Assessing modelling capability in chemistry

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Rationale for developing modelling capability

1. Most chemical explanations of macroscopic phenomena are based on submicroscopic models

A significant feature of the discipline of chemistry is that chemical explanations are based on entities existing at the nanometre level and below. Chemical explanation is also based fundamentally on electron rearrangements in ions, atoms and molecules, and these are not generally amenable to direct observation, even with instruments. Modelling of a wide variety is extensively employed in chemistry to make sense of the processes, which take place, and of the features of these entities, which affect the likelihood of chemical change.

2. Existing school chemical curricula teach chemical models as content to be learned

Science is based on "experimental evidence and models" to evaluate "phenomena and events".

1. Pupils should be taught:

a) that atoms consist of nuclei and electrons
b) about a model of the way electrons are arranged in atoms
c) how the reactions of elements depend upon the arrangement of electrons in their atoms

j) how the rates of many reactions depend on the frequency or energy of collisions between particles

The quotes above are drawn from the consultation materials for the revised National Curriculum (Science) in England (DfEE, 1999), The revision, while maintaining in one section that learners should be taught that chemists use models, treats chemical models as static. They are also seen as equivalent to content in the chemical content section of the curriculum. The emphasis in the text on the phrase *'accepted models'* indicates this approach.

3. Existing school chemical curricula omit the process of modelling

... theories do not come automatically from evidence collected, but may involve creative thought or take the form of models

Implicit in this quote from the revised National Curriculum referred to above is that models simply exist, that they are there to be taught. Other sections from this document over-emphasise the need to teach the provisional nature of models, by focussing mainly on those which have changed, and neglecting to mention that most models are durable. While not changing the character of models as provisional, it is important to recognise that many chemical models have a long lifetime in an atmosphere of rigorous testing and use. Although it is hypothetically possible to imagine that a non-particulate model of chemical change could prove useful, in practice anyone who seriously criticised the general idea that chemical change involved particle entities would be gently led to one side and his or her sanity questioned. The quote also demonstrates an amazing view that models and creative thought are not related!

4. Existing assessment methods tend to ask for rehearsal of the taught use of models in explanations, or in slightly modified novel situations

In examination questions about bonding, especially ionic bonding, or about electrolysis, these are either aimed at testing whether students can use accepted models in a familiar context, or in a slightly modified context. The focus is on application of familiar knowledge or on rehearsal in the examination. I have not seen any question at secondary school level, which refers to the creation of the model itself. It may be felt that this is beyond the intellectual level of the learners at this stage but it seems not to be taught in higher education either. Clearly more careful work needs to be done to verify the generality of this claim but assessment of graduates on initial teacher education courses in England provides some corroborating evidence.

5. Chemical modelling, as a process, can promote commitment to and confidence in chemistry where other methods have failed

Oversby (1998a) has investigated this for pre-service primary student teachers and found this to be the case.

6. Chemical modelling is an authentic chemical activity, and is intrinsically satisfying

Oversby (1998) has made a case for the prime intellectual activity of chemical researchers being modelling. If this is accepted, then chemical modelling is authentic. The evidence for it being intrinsically satisfying is provided by the vast number of research articles based on chemical modelling which are published in the chemical literature. It is also intrinsically satisfying for some novices too (Oversby 1998b)

7. Modelling is an intrinsic element in some National Curricula (eg England)

A case for this is made above.

Chemical modelling capability

As with any new idea, some clarification of its meaning and extent is called for. The following is an attempt to put forward some of the major components and boundaries.

1. Recognition of models - representations of ideas, processes, events, systems, objects
Gilbert (1993) made a well-accepted delineation of the term model as a form of representation. The range of representation is broad and inclusive. The examples provided are not simply representative but include the major classes.

2. Recognition of characteristics of good models (based on Oversby, 1998b)
In this paper only a very brief indication of the issues is attempted.

a. Representational features - points of correspondence and non-correspondence. Models do not exactly correspond to the original, otherwise it would be the original. Explicit recognition of those aspects that correspond to the original is not always recognised. There will be many aspects that do not correspond but here is meant those aspects that might give rise to confusion or misunderstandings.
b. Analogical mapping - drawing on features expected to be in common between the model and the original.
c. Role in explanations - models are a common and essential component of chemical explanations
d. Human creation - models are the product of creativity, of synthesis and are often aesthetic.
e. Types of models - avoiding the tendency to think only of computer-based molecular modelling and ignoring non-traditional forms such as role-play and poetry. In chemistry, models include word

equations, many drawn forms and prose descriptions.

f. Progression in modelling - based on both cognitive psychology thinking (eg progression from concrete to abstract) and natural thinking in chemistry about comparing qualitative and quantitative approaches.
g. Coherence with related models - idiosyncratic models tend to be shunned in chemistry.
h. Clear and systematic failure in explanations - for example, the ideal gas law fails not in a random way but in a manner which promotes modifications which possess rationality. The models created to modify the ideal gas law indicate significant features of the entities, such as their finite size and the existence of attractive forces.
i. Fruitfulness in exploring data from phenomena - the models for dissolution of ionic solutes have promoted the use of data such as measurement of energy changes, entropy changes, and dielectric constants in order to develop the hydration model further.
j. Predictive power in novel situations - the development of generalised kinetic models of organic substitution reactions has lead to greater confidence in predicting products from chemical reactions.
k. Simplicity - the simple ligand model for inorganic complexes has extended the range of data that can be explained using this model.
l. Quantitative if possible - - the transition state model of chemical kinetics has proved useful in explaining why the relation between absolute temperature and rate of chemical reaction is exponential. Such an approach leads to stronger tests of underlying models.

