

Playing with molecules

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Abstract

Recent philosophy of science has seen a number of attempts to understand scientific models by looking to theories of fiction. In previous work, I have offered an account of models that draws on Kendall Walton's 'make-believe' theory of art. According to this account, models function as 'props' in games of make-believe, like children's dolls or toy trucks. In this paper, I assess the make-believe view through an empirical study of molecular models. I suggest that the view gains support when we look at the way that these models are used and the attitude that users take towards them. Users' interaction with molecular models suggests that they do imagine the models to be molecules, in much the same way that children imagine a doll to be a baby. Furthermore, I argue, users of molecular models imagine themselves viewing and manipulating molecules, just as children playing with a doll might imagine themselves looking at a baby or feeding it. Recognising this 'participation' in modelling, I suggest, points towards a new account of how models are used to learn about the world, and helps us to understand the value that scientists sometimes place on three-dimensional, physical models over other forms of representation.

Keywords

Models – representation – imagination – fiction – depiction - manipulation

1. Introduction

Recently, a number of philosophers of science have suggested that we try to understand scientific models by looking to works of fiction. Such proposals draw upon a variety of different analogies between the two. Some begin from the observation that models involve false assumptions (e.g. Cartwright, 1983; Suárez, 2009) or see similarities in the way that models and fiction afford understanding (Elgin, 2009). Others draw parallels between the imagined worlds that both models and fiction appear to invoke (e.g. Contessa 2010; Godfrey-Smith 2006; Knuuttila 2009). While analogies between models and fiction may be suggestive, the real test of fiction-based approaches must be whether they can provide a coherent overall account of scientific modelling. Such an account should not only address the various different philosophical problems posed by models, but must also provide a convincing analysis of the practice of modelling.

One prominent fiction-based approach to models draws on Kendall Walton's influential *make-believe theory* of art (1990). According to Walton, artworks such as novels, paintings, and plays act as props in games of make-believe, like children's dolls or toy trucks. Proponents of the make-believe view of modelling suggest that scientific models might be understood in a similar way. In earlier work, I have argued that this approach may be used to address ontological problems posed by theoretical modelling, and to provide a general account of representation for models (Toon, 2010a, 2010b; see also Toon, forthcoming). Roman Frigg (2010a, 2010b) has drawn on Walton's theory to support a rather different view of theoretical modelling and its ontology, while a broadly Waltonian view of fiction has been put to still different use by Anouk Barberousse and Pascal Ludvig (2000, 2009). In this paper, I ask whether the make-believe view is supported by looking at the practice of modelling. Does the view provide a good account of the way that models are used, and the attitude that users take towards them?

My assessment of the make-believe view will be based on an empirical study of molecular modelling. One advantage of Walton's theory for fiction-based approaches to models, it would seem, is that it extends beyond literary fiction to encompass non-linguistic works such

as paintings or sculpture. My empirical study will examine both hand-held physical models, made out of plastic balls and connecting rods, and computer modelling software. One way to discover that children are engaged in a game of make-believe is to listen to what they say when they are playing the game. If we see a child standing astride a broom shouting ‘giddy up!’ while his friend complains ‘it’s my turn to ride now!’, we quickly guess that they are pretending that the broom is a horse, that standing astride the broom counts as riding the horse, and so on. Of course, such evidence is not conclusive (the children may be hallucinating). Nevertheless, it provides us with some indication that the children are playing a game, and suggests what form their game takes. Similarly, I assess the plausibility of the make-believe approach by examining the actions carried out by users of molecular models, and the way that they talk about those actions. In looking to practice to inform our understanding of models, my study therefore follows work by Daniela Bailer-Jones (2002, 2009), although my methodology will be rather different. While Bailer-Jones’ study used interviews to determine scientists’ views on various aspects of modelling, mine will be based on observations of the way that models are used and, in particular, of how this practice is explained to novices.

I describe the empirical study and its results in detail in Section 2. In Section 3, I will argue that the make-believe view can indeed be used to provide a good analysis of the way that molecular models are used. The claim that models function as props will be shown to capture only part of what is going on in molecular modelling, however. The children playing with the broom not only imagine things of the broom (that it is a horse); they also imagine things of *themselves* (that they are riding the horse, or stroking it). This imaginative *participation* in games of make-believe is a central and distinctive feature of Walton’s theory and, in particular, of his *pretence account* of discourse about fiction. Elsewhere, I have drawn on this account to analyse scientists’ talk about theoretical modelling (Toon, 2010a). In Section 4, I will show that scientists’ imaginative participation in molecular modelling extends beyond merely verbal participation to encompass both their visual and tactile engagement with models. Finally, in Section 5, I shall argue that recognising the importance of this participation changes our understanding of how scientists learn about the world through scientific modelling. As a result, I suggest, we are also able to achieve a better appreciation of the value of three-dimensional, physical models over other forms of representation. Philosophers of science typically focus on abstract, theoretical, models. And yet recent

historical studies have revealed the importance of physical models in many sciences, and of molecular models in particular.¹

2. Molecular models in use

2.1. The study

One way to try to understand a practice is to listen as it is explained to a newcomer. For this reason, the study involved an experienced user of molecular models (the ‘teacher’) and three new to the practice (the ‘students’). The ‘teacher’ was a final year doctoral research student in the Department of Biochemistry at the University of Cambridge, who uses molecular models regularly in her research. The ‘students’ were novices with no education in chemistry or other natural sciences beyond the age of sixteen. The students were set the task of determining the different possible conformations for a number of simple organic molecules, such as propane and cyclohexane, once provided with the correct structural formulae of these compounds. (Different *conformations* of a molecule are different ways in which the atoms within it may be arranged by rotating around, but without breaking, interatomic bonds.) This task was to be carried out using both a ball-and-stick physical model set and a computer modelling program.

