Conceptual Fluency: Switching Between Pre- and Post-Threshold Assumptions of Molecular Dynamics

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Abstract: We present preliminary analysis of chemistry graduate students' and secondary chemistry teachers' assumptions about mechanisms of chemical phenomena, around a set of threshold concepts. Chemistry education literature largely identifies pre-threshold assumptions as naive/alternative conceptions not particularly useful in understanding chemical phenomena. In the context of molecular dynamics, a threshold is considered to exist between thinking deterministically vs. probabilistically. We argue that (a) a deterministic perspective is as useful as a probabilistic one, (b) even experts implicitly exhibit (do not lose) deterministic assumptions, (c) probabilistic mental models are built on top of deterministic models, using multiple instances of the phenomena of interest, and (d) expertise involves willfully switching between pre- and post-threshold assumptions.

Introduction

Research on misconceptions and alternative frameworks has occupied a great deal of effort over the past decades. These endeavors characterize and differentiate between the ways in which students misunderstand the natural world and the models that science offers to explain it. At this point, there is no longer any doubt that alternative conceptions occur. Voluminous evidence supports claims that experts reason differently than novices (e.g. Kozma & Russell, 1997), and that some misconceptions are robust (diSessa, 2006).

Posner et al. (1982) introduced the theory of conceptual change to explain how students' conceptions change when new ideas and evidence are introduced. According to this theory the changes are analogous to the two-phase model of conceptual change in science (Kuhn, 2012; Carey, 1999). Borrowing terminology from Piaget, they called the first phase 'assimilation'. This occurs when learners use concepts they already possess to rationalize new ideas and evidence. The second phase, called 'accommodation', is more radical. It occurs when existing concepts are inadequate to rationalize new ideas and evidence, and the learner must replace or reorganize conceptual understanding. One thread of research proposes a parallel between the historical evolution of concepts in the discipline of science and the development of concepts in a child's mind (psychological recapitulation or the theory-theory view (Carey, 1999; Karmiloff-Smith, 1988; Vosniadou et al., 2008). A similar thread suggests that conceptions (alternative and correct) belonging to ontologically different categories (e.g. direct causal vs. emergent notions notion of a phenomenon, looking at a concept as a 'substance' vs. a more dynamic 'process' notion of the same) are more robust and difficult to remove/rectify, than ontologically similar ones (two different 'direct causal' notions of that phenomenon; Chi, 2008).

Although such models of conceptual change, and the curricular approaches they inspire, stress a qualitative understanding of scientific concepts and an overall constructivist perspective towards learning, many of them downplay or undermine the role of prior knowledge. They do so by considering that, as a result of rational thinking by the learner, correct conceptions will be chosen over (and will replace) misconceptions whenever the learner encounters conflicting ideas (Smith et al., 1993). This has propagated a problematic model of the mind that concepts can be replaced like physical objects.

The 'knowledge in pieces' (diSessa, 1993) perspective on the mechanism of conception and conceptual change suggests that a person's knowledge system consists of numerous simple elements of knowledge, called phenomenological primitives (*p-prims*). These *p-prims* are formed as a result of superficial interpretations of experiences of physical reality by novices, and are organized gradually into a conceptual network. In novices, this network is poorly organized, whereas in experts (through conceptual change), these pieces of knowledge are systematically integrated into larger and more complex systems of knowledge.

Alternatively, Mortimer (1995) has illustrated that a learner can hold several alternative concepts in the mind, and that context influences, but does not determine, the formation and exhibition of such concepts. At any given time, the learner's mind holds a distribution of different related (yet alternative and even contrasting) concepts. The concepts can be characterized, and each learner has a different distribution of these, called a conceptual profile. The conceptual profiles approach mildly denies the very occurrence of conceptual change, and maintains that alternative concepts can not only co-exist but also are necessary as they are often applied pragmatically in corresponding contexts.

There does not seem to exist a consensus among learning scientists (diSessa, 2006) on how conceptual change occurs, what are the mental mechanisms involved, and how can this process (of conception) be intervened with, if at all! A first step in resolving some of this conflict is to establish evidence for whether naïve assumptions or superficial interpretations are indeed replaced by more sophisticated assumptions or conceptual networks when conceptual change occurs, or if sophisticated assumptions and conceptual networks exist alongside naïve assumptions and superficial interpretations that continue to be relied upon. Considering that there are different forms of expertise, specifically expertise as researchers in a discipline and expertise in teaching a discipline, we designed a study to examine what assumptions are relied upon by experts who can be expected to have changed conceptions to at least some degree, if conceptual change occurs.