3. Contexts for demonstrating modelling capability

a. Use of existing models in familiar contexts
b. Use of existing models in novel contexts
c. Creation and use of new models in familiar contexts
d. Creation and use of new models in novel contexts

These are self-explanatory but as yet there is no understanding of whether learners find it easier to appreciate modelling if working within their personally created models, or if working with the accepted models of scientists.

Assessment methodologies

1. Assessment grids

Parts of explanations are given in separate boxes; students have to construct a complete explanation and justify their choice. An example is given below.

2. Question generating

An open-ended response is given to the students and the questions they generate are analysed for modelling capability. An example is provided below.

3. Concept mapping

The ways that students link concepts and create linking propositions is being examined for evidence for modelling capability. This is not reported here.

4. Interpretation of multiple models

Computer based molecular models were used to present different representations to 15 year old students. Students reported perceptions of each type and were requested to express preferences. This is discussed later.

5.Construction of new models to explain phenomena

The CoSim project (Heidelberg/Reading/Essen/Wilceta) is designed to promote model building of particle-based phenomena. This is not reported here but some materials are reported in another paper in this conference.

1. Assessment grids

These are similar to those used by the UK Open University for assessment purposes.

A. Many liquids can dissolve in each other.

B. Particles in a liquid have little space for movement before they collide with other particles.

C. Particles in a liquid move quite slowly and slip by each other.

D. Liquids are runny

E. Liquids spread out quite slowly.

F. The particles in different liquids can into each other's space

G. Particles in a liquid are very close to each other

In an experiment, Sam put some solution of copper sulphate, blue, in a beaker. Then Sam put some water on top of the copper sulphate solution, so that it did not mix straight away. It took a whole day for Sam to see that the blue colour spread part way into the water, and a few days for the blue colour to spread evenly through both liquids. T this time, Sam noticed that there was only one liquid in the beaker.
From the grid of boxes A - G, choose the box or boxes that give the best explanation. Write down this order. Why do you think this explanation is best?

Results
Almost all the students in a class of twenty-five 14 year olds chose descriptive explanations, or an indiscriminate mixture of macroscopic and submicroscopic descriptions. These students had not been explicitly exposed to teaching about chemical modelling. In a related activity with a parallel class, students were given a free hand to explain the experiment in prose. The results were similar to that found in the grids but were more difficult to analyse.

2. Question generating

Gunstone and White (1992) have described this tool. The example used in this work is given below to show its use.

The class was talking about the pictures of ethanol molecules shown. Tam asked the teacher a question but I could not hear what it was. The teacher said: "because each model shows only one way of looking at what the molecule might be." Make a list of all the questions, which might have been asked by Tam.

The great majority of the 14- 15 year old children created questions related to observable characteristics of the particles.

"Why are the atoms drawn at such a large scale?"
"Why are the atoms given these particular colours?"

None thought of questions relating to the apparent solidity of the atoms, or what might be in the space between the atoms, or of the shape of the molecules. Further elaboration and testing of this method is continuing.

4. Interpretation of multiple models

Students were shown a variety of representations of the ethanol molecule from a computer-based molecular modelling program. All the static forms could be rotated in animations. They were asked to pick out features in the model, which they felt corresponded to the actual molecule.

The forms used were:

1. Bonds represented as lines
2. Bonds represented as coloured lines, distinguishing different bonds
3. Ball and stick
4. Slightly open space filling
5. Completely space filling
6. Atoms as chemical symbols, with bonds
7. A stereoscopic form using green and red filters for observation

Students expressed a strong preference, almost unanimous, for ball and stick, and for the form expressed in chemical symbols. Students disliked the space filling forms probably because they obscured the centre of the molecules. Animations were thought to clarify the shape and bonding in the molecules. The commitment to forms explicitly taught, and to atom relationships and bonding, mirrors the concepts taught. It may be that students are more interested in the topology of the molecule in the first place, then go into the detail of bonding when they feel they know the molecule in a general sense. This needs further investigation.

Conclusions

1. Modelling capability is a legitimate learning outcome for all chemistry courses
2. Modelling capability is rarely addressed in secondary schools in England.
3. There are few existing validated instruments for assessing modelling capability
4. Issues such as coherence and progression in modelling capability require validated assessment tools for investigation
5. Some tools may be amenable to written summative assessments but many will only be practicable in coursework
6. Initial outcomes of the research indicate:
    a. There is very little appreciation of the nature of modelling by students in school
    b. There is little explicit teaching about the nature of modelling provided by teachers
    c. There is a limited use of molecular models in learning chemistry at the adolescent stage
    d. There is a remaining confusion between macroscopic behaviours and sub-microscopic explanations based on models

Future work

Some of the interesting areas yet to be explored include:

1. The use of models in novel situations

2. Development and validation of assessment tools in the classroom and examination room
3. Teacher development in using models and understanding modelling
4. Resources for teaching modelling in the chemistry classroom

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