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Integration of multiple external representations in chemistry: a requirements-gathering study

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Abstract: Multiple external representations (MERs) are crucial in the learning and practice of chemistry. Representational competence (RC), the ability to simultaneously process, integrate and transform between MERs, marks expertise in chemistry. A major strand of chemistry education research attributes students' difficulties in learning to difficulty in understanding MERs, particularly the ability to imagine the various inter-connections between them. A dominant model of RC is Johnstone's model of three thinking levels, which describes three different levels of representations in chemistry (symbolic equations, molecular models and reaction phenomena), and treats cognitive load as the core problem underlying student difficulties with MERs. This model is used to design a number of computer interventions in chemistry, mostly focusing on lowering cognitive/working memory load, by simultaneously displaying on a screen, molecular animations, graphs and equations. In contrast to this classical information processing framework, our theoretical approach seeks to understand the internal cognitive mechanisms that support the processing of MERs, using recent cognitive theories such as distributed and embodied cognition. At the intervention level, we focus on achieving integration of MERs, through enactive/embodied interaction design approaches (such as fully interconnected and manipulable interfaces). Before developing the actual form factor of the interventions, we wanted to characterize student difficulties, and how students navigated through existing MERs. For this, we presented a categorization task to students, where 3D molecular animations (depicting only molecular level reaction dynamics, without symbols, text and other representations), graphs, chemical equations and videos of some chemical reactions were given to 6 chemistry undergrad students. Eye-tracking was used to obtain fine-grained data about participants' gaze and eye movement patterns while they viewed these representations. Addition of molecules, molecular aggregation, heat source and increase in velocity of the molecules were frequently attended-to features. Only one student made chemically meaningful groups with animations. Her eye-movement analysis reveals systematic mapping of animation features to chemical equations and other representations.

Keywords: Representational competence (RC), multiple external representations (MERs), chemistry education, molecular animations, categorization, eye-tracking

1. Introduction

Chemical phenomena are understood at multiple levels of detail (electronic configuration, stereo-chemistry or spatial conformation of molecules, stoichiometric ratios etc.), using multiple external representations (MERs) such as reaction mechanisms, molecular diagrams, graphs and equations at each level. A critical aspect of learning chemistry is developing expertise over these MERs. The ability to generate and use MERs in an integrated fashion (for conceptualization, discovery and communication) is indicative of expertise in chemistry. This skill-set is collectively known as representational competence (RC) in chemistry (Kozma & Russell, 1997).

Many problems and difficulties in teaching/learning chemistry are attributed to difficulties in understanding the different MERs in chemistry (Johnstone, 1991, 1993; Kozma & Russell, 1997; Gilbert & Treagust, 2009a & b). The achievement of RC, through many representational transformations, as well as the integration of MERs, is central to learning chemistry.

Currently dominant theoretical approaches, for instance Johnstone's model of three thinking levels (Johnstone, 1982) and versions thereof, describe the different levels of MERs (such as symbolic level, molecular level, etc.) based on the type and level of detail of the chemical phenomenon represented in those representations. This model is combined with working memory models, to

develop a cognitive-load-based characterization of RC in chemistry, which is used to also address student difficulties in dealing with chemistry MERs. This approach considers the simultaneous consideration of MERs by a learner as increasing her cognitive load, while an expert is better able to minimize/handle cognitive load by employing cognitive strategies such as information chunking.

Johnstone's model has inspired and guided the development and use of a number of computer interfaces in chemistry teaching/learning, typically used for making sense of MERs and also developing concept, phenomenon and procedure understanding using MERs (Kozma & Russell, 1997; Kelly & Jones, 2008). Many of these interfaces focus on the simultaneous, dynamic, display of MERs on a screen. However, the effectiveness of such computer interfaces in helping develop RC has been mixed. One possible reason for this could be that these designs are guided by classical information processing theories of cognition, where the role of the interface is to decrease the learner's cognitive load, particularly working memory load. Emerging theories of cognition, such as distributed and embodied cognition, postulate that the roles played by external representations are wider than decreasing cognitive load. For instance, external representations can support operations that are difficult, and sometimes impossible, to do in imagination (Kirsh, 2010). Further, actions could be a way of promoting integration (Chandrasekharan, 2009).

Current characterizations of RC in chemistry, and the interventions inspired by them, do not seek to provide a detailed understanding of the cognitive mechanisms underlying the processing of MERs, and thus offer only a rather superficial account of MER integration. Our research attempts to characterize RC by developing models of the cognitive mechanisms underlying the processing of MERs, particularly integration of MERs (which is how we define RC), and suggest design principles for interventions. Our theoretical approach, as well as interaction designs, are inspired by distributed and embodied cognition perspectives. In this paper, we report findings from an ongoing requirements-gathering phase for an intervention design. For this, we presented a categorization task to students, where 3D molecular animations (depicting only molecular level reaction dynamics, without symbols, text and other representations), graphs, chemical equations and videos of some chemical reactions were given to 6 chemistry undergrad students.

We used Tobii X2-60 static eye-tracker to capture fine-grained data on student eye-movement and gaze patterns across MERs presented to (and handled by) them. This data provides a deeper understanding of how students move through the representations (see e.g. Figure 2). Our preliminary analysis confirms earlier reports on novices' surface-feature-based exploration of MERs, but adds details of eye-gaze and movement patterns. Students struggled/failed in mapping dynamic features from animations to corresponding features in equations.

