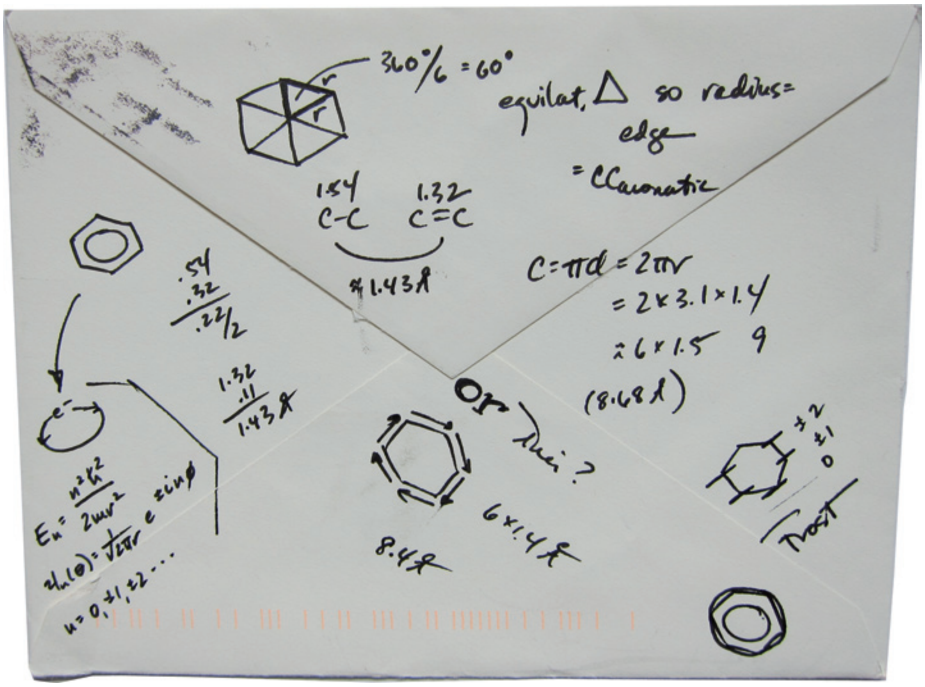
Take a number

Back-of-the-envelope calculations are an important part of chemistry argues **Michelle Francl.**

It's the same awkward scene every September. My physical chemistry students are slinking down in their seats, eyes darting wildly around the classroom, looking at anyone but me. Someone in the back is nervously clicking a pen while the diligent front-row students are flipping frantically through their notes; I briefly wonder if the pair sitting closest to the door are going to bolt.

I count off thirty seconds that feel more like thirty hours; still no one says a word. I firmly repeat the question, "Can anyone tell me roughly the circumference of a benzene ring in metres?" Someone finally has the courage to ask, "Are we supposed to know that?" It's not a game of chemical quizzo, I assure them. How would you figure it out from what you do know, without recourse to a search engine, without wildly guessing?

At a moment in time when many have a search engine in their pocket and trivial access to sophisticated computational resources, it might seem cruelly anachronistic to push students to do this sort of back-of-the-envelope exercise. Why not just look up the number? Is there still any value to a scientist — beyond the gee-whiz factor — in being able to provide rapid and reasonable estimates of values related to their work?



MICHELLE FRANCL

A back-of-the-envelope calculation estimating the circumference of a benzene ring.

> A well-developed sense of the range of possible values gives you a nose for the garbage that can float to the top in a Google search.

The ability to work out a rough value for a quantity with less than complete information may seem more a wild talent than a staid scientific skill. In 1945, on observing that the compression wave from the Trinity nuclear test blew some scraps of paper a distance of 2.5 metres, physicist Enrico Fermi impressed onlookers by giving an on-the-spot estimate of the energy output of the bomb; his estimate ultimately proved to be within a factor of two of the measured yield[1]. There is no doubt Fermi was brilliant, still, he must have felt that a back-of-the-envelope estimation was more than a parlour trick, often challenging graduate students in his classes at the University of Chicago to make estimates of offbeat values such as the number of piano tuners in Chicago. These eponymous Fermi problems are now standard interview fare for finance and tech firms.

So what can a knack for constructing robust estimates get a scientist, aside from a high-paying job with a Wall Street hedge fund? Much, I would suggest. It offers the potential to cobble together a reasonable value when Google doesn't turn up anything useful, allowing an approach to be tested before investing in a thorough literature search to track down the best possible numbers. Likewise, a well-developed sense of the range of possible values gives you a nose for the garbage that can float to the top in a search, as well as for your own experiments that have gone a bit off. Most powerfully though, a comparison of back-of-the-envelope estimates with experimental values can illuminate missing factors in a relationship. If an experimental result is far off from the estimate, it can be a hint that the theoretical framework is lacking. Start looking for new science. Quantum mechanics was born of the mismatch between models of blackbody radiation and experiment.

I would argue that the rewards of being able to roughly assign a number to a quantity, particularly the way it can lead to uncovering new science, make it a far more critical skill for a chemist to master than any single laboratory technique. While I'm not suggesting we should swap courses in analytical chemistry or organic synthesis for a class in making sound guesses (although MIT, among other institutions, routinely teaches a course[2,3] in the art of estimation for scientists and engineers), I am proposing that we consider explicitly embedding such instruction in the chemistry curriculum, and encourage its development throughout the training of researchers.