We present a preliminary analysis from a think-aloud and eye-tracking experiment showing that experts exhibit contradictory assumptions about mechanisms of chemical phenomena depending on the nature of the prompt. We then illustrate how a mixed distributed cognition and neural network model of knowledge representation may provide a possible mechanism of conception and conceptual change.

The experiment

We selected related pairs of assumptions that have been studied sufficiently and are considered to exist on opposite sides of a threshold concept (Meyer & Land, 2006). Threshold concepts are recently and increasingly robustly characterized as conforming to the following main features: 1) they are difficult to grasp, i.e., troublesome, 2) people's thinking becomes transformed when they cross over a threshold, 3) understanding a threshold concept generates interrelations between concepts previously considered unrelated, 4) the transformation is irreversible, and 5) the concepts serve as boundaries that mark a discipline (Loertscher et al., 2014; Talanquer, 2014).

Working within the discipline of chemistry, the threshold concept selected for our exploratory study is characterized by a transition that Talanquer describes as "from a centralized causal process to an emergent process schema" (Talanquer, 2014). This threshold concept centers on transformations of matter. Four related pairs of assumptions appear to straddle the threshold: (a) static vs. dynamic views of molecular behavior, (b) deterministic vs. probabilistic views of chemical phenomena, (c) direct causal vs. emergent views of mechanisms that underlie processes, and (d) object vs. interactions views of structure and properties of matter. Preliminary analysis reported here concerns (a) & (b) only.

Sample and methodology

Eight chemistry graduate students (GS2-GS9) from a university and six experienced secondary chemistry teachers (T2-T7) from schools in the Northeastern USA participated in this study. Participants were recruited from these two populations because they have different kinds of expertise (chemistry content expertise, and expertise in teaching chemistry), and the goal of this study was to examine expertise in chemistry considered broadly. All participants were individually presented with the same visuals, prompts and questions on a laptop screen, and were asked to talk the researcher through her/his entire thinking process. Figure 1 shows the protocol for one of the three experiment trials.

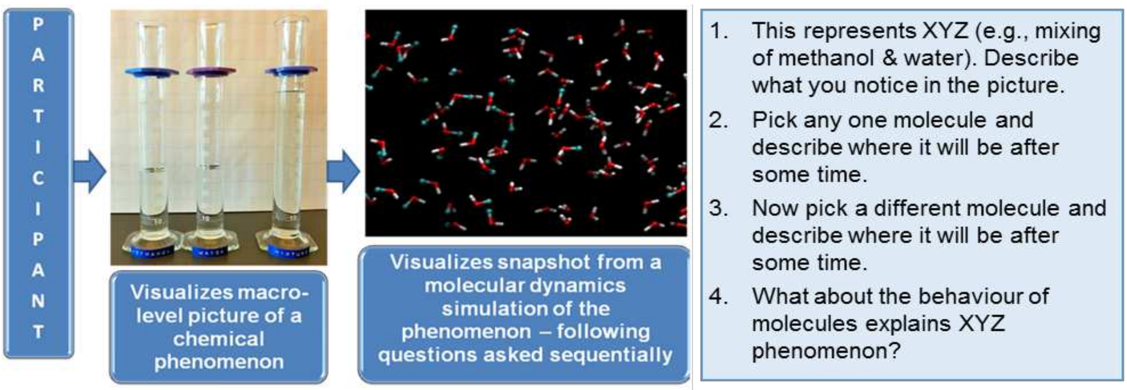

Figure 1.Experiment trial

Questions 2 and 3 were designed to stimulate reliance upon deterministic assumptions, the snapshots were static pictures and the question asked about the immediate timeframe ('what happens next?'). Question 4 was designed to stimulate probabilistic assumptions, as the question requested mechanistic explanation of how molecular-scale dynamics conflate to account for an emergent phenomenon. There were three trials, each involved presentation of four visual stimuli corresponding to a specific chemical phenomenon: a photograph of the macroscopic phenomenon, then three identical copies of snapshots of a molecular dynamics simulation with different questions asked for each of the identical stimuli. Three phenomena were presented: (a) mixing of methanol and water in the liquid phase, (b) formation of ice crystals from liquid water, and (c) combustion of hydrogen gas. Audio and video recorders were used to record participants' explicit thought processes for further analysis. Eye-tracking (Tobii TX2-60) was also employed to capture implicit behavior-level correlates of the deterministic-probabilistic thought processes, as well as differences between those correlates, if any.

Analysis
The think-aloud audios were transcribed. Trains of thought within responses to each question for each participant were characterized as indicating reliance upon either 'deterministic' assumptions or 'probabilistic' ones, based on indicators summarized in Table 1. Other codes, and eye-tracking results are not reported in this paper.

Table 1: Preliminary qualitative coding scheme for think aloud data.