The ball-and-stick models used were a Molymod® ‘Organic Stereochemistry Set’.² These models are made available to undergraduate students at a low price by the Chemistry Department at the University of Cambridge, and are used by students throughout their courses. Indeed, use of such models is recommended in many undergraduate textbooks. At the start of its chapter on stereochemistry, for example, Clayden, Greeves, Warren and Wothers’ *Organic Chemistry* advises students that

In reading this chapter you will have to do a lot of mental manipulation of three-dimensional shapes. Because we can represent these shapes only in two dimensions, we suggest that you make models, using a molecular model kit, of

1 On three-dimensional models in general, see de Chadarevian and Hopwood (2004). On models in chemistry see, for example, Francoeur (1997) and (2000), Francoeur and Segal (2004), Hendry (1999), Meinel (2004), Ramberg (2003) and Roche (2010). Laszlo (2000) offers a chemists perspective on the relationship between molecular models and toys.

2 These model sets are manufactured by Spiring Enterprises Ltd., Gillmans Industrial Estate, Natts Lane, Billingshurst, West Sussex, England.

the molecules we talk about. (Clayden, Greeves, Warren and Wothers, 2001, p. 381)

The model set consists of plastic spheres of different diameters representing standard organic elements, such as carbon, hydrogen, and oxygen. Short connecting devices are included so that these spheres may be attached directly to create ‘compact models’, commonly referred to as ‘space-filling’ models. Alternatively, connecting rods allow the same spheres to be used to form ball-and-stick models. When used in this way, the models also allow the representation of double bonds between atoms using longer, more flexible, connecting rods. It was in this ball-and-stick form that the models were used throughout the study.

The computer modelling software used for the study was the MDL® Chime molecular modelling program. This software is available for free and is widely used.³ It functions as a ‘plug-in’ for internet browser programs and enables users to view chemical structures in a variety of formats, including space-filling and ball-and-stick formats. In addition to viewing molecular models, users may rotate the entire model on the screen using the computer mouse. The program also allows users to move different parts of the model with respect to others, rotating about parts of the model representing single carbon-carbon bonds, for example. The Chime software requires users to input a database of model files, and for this purpose the study made use of the ‘DCU Molecular Viewing Gallery’, of the School of Chemical Sciences at Dublin City University (Pratt, 2006).

The format for the study was as follows. The teacher was first asked to show the student how to carry out the task of determining a molecule’s conformations from its structural formula by demonstrating the process through a simple example, typically ethane. The student then attempted the task themselves, with the teacher allowed to prompt and instruct the student where necessary. Both the teacher and the student were asked to reason out loud as far as possible, and the entire study was filmed with a video camera. The recording was then transcribed. The teacher was allowed to select all of the example molecules used for the study. Neither the teacher nor the students were told anything about the study’s aims, aside from that it was concerned to investigate how people learn using molecular models. The study was repeated three times with the same teacher and three different students. In the

³ MDL® Chime is a product of Accelrys, Inc., 10188 Telesis Court, Suite 100, San Diego, CA 92121, USA. It is available at <http://www.symyx.com/downloads/downloadable/>

excerpts from the transcripts included below, the teacher is denoted by ‘T’ and the students by ‘S1’, ‘S2’ and ‘S3’. Notes in square brackets describe actions undertaken by the teacher and students as they talk, while round brackets show parts of the transcript where their speech was difficult to follow or inaudible. Ellipses indicate pauses.

2.2. Talking about models

Perhaps the most striking feature of the teacher and students’ use of molecular models is their tendency to talk as if they were discussing the molecule itself, rather than a model of it. Here are just a few examples:

T: so what I’m going to do now is take out the double bond [starts disassembling model] so we’re back to just four in a row

S3: hmm

T: and then I’m going to add some other groups to it

S3: hmm

T: so here I’ve got two carbons, the two black ones

S3: hmm

T: and err a red one which is an oxygen and again I just fill up the gaps with hydrogen

...

T: [starts building model] basically, I’m making just some extra carbons to go on...

...

S2: OK...hmm... it can go in a variety of... hmm... all the spaces need to be filled up with hydrogens

...

T: yeah, so basically, when there’s just an extra carbon on, you’re right, there’s loads of different

places they can go, here, or here, or here [indicates parts of the model] and because they're quite small [twists parts of the model] they go anywhere

...

T: [disassembles model] so put the hydrogens back on so it's just a chain of hydrogen and nothing...and...what I'm going to do instead is put on some extra carbons and rather than hydrogen this red one is actually oxygen...and again it needs a hydrogen on it because there's two (holes there) [assembles model] OK, so if you knew that somewhere on our chain of four...

S2: hmm

T: there was an extra carbon with an oxygen and a hydrogen...so these need to go on your chain of four somewhere...what kind of different orientations...

S2: so they can go anywhere where there currently are just a hydrogen...OK, so... well, these could both be coming off the same carbon one, or they could be coming off a different one in any arrangement of that, or obviously off the same one they could both be coming off next to each other or opposite or, erm...[manipulating model]

...

S3: OK, so we're trying to make a molecule, basically

T: yeah

...

T: so what I'm going to ask you to do is to make a similar structure but with four carbons instead of two in it

S3: hmm... so do I have to put the hydrogens on as well?

T: yep...you can start with what I've already made

S3: yep

T: to make it easier rather than starting from scratch

S3: yep, sure, OK, err [picks up physical model] right, so we're going to get four carbons and put

them in a row...so do these carbons all have to be all straight in a line or can I put them ... like, can I put them here?

In each of these examples, the black spheres of the physical models are typically described as ‘carbons’, or sometimes ‘carbon atoms’, the white spheres as ‘hydrogens’, the connecting rods as ‘bonds’, and so on. Both the teacher and the students talk about ‘taking off’ hydrogens or ‘adding’ a double bond. Constructing the model is described as ‘making a molecule’. By contrast, only very rarely did the teacher and students’ discussions explicitly acknowledge that the immediate objects of their attention were not atoms or molecules, but coloured plastic spheres.

2.3. Looking at models

In addition to talking about the model as if it were the molecule, both teacher and student repeatedly speak as if they can *see* the molecule. A good example of this is the way that the teacher explains the difference between the ‘eclipsed’ and ‘staggered’ conformations of ethane. As the first excerpt shows, this way of speaking was not confined to physical models, but was also used when talking about the computer modelling program.