This suggestion, of course, begs the question of whether the art of chemical estimation can even be taught, or is it like happiness in the eyes[4] of nineteenth century

American novelist Nathanial Hawthorne: “when it comes, [it] comes incidentally. Make it the object of pursuit, and it leads us on a wild-goose chase, and is never attained.” Well-developed theories of estimation exist, both because computer scientists[5] would like to enable computers to make rough estimates better than they currently do (ask Wolfram Alpha for the carbon–carbon bond distance in ethanol, for example) and because cognitive psychologists[6] would like to help people make rough estimates better than they currently do (ask a chemistry student for the carbon–carbon bond distance in ethanol, for example).

Encourage students to become as familiar with anchoring values as they are with chemical trends.

Norman Brown and Robert Siegler’s ‘metrics and mapping’ frame[6] is particularly helpful in understanding how chemists might generate useful estimates from an incomplete data set. In this framework, mapping is an understanding of the relative ordering of critical data; for example, X–H bonds are shorter than X–X bonds. Metrics capture the reliance of estimates on key values, including fundamental constants, unit conversion factors and anchoring values. Anchors are those bits of trivia (the average carbon–carbon single bond length) that can be leveraged by an ordered relationship (aromatic bonds are longer than single bonds) and tempered by a grasp of the reasonable distribution of related values around the anchor value (carbon–carbon bonds are never shorter than 100 pm) to yield a reasonable estimate.

Open any introductory or organic chemistry text and it’s clear that fundamentally much of chemistry is the art of mapping; we explicitly teach chemists to deftly wield relative orderings of quantities from electronegativities to pK_a values to produce rational and robust predictions of chemical behaviour. We hold a significant subset of these relationships in equation form, often committed to memory in our early years of training: $PV = nRT$, for example.

Lists of chemical metrics, typically fundamental constants and unit conversions, are found inside the covers of most chemistry texts, but it’s the anchoring values that I suspect we have difficulty articulating. What anchor values would most benefit students as they seek to hone their chemical intuition? Sanjoy Mahajan, who teaches MIT’s course on estimation, gives students a page of “numbers for the backs of envelopes”, a list of key metrics for scientists and engineers[7]. I recently asked a few hundred of my closest chemical friends on Twitter and Facebook what should go on such a sheet for chemists, what they might encourage students to master. Schematics of periodic trends and the electromagnetic spectrum are obvious candidates for mappings, but the list of suggested anchors varied wildly with subfield. There are very few values that a majority of chemists cling to: room temperature is 300 K; the length of a single carbon–carbon bond is 154 pm; the atomic masses of C, H, N, O, S and Cl.

In addition to metrics and maps, chemists keep a variety of hacks in their armament. These are often drawn and wielded instinctively, ranging from the quick and dirty conversion[8] from Fahrenheit to Celsius, $2C + 30 = F$, for the SI-impaired chemistry student (or chemist), to the trick — often a real mystery to students accustomed to calculators displaying eight or more digits — of doing a calculation carrying just one significant figure along to get an order of magnitude estimate.

I urge chemists to explicitly develop in our students the ability — and the courage — to routinely make reasonable estimates of chemical values. Assign the occasional chemical Fermi problem. Think aloud. Point out the hacks you use. Post the latest XKCD *What If* feature[9]. Encourage students to become as familiar with anchoring values as they are with chemical trends, and to routinely calculate values to one significant figure. The development of chemical intuition need not be intuitive, nor incidental. ❐

Michelle Francl is Professor of Chemistry on the Clowes Fund for Science and Public Policy and is in the Department of Chemistry at Bryn Mawr College, Bryn Mawr, Pennsylvania 19010-2899, USA.
e-mail: mfrancl@brynmawr.edu

References

1. http://www.dannen.com/decision/fermi.html
2. Mahajan, S. *6.055J The Art of Approximation in Science and Engineering, Spring 2008* (MIT OpenCourseWare, accessed 15 July 2013); http://web.mit.edu/6.055
3. Mahajan, S. *Street-fighting Mathematics: The Art of Educated Guessing and Opportunistic Problem Solving* (MIT Press, 2010).
4. Hawthorne, N. & Hawthorne, J. *Passages from the American Notebooks* (Houghton, Mifflin and Co., 1900).
5. Paritosh, P. K. in *Proc. 26th Cognitive Science Conference* (eds Forbus, K., Gentner, D. & Regier, T.) 1083–1088 (Cognitive Science Society, 2005); http://csjarchive.cogsci.rpi.edu/Proceedings/2004/CogSci04.pdf
6. Brown, N. R. & Siegler, R. S. *Psych. Rev.* **100,** 511–534 (1993).
7. http://web.mit.edu/6.055/notes/constants.pdf
8. http://lifehacker.com/5917331/quickly-convert-between-fahrenheit-and-celsius-without-a-calculator
9. http://what-if.xkcd.com/