energy of reaction, Δ<sub>r</sub>G°.

mol is taken as an exact integer value. Well-crafted names of the quantities can carry a lot of information in themselves (what kind of quantity, which sample). Additional information that might help in solving the problem can be added as comment; a typical example is a balanced chemical equation necessary for stoichiometric problems (Figure 2). With these capabilities, setting up a problem with PQcalc captures the science context as well as the numeric data. Consequently, PQcalc not only performs calculations but also supports students in deciding what type of problem is at hand, and what the path to a solution might be.

### Solving the Problem

Although PQcalc helps find the path to the solution, it is up to the students to figure out which relationships between quantities are relevant to the problem and to solve these relationships algebraically for the unknowns before letting PQcalc do the arithmetic.<sup>4</sup> This division of labor is intentional. Students focus on the higher-order tasks, learning which relationships apply under which circumstances and practicing how to manipulate a formula without substituting values first. Once they have completed this difficult task, they can quickly enter the solution in terms of the already defined quantities and press “go” to see the calculation and the result.

### Viewing the Calculation and Interpreting the Result

Calculations done with PQcalc are shown step by step so that students can follow the arithmetic (Figure 3). First, the input is mirrored but formatted for better readability. Then, the known values—including units—are substituted, and mathematical operations are performed one step at a time. This detailed “showing your work” allows the discussion of operator precedence, fractions, unit cancellation, and properties of

functions such as square root or logarithm. If the requested calculations lack physical sense (e.g., attempts to add quantities of different dimensions or to take the logarithm of a unit), specific detailed error messages are shown. Finally, the result is displayed with units and the appropriate number of significant figures (the error propagation algorithm is given in the manual provided as [Supporting Information](#)). Units are chosen to mirror units of the quantities entered previously, for example, if energies are entered in kilojoules, answers will be in kilojoules as well. If units other than those given are more appropriate or convenient, it is possible to convert to these, as shown in Figure 3 (bottom).

## ADAPTING TO THE LEARNER

To accommodate different levels of learners, PQcalc has switches to change the amount of output and the available features. To make beginners aware of conventions for naming quantities (e.g., *t* has dimension of time and *T* has dimension of temperature), a switch turns on warning messages if names and units do not seem to match. Also, student input is first mirrored in plain text and then shown with math and chemistry markup to aid in understanding how math is communicated in plain, linear text. To reduce visual clutter for intermediate students, mirroring input can be switched off. To save screen space when working on multistep problems, advanced students can choose to omit the intermediate steps of calculations. In addition, they may choose to show uncertainties in the last digit explicitly (e.g., 2.31(7) g instead of 2.31 g) to provide slightly more information on errors. Being able to switch on or switch off features maximizes the support for beginning students while also enabling more complex calculations performed by advanced students. If desired, the instructor can preset switches by giving students a slightly modified link to PQcalc as explained in the user manual.

### Accessibility

Students can use PQcalc whenever they have access to the Internet. As browser-based software, PQcalc works with a wide range of devices, from desktop to mobile phone. Because the input is plain text, it is easy to disseminate problems and solutions. The math markup is built on widely used software packages (LaTeX and MathJax<sup>5</sup>), making it possible to adapt it for the visually impaired.<sup>6</sup> These features allow to integrate working with PQcalc into the class room, the lab and for home work, making one single tool available to everyone in multiple settings.

## USE IN THE CLASSROOM

PQcalc has been designed as a tool an instructor can work with as well. With the rich formatting, it allows the instructor to communicate model solutions to practice problems in presentations or worksheets. Because the tool runs in a browser, it becomes possible to project it during class and use it while discussing how to tackle a given quantitative problem. Thanks to a simple “undo” mechanism, the class can explore unproductive or incorrect steps, discuss, back up one step, and then figure out the steps that lead to the solution. The Python source code for PQcalc is open access and may be run on local servers and adapted to specific needs.

### Keeping Students Accountable for the Arithmetic

One concern with providing a powerful calculator to students is that students will treat it as a black box and lose basic math abilities. PQcalc has a switch that will hide all units in a

calculation, giving students practice in unit manipulation. Another switch hides all the numbers while showing the units. This is a prompt to practice doing the arithmetic with a pocket calculator, as they might be required to in a standardized exam. If an instructor does not wish students to use PQcalc for a given homework assignment, the use of certain “magic” numbers (such as “19.9351”) in a problem will be detected by PQcalc, and the calculator will not proceed with the calculation.

## ■ CONCLUSION

PQcalc is a powerful tool that adapts to the level of the learner and to the requirements of the class room. It is freely available and can be integrated into science courses to help students learn how to reason quantitatively. It supports students’ problem solving by encouraging them to represent the problem clearly, by maintaining a rich context while working on the numerical aspects of the problem, and by allowing students to document the concepts and the logic underlying the path to a valid solution through rich annotations.

## ■ ASSOCIATED CONTENT

### 📄 Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: [10.1021/acs.jchemed.5b00366](https://doi.org/10.1021/acs.jchemed.5b00366).

User manual provided as Supporting Information (PDF).  
Open source code available at [github.com/ktheis/pqcalc](https://github.com/ktheis/pqcalc).  
Program available via [bioinformatics.org/pqcalc](https://bioinformatics.org/pqcalc).

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### Notes

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