T: so if we look down this middle carbon-carbon bond [holds up model to S3’s eye line] it’s that one there and you can see that these hydrogens are lined up

S3: hmm

T: but they can twisted and they can be like that [rotates model]

S3: aha

T: so, yeah, different isomers basically, so you can also... so you can see it on the plastic models but you can also see it on the computer [takes mouse]

S3: aha

T: so I’ve got it opened here... I’ll try and stop it rotating... so here you can see the hydrogens are all lined up in front of each other

...

T: basically, the way they're named [picks up physical model] is from when you look down the middle bond what you see...

S2: oh [takes model] so this one is that [presents one orientation of physical model] basically

T: yeah, so the first one, the eclipse one, is when you look down the middle and they're both in line

S2: hmm

2.4. Manipulating models

Many historical and sociological studies of three-dimensional, physical models have stressed the importance of the physical manipulation that they allow. For example, Eric Francoeur notes that, when used in research, molecular models 'are not simply observed. They are submitted to various manipulations, assembled, probed and measured' (2000, p.12). This is certainly born out by my own study. Both the teacher and the students almost continually manipulate the models while reasoning through the problems set. The different acts of manipulation carried out on the models may be divided into three rough categories: building the model or taking it apart; twisting different parts of the model around; and rotating the entire model. Once again, it is striking that, while manipulating the models, the teacher and students almost always speak as if they were manipulating the molecule itself.

T: think about maybe keeping the middle two carbons [gestures a straight line then points to the centre of the model then gestures a twisting motion] straight initially and then seeing what different things you can do

S1: so I guess obviously you can have the carbons facing (inaudible), you know [gestures using model, turning it into a different orientation] and then basically the same down or up. And then obviously the end ones are much more... I can rotate those (inaudible)

...

T: [...] So what you can see here is basically all the bonds can twist round in various different shapes [twists model] but what would happen if we took two of these hydrogens off [takes off white sphere from model] you're losing two hydrogens and instead you can add a double bond

[adds two longer connecting rods] so maybe you could look at what difference that makes to the orientations [passes over model to S1]

S1: [picks up model] well, it makes it much more fixed [tries to twist model across double connecting rod, and rotates around end of single connecting rods] so you've got much less movement... basically the ends can twist and that's about it... that's the main thing

T: that's right. With single bonds you can get a lot of movement around them but with double bonds you can't.

...

T: because there's another hole there which is the equivalent of another electron they'll be one (inaudible) [builds model] and do the same on the other side... is there, how to ask it?... how many orientations I guess are there?

S1: well, I guess you can twist these up and around again [twists model] although again that might be problematic (inaudible) [shows that two parts of the model knock into each other] yeah, I mean, they're single things as well, so you can twist the lower half and the upper half around

T: hmm

S1: and you can also twist each branch

T: yeah, branches of the chain

S1: sort of around [twists different parts of the model] and then I guess with these in you can sort of move the hydrogens [twists other parts again]

...

T: erm, right now you're twisting around that middle bond

S3: oh yeah

T: twisting around but when you've got the double bond in

S3: we can't twist it... yeah yeah you can't twist around that way

T: basically double bonds are quite fixed, you can't twist them

...

T: but the hydrogens never kind of hit together did they?

S3: before?

T: like with these extra groups on

S3: No.

Manipulation is also important in the use of computer models. The teacher points out that the computer model will 'let you twist things' and, once again, both the teacher and the students often talk as if they were manipulating the molecule itself:

T: ... Also on this programme it'll let you twist things round. . . so if you go to this thing called sculpt mode, it lets you just twist things. [. . .] so you can play about with it, like you can with the model here [picks up physical model] you can do similar things

...

T: ... basically if you click on one of the atoms and drag a bit it'll let you play around a bit... so if you drag on a hydrogen you don't get much movement because they can't move much...

...

S2: hmm... [manipulating computer model using mouse] so this is showing me that I can rotate that and I can rotate that...

T: hmm

S2: and I can't rotate the carbons... is that right, should I be able to rotate the carbons?

T: yeah they should do a bit... that's what we (inaudible) but when you move one of the atoms on the computer what happens to the other ones... do they all stay the same, or...

S2 : well, if I move the middle ones the other ones move as well but on the outside ones I can do things quite freely

2.5. Play, pretence and realism

One aspect of the teacher and students' discourse that is particularly striking for our purposes are their explicit references to the use of molecular models as 'play'. Frequently, the teacher points out that molecular models allow you to 'play about with' the model or molecule. Molecular models are said to be 'fun' to use, and both teacher and student laugh and joke while using them. At one point, the teacher explicitly refers to pretence:

T: [building model] so now if we pretend that, rather than just being a carbon like this there's actually an extra ...what to put on? maybe add an oxygen onto it. That's the red one [points to model] that's oxygen.

One student uses this language while expressing scepticism over the use of molecular models:

S3: I mean it's nice to play with but it doesn't seem like it... I don't... I'm more trustworthy of that really [points to structural formula]

This comment must be seen as an exception, however. In general, references to play and pretence do not go hand-in-hand with scepticism over molecular models' representational accuracy. Indeed, the teacher, experienced in their use, most often exhibits a strongly realist attitude. Introducing the main task of the study, for example, she says:

T: so I'm just going to try and get you to think a bit about how from what you know... if you know what atoms are in a molecule how that can translate into a 3D-model of what the molecule actually looks like

3. Molecular models as props

Having seen something of the way that molecular models are used and talked about, let us now introduce the make-believe approach (Section 3.1) and consider whether it may be used to analyse molecular models (Section 3.2).

