Chapter 3

MODELS AND MODELLING IN CHEMICAL EDUCATION

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INTRODUCTION

As chemistry is concerned with the properties and transformations of materials, chemists are essentially modellers of the substances that constitute such materials and of their transformations. In doing so, they seek to make predictions about the necessary conditions both for the occurrence of a desirable transformations and for the avoidance of undesirable ones. Chemists model both the phenomena they observe and the ideas with which they try to explain such phenomena - that is, at both the macroscopic and the sub-microscopic levels (Johnstone, 1993) - by the use of analogy with what they already know. The outcomes of such a process are expressed in a concrete, visual, mathematical and/or verbal mode of representation, sometimes by using special symbols that constitute chemical language (e.g., formulae of compounds). Moreover, chemists are able to transform models in one mode of representation into equivalent representation in other modes (Kozma & Russel, 1997). Such models may be focused on different attributes of representation (their relationship to quantification, their behaviour through time, and the reproducibility of their behaviour (Boulter & Buckley, 2000)). Thus chemical knowledge about a range of phenomena is produced and communicated with the use of several models, which evolve and are changed as the field of enquiry advances. In the second half of the last century, such a central role for the production and use of models in the growth of chemical knowledge was generally recognised by chemists, philosophers of chemistry, and by chemical educators (Bailer-Jones, 1999;

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Erduran, 2001; Francoeur, 2000; Giere, 1999; Hardwicke, 1995; Luisi & Thomas, 1990; Nersessian, 1999; Ramberg, 2000; Suckling et al., 1980; Tomasi, 1988; Trindle, 1999). Modelling is so common in chemistry that it has become 'the dominant way of thinking' (Luisi & Thomas, 1990, p. 67) as the subject has matured, something that chemists do 'without having to analyse or even be aware of the mechanism of the process' (Suckling et al., 1980, p. 26). This seems to be so because the explanations of the natures of substances and of their transformations are essentially abstract. Thinking with models enables chemists to visualise the entities or processes that are being enquired into, to more readily plan experimental activities on them (Tomasi, 1988), and to support the processes of reasoning and constructing knowledge (Nersessian, 1999).

It seems likely that chemical ideas have been visually, mathematically, or verbally modelled since they began to be produced. However, the production of the first concrete models for atoms by John Dalton at the beginning of the nineteenth century was a landmark in the way that models have contributed to the development of chemical knowledge. Following him, leading chemists, such as Kekulé, Van 't Hoff, Pauling, Watson and Crick have made increasing use of concrete models to present, develop and discuss their ideas about molecular structures. This enabled them to predict the behaviour of the substances they were modelling and to speculate about the spatial arrangements of atoms and functional groups in their structures (Francoeur, 2000). Molecular models thus became obligatory tools in the study of the stereochemistry, properties, and reactivity of substances which, in turn, corroborated the atomic theory (Francoeur, 1997).

In recent years, computational models and modelling have been comprehensively established in chemical research. Two factors seem to have contributed to this. First, the study of the dynamics of chemical reactions – the mechanisms through which they occur – required the production of more complex models once static and rigid molecular models, as well as their two-dimension representations (formulas and equations – even when curly arrows are used), were shown to have a limited utility for this purpose. Second, the introduction of quantum mechanics provided chemistry with a new research programme (in Lakatosian terms) which allowed chemists to go beyond qualitative descriptions and even to predict the properties of materials which have not yet been synthesised (Erduran, 2001; Mainzer, 1999). The possibility of both combining a large amount of data, from several sources and about different aspects of materials, and of moving readily between different levels of representation (Ealy, 1999), has made computational models and modelling an essential tool for investigating known and new substances and their transformations. The approach is also vital in probing the properties and uses of new materials – undoubted one of the currently most important areas of chemical research.

MODELS AND MODELLING IN CHEMICAL EDUCATION: THE LEARNER'S PERSPECTIVE

The essential roles of models and modelling in chemistry ensure that they must not be neglected in chemical education. On the contrary, learning chemistry involves: (i) coming to know the major models already produced by chemists, as well as the scope and limitations of such models; (ii) appreciating the role of models in the accreditation and dissemination of the products of chemical enquiry; and (iii) creating and testing chemical models produced by an individual and/or a group (Justi & Gilbert, in press a). Therefore, a comprehensive understanding of models and modelling is essential for students' learning of chemistry.

From an interview-based enquiry involving mixed-ability seventh and eleventh grade students in the USA. who had not been taught about models (but not exclusively as part of their chemical education), Grosslight, Unger, Jay & Smith (1991) proposed that students' notions of the 'nature of model' formed a distinct hierarchy of stages. Students in Level 1 thought of models either as toys or as copies of reality. These sometimes have aspects or parts of the real thing omitted and are produced just to provide copies of objects or actions. Students in Level 2 thought of models as being created for a purpose. The emphasis on some components is therefore altered, but the template of reality still predominates. The model is tested solely in terms of its fitness for the predetermined purpose. None of these students reached Level 3, which had been identified in corresponding interviews with 'experts' (educated adults with an interest in the area of models). A Level 3 understanding was found to have three components: a realisation that a model is created to test ideas, rather than as a copy of reality; an acceptance that the modeller has an active role in its construction for a specified purpose; and the view that models can be tested and changed in order to inform the development of ideas.

These levels were used by Harrison & Treagust (1996) whilst investigating students' mental models of atoms and molecules. Most of the students in their sample (58%) were classified at Level 1 because they thought that there was a strong correlation between the structure of the models and reality. For instance, almost all of these students said that 'an atom is like a ball or sphere'. The other 42% of the students were said to be at Level 2 because they were able to express some difference between

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