Communicating Chemistry: the Challenges and the Opportunities

*Peter Atkins**

En su presentación, el Dr. Peter Atkins nos habló de los retos y las oportunidades alrededor de la química (ver la portada de este número, tomada con la autorización del autor). Se refirió a los retos con el color rojo y los describió como *La Abstracción, La complejidad* y *Las matemáticas*, mientras que las oportunidades llevaron el color verde y fueron *Los conceptos, El currículo* y *Los Gráficos*.

In his presentation Dr. Peter Atkins spoke to us about the challenges and the opportunities around chemistry (see the frontispiece of this issue, printed with the permission of the author). He referred to the challenges with the red color and describes them as Abstraction, Complexity *and* Mathematics, *while opportunities took a green color and were* Concepts, Curriculum *and* Graphics.

The challenges we face are numerous. I shall concentrate on just three, which are the abstract nature of our subject, the disheartening role of mathematics, and the complexity of our subject. At the same time we should recognize that there are many opportunities for the development of chemical education. Once again, I shall concentrate on just three, which are the role of computer graphics, the identification of core concepts, and the control we have over the curriculum. Many of my remarks will apply to the public appreciation of chemistry as well as to my principal target, the general education of a chemist.

The overall strategy of education should be to build a bridge—a bridge between the familiar macroscopic world of everyday entities and the imagined underworld of atoms. Our students should be able to move in both directions easily and effectively: they should be able to move from the imagined to the perceived and from the perceived to the imagined. Whenever they look at an everyday object they should be able to imagine it in terms of its atoms. Another central idea that we should be sure to convey is that the role of science is to discover the simplicity that lies below complexity. The world ultimately is very simple: its complexity stems from the manner in which those simplicities interact.

I shall concentrate on three components of the challenge that confronts us. One challenge is the abstract nature of many of our concepts. Another challenge is the complexity of our subject: there are many details that must be mastered. Thirdly, there is the ever-present problem of mathematics, and how we overcome fear of it. I will also concentrate on three components of the opportunities that we have to overcome these challenges. One opportunity of great importance is the availability of graphics, particularly computer graphics of various kinds. Another opportunity is our ability to identify the truly important concepts that underlie chemistry. Thirdly, we have the curriculum under our control, and can use it sensibly to overcome the challenges. I shall examine some aspects of these three challenges and see how they can be overcome by a selection of the three opportunities I have mentioned.

The challenge of abstraction

Chemistry is an abstract subject, even though it deals with the most tangible of entities. As soon as chemists start to talk, they use language and concepts that many perceive as abstract. That includes the basic currency of atoms, bonds, molecules, and entropy, and even such seemingly familiar term as energy. The challenge is to make these concepts seem tangible. The opportunity is the use of computer graphics. We now have wonderful opportunities to display images of molecular models, and such images help us to convey that molecules are actual entities. W can display images of small molecules, biological macromolecules, and solids. But the use of imagery does not stop at molecules: we can use graphical images to display the core ideas of the principles of our subject. My favourite example here is entropy and the second law of thermodynamics, which is easy to illuminate graphically.

Let me say a few words about the second law, as it is so important for everyone to understand it, yet it is often presented in such a confusing way. All it implies (in its molecular interpretation) is that matter

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* University of Oxford, UK.
Correo electrónico: peter.atkins@lincoln.ox.ac.uk

and energy tend to disperse in disorder. The crucially important point, though is that that dispersal may be used to drive a *local* decrease in disorder. Thus, when a hydrocarbon fuel burns in an engine, the atoms disperse as carbon dioxide and water molecules, and the energy liberated by the combustion also disperses. The mechanical structure of the engine enables us to capture this dispersal and use it to do work, which may be the organization of a pile of bricks into a building. Alternatively, the fuel might be our food, and as it is digested, the chain of metabolic processes in our body might be used to drive another local, structure-forming process, the organization of a collection of amino acids into a protein. More fancifully, the same metabolism of food might be used to organize the random current in the neurons of our brain, and result in the construction of a work of literature, of music, of art, or the carrying out of a noble deed. *Globally* the universe has become more disordered but *locally* there might be the emergence of structure. We have truly found the engine of the universe.

Complexity

The problems of complexity stem from the fact that, regrettably, many of our instructors (especially in high schools) are under-prepared. Through no fault of their own, they may be forced to teach a subject for which they have not been trained, or for which they themselves were badly taught. But chemistry is intrinsically complex, because it involves fine judgements about the competition between disparate influences. Thus, in some cases thermodynamics might be the dominant cause; in others it might be kinetics, and so on. It is very difficult for students to know which of the whole array of explanations is relevant to a particular observation. Thirdly, there are large numbers of concepts to master, ranging from classical thermodynamics to bizarre aspects of quantum mechanics. Fourthly, there are many facts that should be remembered: ours is a concept-rich and fact-rich subject, and we should not hide that from our students.

The organization of the curriculum plays an important role here. Although there is a current fashion to blend the three classical divisions of chemistry (physical, inorganic, and organic), I think that there are strong arguments for keeping them separate. Principally, each division requires a different mode of thought, and the beginning student can probably cope with the subject better if these modes of thought are kept separate. Of course, in later years of the course, it is essential to become able to migrate freely between the three divisions, for many of the best chemists work at the intersection of all three.