3.1. Props and games

Suppose that David and Anna are playing with a doll. In Walton's terminology, the doll is a *prop* in their game of make-believe. David and Anna imagine that the doll is a baby and, depending on what happens to the doll, they imagine various things happening to the baby: if the doll is in the cot, they imagine the baby is in the cot; if doll's 'eyes' are closed, they imagine that the baby is asleep, and so on. Walton calls the rules by which props prescribe imaginings *principles of generation*. Thus, it is a principle guiding David and Anna's game that if the doll's eyes are closed, the baby is asleep. It is not a principle that, if the doll is made of plastic, the baby is too. Principles of generation are normative: they say what participants should imagine, given the state of the props, if they are playing the game correctly. Walton calls imaginings that are prescribed within the game *fictional*. Thus, it is fictional in David and Anna's game that the doll is a baby, that at the moment it is asleep, and so on. Notice that what is fictional is not the same as what is actually imagined. If neither David nor Anna have noticed that the doll's eyes are closed, for example, they might not imagine that the baby is asleep, but it nevertheless remains fictional that this is the case.

Walton uses his framework to develop a theory of representation: representations, he suggests, 'are things possessing the social function of serving as props in games of make-believe' (1990, p.96). He argues that this concept of representation may be applied to novels, paintings, sculptures, plays, and many other works. Consider, for example, a marble statue of Napoleon on horseback. According to Walton, the statue, just like a doll, acts as a prop in certain games of make-believe. It prescribes viewers to imagine certain things (that Napoleon is riding a horse, that he wears a look of determination, and so on). Of course, the principles governing viewers' interpretation of the statue are rather different from those in the children's game. Presumably, for example, the children imagine the baby to be the same size as the doll; but viewers of the statue are not supposed to imagine that Napoleon is 10 feet tall just because his sculpted form is that high. The principles governing games featuring novels and paintings will be different again; they will be conditional upon the text of the novel or the distribution of oil on the canvass.

Thus, Walton argues that many things that we might call works of art or fiction, like novels, paintings and sculptures, may all be understood as props in games of make-believe. Where

these works represent actual objects, Walton claims, they do so by prescribing imaginings about them. Thus, both the statue and *War and Peace* represent Napoleon by asking us to imagine things about Napoleon, such as that he rode a horse or that he invaded Russia in 1812. In Walton's terminology, then, the statue makes it *fictional* that Napoleon rode a horse, and *War and Peace* makes it fictional that Napoleon invaded Russia in 1812. (Recall that to say a proposition is fictional in Walton's sense is merely to say that there is a prescription to imagine it; this is perfectly compatible with truth. This notion of fiction is therefore very different from another recently applied to scientific models, stemming from the work of Hans Vaihinger. In Vaihinger's sense, fictions are elements of theories that 'contradict' reality and are known to do so (Fine, 1993; Suárez, 2009).)

Two further features of Walton's view should be mentioned. The first concerns principles of generation. Often, the rules of children's games are declared explicitly ('let's pretend this is the pony!'). But principles of generation need not be explicitly defined, and the rules guiding our imaginings with most works remain implicit. The second point that should be noted concerns what Walton calls *reflexivity*. As well as prescribing imaginings, dolls are also the objects of those imaginings: David and Anna imagine *of the lump of plastic* that *it* is a baby. Dolls are thus *reflexive* props. This is not a necessary condition for something to count as a prop, however. The text of *War and Peace* may ask us to imagine things about Napoleon, but clearly we are not to imagine the page of text itself to be Napoleon. Nevertheless, some works of fiction are reflexive. For example, when we read an epistolary novel we may be supposed to imagine that the text we are reading is from a character's letter or diary.

3.2. Molecular models

Proponents of the make-believe approach to modelling suggest that we should understand scientific models in the same way that Walton analyses novels, paintings and plays, as props in games of make-believe. Can this framework be used to give a good account of the role of molecular models and the way that they are used?

Let us begin with physical models. As we saw, both the teacher and the students routinely talk about the models as if they were molecules. Attaching a black sphere to the model they

describe themselves as ‘adding a carbon’, while removing a white sphere is ‘taking off a hydrogen’. Connecting rods are almost always described as ‘bonds’. I suggest that the teacher and student imagine the model to be a molecule, just as a child imagines a doll to be a baby and refers to its parts as the baby’s ‘mouth’, ‘arms’ and ‘legs’. These imaginings are not random, but are guided by the model, together with certain rules: the student imagines that each carbon atom in ethane bonds with three hydrogen atoms because the black spheres of the model are connected to three white spheres, and because she understands that if two spheres are connected this means that the corresponding atoms share a bond. And these rules are normative: the student knows that if she were instead to imagine that the carbon were bonded to three oxygen atoms, she would have misinterpreted the model.

Taken together, these observations make molecular models props, in Walton’s sense: the models prescribe users’ imaginings according to certain rules. Physical molecular models are *reflexive* props: users imagine the models *themselves* to be molecules. Moreover, like the statue of Napoleon, the models represent actual objects, namely types of molecules, such as ethane, butane or cyclohexane. According to the make-believe view, this is captured by saying that users of molecular models are supposed to imagine that, for example, ethane consists of two carbon atoms, and so on. This may seem the wrong way of expressing the user’s attitude to molecular models: surely scientists *believe* that ethane contains two carbon atoms. The make-believe view need not deny this: one can imagine something that one believes to be true. (Consider the reader of *War and Peace* who imagines Napoleon’s invasion of Russia.) But perhaps we should drop talk of imagining altogether, and speak rather of prescriptions to believe?⁴ It is clear, however, that some of the content of molecular models is false, and known to be so: the atoms making up the molecule are represented as having definite sizes and locations, for example, although the truth is known to be rather more complicated. It seems that we are merely to imagine that such assumptions hold, not to believe them.

The make-believe view of molecular models receives further support from participants’ own descriptions of their use as ‘play’ or ‘pretence’. We have seen that this way of speaking was perfectly compatible with a realist attitude towards molecular models. And, on the analysis I have outlined, the two do not conflict: molecular models can function as props in games of

4 I am grateful for Aaron Meskin for raising this point with me.

make-believe, while many of the imaginings that they prescribe may be true, and believed to be true. The ethane model asks us to imagine that ethane consists of two carbon atoms, each bonded to three hydrogen atoms, and that these atoms have a certain definite size and structure; in Walton's terminology, the models make these propositions fictional. Some of what the model makes fictional is true (that ethane consists of two carbon atoms) while some is false (that they have a definite location).