Mental model/code	**Indicators/Markers**
Deterministic	Linear explanations of reaction mechanisms (uncertainty of events ignored), explained molecular/reaction behavior deemed **certain**
Probabilistic	Non-linear explanations of reaction molecular behavior, uncertainty/affecting factors considered, particular behavior of molecules/reactions as a **function of probability**

Findings
For the 'single molecule behavior' questions (Q2 & 3 - Figure 1, total six questions across three trials), eight participants provided probabilistic explanations (e.g. Transcript 1). They indicated the 'likelihood' of a molecular event depending on the properties of the picked molecule and its surrounding, and other possible factors that could affect that reaction. Four participants provided deterministic explanations (e.g. Transcript 2). One participant (T4) tended to use probabilistic and deterministic perspectives equally often interchangeably.

1. Transcript 1 (GS7): So.. the oxygen molecule near the bottom right, I don't know where it'll be, but it won't be where it is right now. And.. uh.. it may not be an oxygen molecule if it collides.. um.. with a hydrogen atom or molecule.. um.. with enough force to break the bond. That's about it.
2. Transcript 2 (T2): Let's pick another one.. to the right of those methanols, there are three water molecules in close proximity and the same thing I think would happen. The more negative oxygen side would be attracted to the more positive hydrogen side of the other two water molecules. And therefore they would move close together. That's it.

For the 'mechanism' questions (Q4 - Figure 1, total three questions over all trials), all participants (except T6) tended to provide 'likelihood' explanations. Interestingly, these overall seemingly probabilistic answers 'emerged' out of different small and isolated instances of deterministic explanations of molecular events. In summary, most participants relied upon both deterministic and probabilistic explanations while answering the 'single molecule behavior' as well as 'mechanism' questions. Thus, it seemed difficult and inappropriate to call a participant either a deterministic or a probabilistic thinker.

Discussion and conclusions
In this study, the 'single molecule behavior' questions were intended to cue for pre-threshold (deterministic) assumptions, while 'mechanism' questions were intended to cue for post-threshold (probabilistic) assumptions, if the participant had developed these assumptions.

Preliminary findings indicate that participants employed both pre- and post-threshold assumptions quite pragmatically. Deterministic assumptions were often exhibited among some participants when behavior of a single molecule was in focus. Meanwhile, the same participants seemed to employ probabilistic assumptions when explaining macro-level manifestations of molecular interactions. Deterministic models of phenomena offer executive control over variables by lowering cognitive load, and allowing externalization, (through representations and actions, Kirsh, 2013). Probabilistic models provide holistic understanding of chemical phenomena. Below we briefly discuss a possible general mechanism of conception indicating how assumptions lying on both the sides of a threshold can co-exist/exhibit. We present here a theoretical proposal based on recent advances in cognition. Our preliminary empirical findings described above are used to illustrate the promise of the argument.

A neural network model of conception

Neurons in the brain are connected to each other, forming a web. The networks formed out of these connections can exist in multiple activation states. Several neuro-imaging experiments and studies in distributed cognition show that specific activation patterns in the brain are coupled with specific elements in the external world (such as entities, phenomena, and their representations or models). There may not be a direct one-to-one correspondence between activation patterns and the external world, but the coupling has biological correlates.

We imagine a conceptual network supported by (possibly built upon) this biological neural network. Unlike in a semantic network, experiences of worldly events are coded as activation patterns in this conceptual neural network, so are scientific experiences of worldly events - through either direct exposure to those phenomena and/or multiple external representations and models of those phenomena (Pande & Chandrasekaran, 2016). In our view, a collection of related activation patterns is exhibited as assumptions/generalizations built upon relatively concrete experiences. Any new experience around corresponding worldly element leads to a reorganization of the existing network (or activation patterns), thus, changing the assumption. The extent of this change would depend on the (virtual) size of the previous network - richness and diversity of previous experiences. This property of the networks makes some assumptions robust, for instance the assumption among children (and even adults) that 'the earth is flat' as deemed robust by previous research. We argue that this, and assumptions alike, are not only retained in the network but also used implicitly.

This neural network model makes possible understanding 'alternative conceptions' as natural conceptions that can have validity under some circumstances, endowing them with utility. Thus, they should not be viewed as 'things to be dealt with'. There is no qualitative/mechanism level difference in the formation as well as nature between alternative and so called 'correct' concepts. This view is sympathetic with the *p-prims* as well as conceptual profiles approaches. From our perspective, the more diverse one's experiences around a concept, the richer the network/activation patterns may be. Expertise, therefore, is redefined as the ability to willfully switch between multiple assumptions/activation patterns. In other words, the conceptual neural network perspective predicts conceptual fluency rather than conceptual change, as a model of learning.

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