Another way to reflect on the organization of a modern course in chemistry is to reflect on the techniques that are currently driving chemistry forward. I think that these techniques currently include:

- Computation
- Lasers
- NMR
- Diffraction
- Surface microscopy
- Electrochemistry
- Catalysis
- Synthesis
- Nanoscience

By thinking about a course that uses these techniques as a guide, the course will appear modern and exciting.

A third way to tackle the challenge of complexity is to attempt to identify the core concepts that underlie chemistry. I have spoken on a number of occasions about the distillation of chemistry into its core ideas, and have suggested the following nine principles:

1. Matter consists of atoms.
2. The elements form families that can be understood in terms of atomic structure.
3. Atoms form bonds by sharing electron pairs.
4. The shape of the resulting molecules is of paramount importance.
5. There are residual forces between molecules.
6. Energy is conserved.
7. Matter and energy tend to disperse.
8. There are barriers to reaction.
9. There are only four types of reaction*.

If we could ensure that our students knew at least these principles and their principal ramifications; then we would have done a good job.

Mathematics

The greatest challenge of all: how can we instil in our students an appreciation of the importance of mathematics? The challenge stems from a number of sources. One is that our students are often under-pre-

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* Proton transfer (acid-base); electron transfer (redox); electron sharing (radical); electron-pair sharing (Lewis acid-base).

pared in mathematics, and increasingly (in some, not all parts of the world), are simply not taught enough before they come into our hands. But it is deeper than that. Many people who study chemistry are comfortable with tangible entities but are uncomfortable with abstract concepts. We should accept that you can be a really good chemist even if you are incompetent at formulating or even following a mathematical argument. It may be wrong to expel a chemist from a course simply because he or she is an incompetent mathematician: the skills of chemistry are quite different. Thirdly, there is often in our teaching a gap between the symbol that appears in an equation and the physical, tangible concept it represents.

One great opportunity to overcome this challenge is computer graphics. We can use computer graphics to explain abstract concepts (although there may be some that defy even that aid). We should also recognize that modern science is undergoing a paradigm shift: until a couple of decades ago, science proceeded analytically, and the primary aim was to deduce conclusions analytically from theoretical expressions. Now, increasingly, attention is turning to numerical analysis, and whole regions of science that were previously inaccessible have become open to study (complexity, chaos, and so on). We should acknowledge this paradigm shift in our courses. Thirdly, even conventional analytical mathematics –algebra, trigonometry, calculus– can be made much more interesting if it is carried out on a computer using mathematical software.

Basically, though, mathematics should be developed in our courses by:

1. Motivating every equation.
2. Interpreting every equation.
3. Demonstrating the *power* that it puts into our hands as scientists.

I concluded the lecture by trying to identify what I regard as the central equations of physical chemistry, and for completeness, offer my suggestions here. For thermodynamics, the two central concepts are the perfect gas equation of state, $pV = nRT$, and the chemical potential, $\mu = \mu^\circ + RT\ln a$. The former is a kind of guide for the formulation of the latter, and the latter, through seeking conditions for the equality of the chemical potentials of substances in various phases underlies the description of all physical and chemical equilibria. These merge in probably the single most useful equation of all chemical thermodynamics, $\Delta_r G^\circ = -RT\ln K$ and the crucially important link between thermodynamics and electrochemistry, $\Delta G = w_e$. The relation that governs the response of systems to changes in the conditions is $\mathrm{d}G = V\mathrm{d}p - S\,\mathrm{d}T$, and summarizes almost everything we need to know.

In quantum chemistry, the De Broglie relation, $\lambda = h/p$, summarizes the central concept of duality. Stemming from duality is the aspect of reality that distinguishes quantum mechanics from classical mechanics, namely superposition: $\Psi = \Psi_A + \Psi_B$ with its implication of the roles of constructive and destructive interference. Then of course, there is the means of calculating wavefunctions, the Schrödinger equation, $H\Psi = E\Psi$.

In chemical kinetics and dynamics, there are three central equations. One is the form of a rate law, $\mathrm{d[A]/dt} = f([\mathrm{A}],[\mathrm{B}]\ldots)$, and all its implication for the prediction of the outcome of reactions, and their mechanisms, and the Arrhenius relation, $k = A\exp(-\mathrm{E_a}/RT)$, with its implications for the temperature-dependence of reaction rates. Lurking behind discussions of this kind is the diffusion equation, in its various flavours starting from the vanilla $\partial\Psi/\partial t = -D\partial^2\Psi/\partial x^2$.

An equation that brings all these others together is the Boltzmann distribution, $N_i/N = \exp(-\varepsilon_i/kT)/q$. To a large extent, this equation summarizes the whol of chemistry. First, it is derived from the most primitive of assumptions (the random distribution of entities over available energy levels subject to a couple of obvious constraints) and consequently applies universally. Because it uses the concept of energy levels yet can be used to calculate thermodynamic properties, it is a bridge between the microscopic and macroscopic worlds. Third, because it is essentially a way of distinguishing populations that are stable ($\varepsilon_i < kT$) from those that are volatile ($\varepsilon_i > kT$), it captures the essence of the two pillars of chemistry: structure and change.

Conclusion

I would like to conclude with two simple messages. One is that the education of a scientist should install the view that behind every complexity there is an underlying simplicity. The second point is that science opens our eyes–it deepens our enjoyment. If we keep those two thoughts in mind, and convey them to our students, we shall have done well. ◪