What are the principles of generation that govern the use of molecular models? These will vary for different types of models. They have also changed dramatically over time.⁵ The principles guiding the use of the models in our study seem to have been as follows. First, there were a number of principles concerned simply with the way that the balls in the model are connected. If two balls are joined by a connecting rod then, fictionally, the corresponding atoms are bonded together. Ball-and-stick models also represent the shape of the molecule: if the connecting rods are distributed in a certain way about an atom, then, fictionally, the bonds between atoms in the molecule are also distributed in that way. Since the spheres of the Molymod models are made to scale, it is also the case that if one sphere is larger than another, then the corresponding atoms share the same relative sizes. But, of course, not all aspects of the shape of the model are 'carried over' to the molecule. Used as ball-and-stick models, for example, the Molymod molecular models do not represent to scale the distance between bonded atoms, nor, of course, do they represent bonded atoms as being joined by small 'interatomic sticks'. Finally, in addition to representing the bonds between atoms and their spatial distribution, the ball-and-stick models also represent the way in which these bonds allow atoms to move within the molecule: single connecting rods allow for free rotation; double connecting rods do not. Another principle guiding the use of the models, therefore, is that if one part of the molecule is free to rotate in a certain direction, then, fictionally, the corresponding part of the molecule is also free to rotate in that direction.

Let us now turn to the computer modelling program. There are a number of important differences between the physical and computer models. One is that the computer models are not reflexive. Pictures are, in general, not reflexive props: we do not imagine of the framed sheet of canvass entitled *Napoleon Crossing the St. Bernard* that it is Napoleon. Similarly, users of the computer model do not imagine that the computer display is the molecule that it

⁵ For example, early chemical models were not intended to show the spatial arrangement of atoms (e.g. Meinel (2004); Ramberg (2003)).

represents. Nevertheless, I believe, the computer model may still be considered as a prop in Walton's sense. The teacher and students imagine things of molecules when viewing the computer model, and those imaginings are guided by the display they see on the screen. Seeing a display depicting two overlapping spheres, for example, users imagine that the corresponding carbon atoms in the ethane molecule share an interatomic bond. Seeing that the two larger spheres can be rotated with respect to each other the user imagines that the two atoms may also rotate in that direction.

Our empirical study thus provides some support to the make-believe view. Of course, the evidence is not conclusive: there are other possible interpretations of the teacher and students' actions and talk about molecular models. This is particularly clear in the case of the computer models, where the analogy to games played with physical objects such as dolls or broom handles is perhaps less strong. Support for the make-believe view is made more compelling, however, when we consider users' active participation in modelling. That is the subject of the next section.

4. Playing with molecules

If the discussion so far is correct, then it seems that molecular models may indeed be analysed as props in games of make-believe. If we pay attention only to the models themselves, however, we will miss an important part of what is going on in molecular modelling. To offer a better analysis, I believe, we must recognise the importance of users' active *participation* in modelling. This participation also serves to lend further support to the make-believe view. In this section, I will introduce the concept of participation as it appears in Walton's theory (Section 4.1). I will then go on to show how this concept may be used to understand users' engagement with molecular models (Sections 4.2 - 4.4).

4.1. Participation and depiction

One of the most important aspects of Walton's view is his claim that, when we read a novel or

look at a painting, we participate in the fiction. As readers or viewers, Walton believes, *we ourselves become props in the games of make-believe we play with these works*. This claim follows closely from the analogy he draws between representations and children's games. Suppose Anna raises a cup to the doll. In doing so, she makes it fictional that she feeds a baby. Like the doll, Anna herself is a prop in the game: Anna's actions, together with the principles of the game, prescribe imaginings. Anna is also an object of the imaginings she prescribes: participants in the game are to imagine *of her* that she is feeding a baby, and *of her act of raising the cup to the doll* that it is feeding a baby. Similarly, according to Walton, we also participate in games we play with novels or paintings, by acting as reflexive props. For example, reading the early pages of *Dracula* I am to imagine that I am reading the character Jonathan Harker's journal; it is fictional of me that I am reading Harker's journal. When I look at a painting like *Napoleon Crossing the Saint Bernard* I am to imagine that I see Napoleon on horseback; it is fictional that I see Napoleon on horseback.

Of course, children's games usually allow for a greater degree of participation than representations like novels or paintings. Children playing with a doll, by moving closer to the doll and picking it up, or putting it down on a pillow, can fictionally move closer to and pick up a baby, or put one to bed. Getting up from your seat in the audience for *Macbeth* and approaching the stage to embrace the lead actor does not count as fictionally approaching or embracing Macbeth. Indeed, neither action would count as fictionally doing anything. Moreover, different representations allow for different forms of participation. Viewing *Napoleon Crossing the Saint Bernard* we may fictionally see things, notice them, or point to them. But if we were to evade the gallery guards and touch the painting this would not count as fictionally touching Napoleon. Touching certain sculptures may count as fictionally touching their subjects, however. Perhaps when a worshipper touches a statue of Christ it is fictional that they touch him. Plays, films and some musical pieces, it seems, allow audiences fictionally to hear things.

Participation underpins Walton's treatment of a number of important problems in aesthetics. As we have already noted, it plays a key role in his deflationary, pretence account of discourse about fictional characters. On this account, utterances about fictional characters are understood as acts of verbal participation in the game we play with fiction. If we say 'Dracula is a vampire', for example, we are not really asserting something about a fictional entity; we

are pretending to make an assertion in the game we play with Stoker's novel.⁶ Participation is also central to Walton's analysis of depiction. Consider someone who looks at *Napoleon Crossing the Saint Bernard*. As we saw above, according to Walton, when the viewer looks at the painting she imagines that she sees Napoleon. Moreover, the viewer imagines *seeing* Napoleon. However, this is not sufficient to distinguish pictures from other forms of representation. Someone reading *War and Peace* may also be expected to imagine seeing Napoleon, or St. Petersburg. What is distinctive of depiction, Walton thinks, is that the viewer of the painting not only imagines seeing Napoleon, but also imagines *of her looking at the painting* that it is an instance of looking at Napoleon. This is not true of the novel: the reader may imagine seeing Napoleon, but she does not imagine of her reading of the novel that it is seeing Napoleon.⁷

4.2. Manipulating molecules

In previous work, I have made use of Walton's pretence account of discourse about fiction in an attempt to understand scientists' talk about theoretical modelling (Toon, 2010a; cf. Frigg, 2010a). The present study suggests that scientists' imaginative participation in modelling goes far beyond merely verbal participation, however.

Consider first the teacher and students' manipulation of molecular models. We saw the importance of these acts of manipulation in Section 2.4. Physical molecular models can be put together, twisted, rotated, and finally taken apart and reassembled. Each of these acts are described as if they were carried out on the molecule itself. The teacher and students describe themselves as 'taking off hydrogens', for example, or 'twisting around that middle bond'. I suggest that the way in which users talk about manipulation of molecular models shows that they participate in the games of make-believe they play with molecular models in a variety of ways, just as children participate in their imaginative games.

When Anna raises a cup to the doll she imagines feeding a baby, and imagines of her act of raising the cup that it is the act of feeding a baby. Her act of raising the cup becomes a reflexive prop in the game. Similarly, I suggest, when the user of a molecular model twists

6 Of course, Walton's analysis of discourse about fictional characters is far from universally accepted. Friend (2007) gives a very helpful review of this debate.

7 For criticism of Walton's account of depiction see, for example, Schier (1986).

the model, she imagines herself twisting the molecule itself, and she imagines her act of twisting the model to be the act of twisting the molecule. The user's act of twisting the model is a reflexive prop: she is to imagine that it is the act of twisting the molecule, just as the children are to imagine that raising a cup to the doll is feeding a baby. It is fictional that the user's manipulation of the model is manipulation of the molecule.

Precisely what form of participation molecular models allow is a matter of what actions users can perform vis-à-vis the models such that they are imagined to be actions vis-à-vis the molecule. In the case of the ball-and-stick models used in the study, users of the models can fictionally build or disassemble molecules and fictionally twist different parts of them around. They can also fictionally rotate the molecule, and determine that two of its atoms will hinder each other. In so-called 'open' or 'skeletal' molecular models, on the other hand, the distances between atoms in the molecule are represented to scale and users can measure the distance between different parts of the model. And it seems that these acts of measurement are also (at least sometimes) construed as if they were carried out on the molecule. Francoeur quotes English chemist Derek Barton, who remarks of some skeletal models that

[t]he accuracy of manufacture and scale of these models is such that quite satisfactory measurements with a metre rule can be made of the distance between atomic centres. (Francoeur, 2000, p.9)

What about computer modelling? As we saw in Section 2.4, computer modelling also allows users to manipulate the model displayed on the screen. Just as with physical models, when users perform these 'virtual' manipulations they appear to imagine them being performed on the molecule itself. While using the mouse to rotate parts of the model, for example, one student asks 'should I be able to rotate the carbons?' Of course, users' virtual manipulation using the mouse is very different from the physical acts of manipulation allowed by physical models. We will consider the importance of this in Section 4.4.

4.3. Seeing molecules

Earlier we saw that, when looking at the models, the teacher and students speak as if they are looking at the molecule itself. Demonstrating the computer model, for example, the teacher

remarks, ‘here you can see the hydrogens are all lined up in front of each other’. Moreover, it seems clear that the teacher and student do not simply imagine seeing the molecule, as they might while reading a textbook; they also imagine of their act of looking at the model that it is looking at the molecule. The teacher directs the students to ‘look down this middle carbon-carbon bond’ in order to distinguish between staggered and eclipsed forms of ethane and points at the relevant part of the model to direct their attention there. Such actions suggest that users imagine of their visual actions vis-à-vis the model that they are visual actions vis-à-vis the molecule.

It seems, then, that molecular models are depictions, in Walton’s sense. The teacher and student relate to the model in a similar manner to that in which the viewer of *Napoleon Crossing the St. Bernard* relates to the painting. Of course, although the teacher and student speak as if they were looking at the molecule when viewing the model, they are well aware of the distinction between the two. Similarly, the viewer of the painting is well aware that she is looking at a piece of canvass, even while she imagines seeing Napoleon. Many features of the model are not ‘carried over’ to the molecule: we don’t fictionally see carbon atoms as black and hydrogen as white. But the same is true of many depictions: we don’t fictionally see the subjects of line drawings as composed of black and white lines. Compared to the painting, molecular models are relatively lacking in what Walton terms *richness*. Richness consists in the variety of visual actions that, by virtue of actual visual actions we perform regarding the work, we may fictionally perform. Looking at the painting, we may first fictionally scan the horizon, before peering closer, fictionally examining the red of Napoleon’s cloak, or the texture of the horse’s mane. The visual games allowed by molecular models are not particularly rich: we can fictionally see the molecule as having a certain structure, but not, of course, its colour or the texture of its surface.

Francoeur points to an important objection that might be made to the claim that molecular models are depictive:

Molecular models can be considered a mode of visual representation, in the sense that they allow us to visualize molecular structure. Yet, arguably, no chemist would propose that models, even in their more elaborate forms, are about what molecules “really” look like. In fact, any argument to that effect is bound to be

considered technically moot, since, as a prominent biophysicist has noted, “for something smaller than the wavelength of light, there is no such thing as showing how it really looks on the molecular level”. (Francoeur, 1997, p. 12. Quote from Richardson et. al., 1992, p. 1186)

The make-believe account helps to alleviate the sense of paradox somewhat. On a resemblance account of depiction, for example, it would be hard to see how molecular models could count as depictive at all. According to resemblance accounts, pictures represent their objects because they look like them; how could molecular models look like molecules if molecules have no appearance? It seems rather less problematic to say that we *imagine* ourselves looking at molecules.

Things are not so straightforward, however. Many molecular models are built to scale. They would therefore seem to represent molecules as being smaller than the wavelength of light. On the make-believe account, this means that we are to imagine that the molecules are smaller than the wavelength of light. But now it appears that we are asked to imagine a contradiction: we are both to imagine seeing molecules and to imagine that they cannot be seen. Similar problems arise for many pictures. When we look at the panels of the Sistine Chapel, for example, it seems we are to imagine seeing the Creation. And yet we are also to imagine that the Creation is unseen. There are number of different solutions we might adopt to such problems. For our purposes, we may simply note that the presence of a contradiction like this need not lead us to deny that molecular models are depictions.

4.4. Touching molecules

In contrast to our normal use of the term, Walton applies his definition of depiction to senses other than sight. Thus, a musical work that represents the chirping of birds may be depictive with respect to hearing: when we hear the music it is fictional that we hear birdsong, and it is fictional of our listening to the music that it is listening to birdsong. And a teddy bear may be depictive with regard to touch: it is fictional of our touching the teddy bear that it is touching a bear. I believe that, as well as being depictive with respect to sight, the physical molecular models used in our empirical study are also depictive with respect to touch.

To see this, suppose the scientist tries, and fails, to twist the model in a certain direction. When she does so, she feels the model exert pressure against her hand. In Section 4.2 we saw that scientists manipulating molecular models imagine themselves manipulating molecules. In this case, then, the scientist imagines her action to be that of trying and failing to twist the molecule. It follows, I suggest, that the scientist also imagines the pressure she feels against her hand to be exerted by the molecule. A comparison with dolls is helpful here. Suppose a child goes through the action of ‘feeding’ her doll and finds that its ‘arms’ get in the way. If she imagines her action to be that of feeding a baby, then it seems that she imagines the pressure exerted on her hands by the doll’s ‘arms’ as they impede her to be exerted by the baby’s arms.⁸

Physical molecular models are thus depictive with respect to touch. Once again, however, the games allowed by molecular models are not particularly rich. A teddy bear allows for a rich variety of different tactile actions, each of which may be imagined to be tactile actions involving the bear: we can fictionally squeeze the bear tightly or softly, feel the texture of his fur, and so on. Feeling the model resist twisting in a certain direction counts as fictionally feeling the molecule resist twisting in that direction. But feeling the texture of the balls and sticks that make up the model does not count as fictionally feeling the texture of the molecules. Nevertheless, the depictive character of scientists’ tactile interaction with physical models is important, as we shall see in Section 5. It is also an important way in which they differ from computer models.

Computer molecular models are not depictive with respect to touch. As we have seen, computer models allow for various forms of participation. Users can manipulate the model displayed on the screen, and when they do so they imagine manipulating the molecule itself. But, of course, the scientist using a computer model does not manipulate the model with her bare hands; she does so by moving the mouse and witnessing its effect on the screen. It is this ‘virtual’ manipulation that the scientist imagines being carried out on the molecule, not the actual, physical motion her hand makes with the mouse. And the tactile element is therefore lost. When she moves the mouse to perform this virtual manipulation the scientist does, of course, feel the mouse press against our hand. And an accomplished user of computer models

⁸ Of course, there are many puzzles one could raise in this regard, just as there are regarding the visual depiction of molecules. For example, isn’t it fictional that we cannot touch molecules? Once again, it seems that the threat of contradiction does not prevent us from engaging in such imaginings.

may even imagine feeling the molecule resist as she does so. But she does not imagine of the steady, even, feel of the mouse in her hand that it is the feeling of a molecule pushing back against her. For this reason, computer models (or at least those used in this study) are not depictive with respect to touch.⁹

5. Imagined experiments

To sum up so far: I have argued that molecular models may be analysed as props in games of make-believe, and that users of molecular models participate in these games. Users of molecular models not only imagine things about molecules; they also imagine themselves looking at molecules, picking them up and twisting them around. If this is correct, and scientists do engage in these sorts of self-imaginings, then clearly it is an advantage of the make-believe account that it is able to capture this feature of the use of molecular models. And users' participation in modelling lends further support to the analogy the account draws to games of make-believe. Still, one might wonder whether this participation is important. Is scientists' imaginative participation in modelling any more than an interesting psychological curiosity? I believe that scientists' participation in modelling is important. In particular, I think, it suggests a different view of how scientists use molecular models to find out about the world, through what I shall call *imagined experiments*.

We commonly think of learning about the world through scientific modelling as taking place in an indirect, two-stage, manner. First, scientists investigate the properties of the model. Second, they then use similarities between the model and the system being modelled to translate what has been learned about the model into information about the system. This might be a good description of the way that some physical models are used. For example, consider an engineer using a scale model to carry out tests. In this case, the engineer may well first determine the properties of the model, and then go on to calculate how these results 'scale-up' for the full system. Recognising scientists' participation in modelling, however, suggests that physical models may sometimes be used to find out about the world in ways not captured by the two-stage view.

⁹ However, there are some molecular modelling computer programs being developed that allow for tactile engagement. See Francoeur and Segal (2004).

To see this, let us again consider children playing with a doll. It is often noted that children's games of make-believe play an important role in teaching them about the world.¹⁰ To return to our previous example, suppose Anna raises a cup to the doll's 'mouth'. When she does so Anna imagines her action of raising the cup to be that of feeding a baby. Intuitively, it seems that Anna can learn something about caring for a baby through actions such as these. She may, for example, learn (at least partly) *how* to feed a baby. And here it is clearly important that Anna does carry out an action, rather than simply saying to herself 'imagine feeding a baby is like this...'. Doing so, it seems, further enhances Anna's experience, since she rehearses an action (at least partly) close to that of feeding a baby. Moreover, it would appear that through these imagined actions, Anna may learn things *about* babies. If Anna raises the cup and the doll's 'arms' get in the way, she imagines that the baby's arms have got in the way of her feeding it, and so learns that babies' arms can get in the way when you feed them.

Notice how poorly a two-stage account would characterise Anna's learning process. Similarities between the properties of the doll and the baby are, of course, important for underpinning her learning: if the doll had three arms, it would seriously lead her astray. But Anna does not first attend only to the doll's properties, and then go on to 'translate' this into knowledge about babies. Instead, her interaction with the doll is itself shot through with her imaginings about the baby. Anna imagines the actions that she carries out with the doll to be actions performed with a baby, and it is through these imagined actions that she learns both how to feed a baby and that their arms can get in the way when you do so.

I suggest that molecular models sometimes teach scientists about the world in a similar way. Suppose that a scientist tries, and fails, to twist the model in a certain direction, and thereby learns that the molecule is rigid in that direction. In doing so, I think, the scientist does not first discover that the model is rigid and then infer that, since the model and molecule share the relevant properties, the molecule is rigid also. Instead, she imagines her actual manipulation of the model to be the manipulation of the molecule, and it is these imagined actions that teach her about the molecule's properties. The scientist imagines the twisting action she performs on the model to be a twisting action performed on the molecule. And imagining trying, and failing, to twist the molecule allows her to discover that, fictionally, the molecule is rigid in that direction. If the imagined actions that the scientist performs are

¹⁰ On make-believe and pretense in children's games see, for example, Leslie (1987), Singer and Singer (1990), Sheikh and Shaffer (1979), Weisberg and Bloom (2009) and Wyman et. al. (2009).

accurate – that is, if what she imagines trying to twist the molecule at that point to be like is close to what trying to twist the molecule at that point would actually be like – then she is able to learn about the molecule’s actual properties. Unlike the child playing with the doll, of course, the scientist doesn’t want to learn *how* to twist the molecule, because we can’t twist molecules with our bare hands. But this form of learning is important with other physical models, such as the silicone models used by doctors to teach breast self-examination (cf. Francoeur, 1997).

Recent historical studies of a wide variety of physical models in the sciences have stressed the importance of the bodily, tactile engagement that they allow.¹¹ In his study of the history of molecular models in research, for example, Francoeur observes that ‘the way models mechanically resist or yield when one tries to have them adopt some configuration constitutes a physical, embodied experience of ‘allowed’ or ‘non-allowed’ spatial configurations’ (1997, p. 16). The value of this tactile element in molecular modelling is stressed by chemists themselves, and is often cited as the main advantage of physical models over computer modelling programs. Thus, in her discussion of molecular models for a Biophysical Society National Lecture, biochemist Jane Richardson (quoted above by Francoeur) notes that ‘the real virtue of [‘space-filling’ physical models] is the physical “feel” for the bumps, constraints, and degrees of freedom one obtains by manipulating them’ (Richardson et. al., 1992, p. 1186, quoted in Francoeur, 1997). Within the philosophy of science, Tarja Knuuttila has recently stressed the way in which our learning from models depends upon their ‘material dimension’ (2005, p. 1267).

Recognising the role of scientists’ imagined experiments with models allows us to appreciate the importance of the tactile engagement that physical models allow. In Section 4.4 we saw that physical molecular models are depictive with respect to touch: when users manipulate physical models they experience sensations of touch which they imagine to be caused by manipulation of the molecule. This allows scientists to investigate the properties of molecules in a kind of ‘imagined analogue’ of the way in which we discover the properties of normal everyday objects. We might find out whether a piece of metal is rigid by trying to bend it and feeling it resist. Similarly, using physical models, scientists can find out whether a molecule is rigid by carrying out imagined actions, fictionally bending or twisting the molecule and

¹¹ See, in particular, the papers collected in de Chadarevian and Hopwood (2004).

feeling resistance that it exerts. Computer models do not allow us to utilise our sense of touch in this way. For that reason, physical models even now retain a crucial advantage over their computer counterparts, despite the considerable advantages that computer modelling has introduced.¹²

6. Conclusion

A number of authors have looked to the make-believe view in order to address philosophical problems raised by scientific modelling. I have argued that the view also gains support when we look at the way that models are used. Users' interaction with molecular models, and the way that they talk about what they are doing, suggests that they do treat these models as props that guide their imaginings in various ways. As we have seen, this not only includes imagining the balls and sticks of the models to be atoms and bonds; users of molecular models also imagine themselves looking at molecules, picking them up and twisting them around. These imagined actions are central to the way that such models teach us about the world, and help to explain the value of the tactile, manipulable properties of physical models in particular.

Of course, questions remain concerning the wider applicability of this view. The study I have presented focussed on the relationship between a teacher and student, in order to uncover aspects of the practice of molecular modelling that might otherwise remain hidden. Since the teacher was herself trained as a member of the research community, it seems likely that the attitude to models uncovered in the study will also be reflected in the way that they are used in cutting-edge research. But further studies may, of course, reveal surprises here. We might also ask how far the account I have offered may be extended to cover other forms of modelling. In some cases, the analysis would appear to proceed along similar lines. A woman using a silicon breast model, it seems, is to imagine that she is examining her breast. The student taking apart one of Felice Fontana's wooden anatomical models was to imagine himself '[t]aking apart an entire man piece by piece' (Mazzolini 2004, p. 59). Some models might allow for only limited participation, however, or for participation of different forms. The Phillips machine models the economy using coloured water in a hydraulic system

¹² This includes, for example, the relative ease with which computer models allow the user to build models of large molecules and their ability to simulate more complex interactions between atoms within a molecule.

(Morgan and Boumans, 2004). Perhaps the user who manipulates the machine, opening and closing valves or changing the 'slides' to produce different functional relationships, imagines herself controlling the economy. As I see it, these questions will have to be decided from case to case. But I hope at least to have shown that the make-believe approach offers resources for developing a more general account of scientific modelling, and to have pointed to some of the insights that such an account might provide.

Acknowledgments

I would like to thank Soraya de Chadarevian, Stacie Friend, Roman Frigg, Martin Kusch, Tim Lewens, Aaron Meskin, Kendall Walton, and three anonymous referees, for their very helpful comments and criticism. Material from this paper was presented at the Inaugural Conference of the Centre for Literature and Philosophy at the University of Sussex in June 2008 and a Departmental Seminar in the Department of History and Philosophy of Science at Cambridge in November 2008. I would like to thank participants at both of these events for their helpful comments and questions. Research for this paper was supported by the Arts and Humanities Research Council, the Darwin Trust of Edinburgh and the Williamson and Rausing Funds of the Department of History and Philosophy of Science, Cambridge. I am very grateful to all of these institutions for their generous support. I would also like to thank all of the participants in the empirical study.

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