2. RC characterization and investigation approaches in chemistry

A significant strand of research in chemistry education reports descriptions of students' use of multiple representations, transformations of these representations, and the difficulties students face while doing both of the above. Studies show that students lack a clear understanding of basic concepts such as oxidation numbers, ionic charge, atoms and atomic structure, formal rules for writing molecular formulae, as well as meaning of subscript numbers and brackets and coefficients (Garforth, Johnstone & Lazonby, 1976; Savoy, 1988), and eventually fail to associate the symbols and numbers with substances and phenomena (Yarroch, 1985; Herron and Greenbowe, 1986; Nurrenbern & Pickering, 1987; Hinton & Nakhleh, 1999; Sanger & Phelps, 2007). Ben-Zvi, Eylon, & Silberstein, (1988) propose that students' thinking about phenomena relies primarily on perceptual/sensory information but since current pedagogical practices hardly provide perceptual/sensory assistance, students do not understand chemical symbols in terms of their macro and micro-level instantiations.

A more direct approach to characterize RC describes expert-novice differences in the use of MERs of chemical phenomena and their transformations (Kozma & Russell, 1997; Kozma, 2003), by using (in combination or in isolation) the influential working memory model (novices have less skills to manage cognitive load; Johnstone, 1982), context and practice (novices are less exposed to these; Ben-Zvi, Eylon, & Silberstein, 1988) and conceptual understanding (novices lack rich conceptual ground to counter cognitive load; Cook, 2006; Nitz, Nerdel & Prechtl, 2012). Kozma and Russell (2005) identified specific skills among chemistry experts, viz., (a) using representations to describe chemical phenomena, (b) generating and/or selecting appropriate MERs according to specific needs,

(c) identifying and analyzing different features of MERs, (d) comparing and contrasting different MERs, (e) making connections across different representations, relating/mapping features between MERs, (f) understanding that the MERs correspond to phenomena but are distinct from them, and (g) using MERs to support claims, draw inferences, and make predictions.

Experts also seem to better transform between static (such as equation & graphs) and dynamic representations (such as reaction mechanisms; Wu & Shah, 2004; Kelly & Jones, 2008; Nakhleh & Postek, 2008) while students face difficulties in producing static representations (e.g. sketches; Madden, Jones & Rahm, 2011) of the (imagined) dynamic particulate interactions. Understanding chemical phenomena involves building of internal (mental) models that simulate the behaviors of many individual molecules/atoms, their collective behaviors and properties (Levy & Wilensky, 2009) and effects of various parameters on such behaviors.

To improve students' conceptual understanding by linking and transforming between representations, interventions (guided by the above research and theoretical approaches) have focused on the use of computer interfaces, mostly based on the classical information processing approach to cognition, particularly Baddeley's working memory model (e.g. SMV Chem, visChem, 4M:Chem, EduChem HS, eChem, etc.). These interfaces, seek to lower the load on students' memory, by allowing learners to view multiple representations simultaneously on screen.

In contrast to this traditional memory-based approach focusing on simultaneous display, recent work, such as the Connected Chemistry Curriculum, focuses on interlinking representations through *manipulable* simulations and animations. Based on the Netlogo 2D interface, the manipulability feature may help students better transform between static and dynamic representations. The developers of this curriculum report, through control-experimental group studies, that the curriculum improves generation, handling and understanding of chemistry MERs, particularly the submicroscopic ones, among students, when compared to conventional text/lecture based curricula (Stieff & Wilensky, 2003; Stieff & McCombs, 2006). Such manipulable simulation interfaces have often been coupled with other scaffolds (such as exercises, quizzes, activities and teacher guides; Zhang & Linn, 2011) and have been effective in improving students' representations and understanding. Computer interfaces for RC assessment have also been explored, and could prove useful in characterizing RC. For instance, by examining students' use of a multi-representational molecular mechanics animation using eye-tracking, researchers show that students mainly use graphical and model representations in animations, often ignoring the equations (Stieff, Hegarty & Deslongchamps, 2011).

Despite this rich set of studies, there is no theoretical account of the cognitive mechanisms underlying RC, or efforts to develop interventions based on recent cognitive models.

3. Study and Research Questions

Here we report an ongoing requirements-gathering phase for an intervention design. The studies in this phase seek to characterize specific problems faced by students, and how they navigate through existing MERs. 3D molecular animations (depicting only molecular level reaction dynamics, without symbols, text and other representations), graphs, chemical equations and videos of some chemical reactions were given to 6 chemistry undergrad students. Our primary research question was:

How do students understand the reaction dynamics through animations and other representations? At the operational level, our questions include:

- What are the commonly/frequently attended-to features in bare/raw animations, and how are they used to establish links with other representations?
- Do students make chemically meaningful groups/correspondences between bare/raw animations and other representations?
- What are the correctly and incorrectly referred-to features in bare/raw animations, and other representations, in cases of chemically meaningful correspondences?

4. Materials, sample and methodology

Materials for the categorization experiment included, for five pre-determined general chemical reactions, bare 3D molecular animations, laboratory videos, chemical equations and graphs. We

developed bare/raw 3D molecular animation for five general chemical reactions. Each animation depicts only the molecular dynamics/mechanism of that reaction, and does not have any other embedded representations, such as text, narrative, or symbols. Free and open videos of the five chemical reactions (being performed in laboratories) were procured from on-line sources. Equations and approximate graphs were generated using an image editing software. Each representation was validated for content, conceptual and representational correctness, by two chemistry experts and one cognitive science expert. Figure 1 shows the preparation and execution of the experiment in detail.

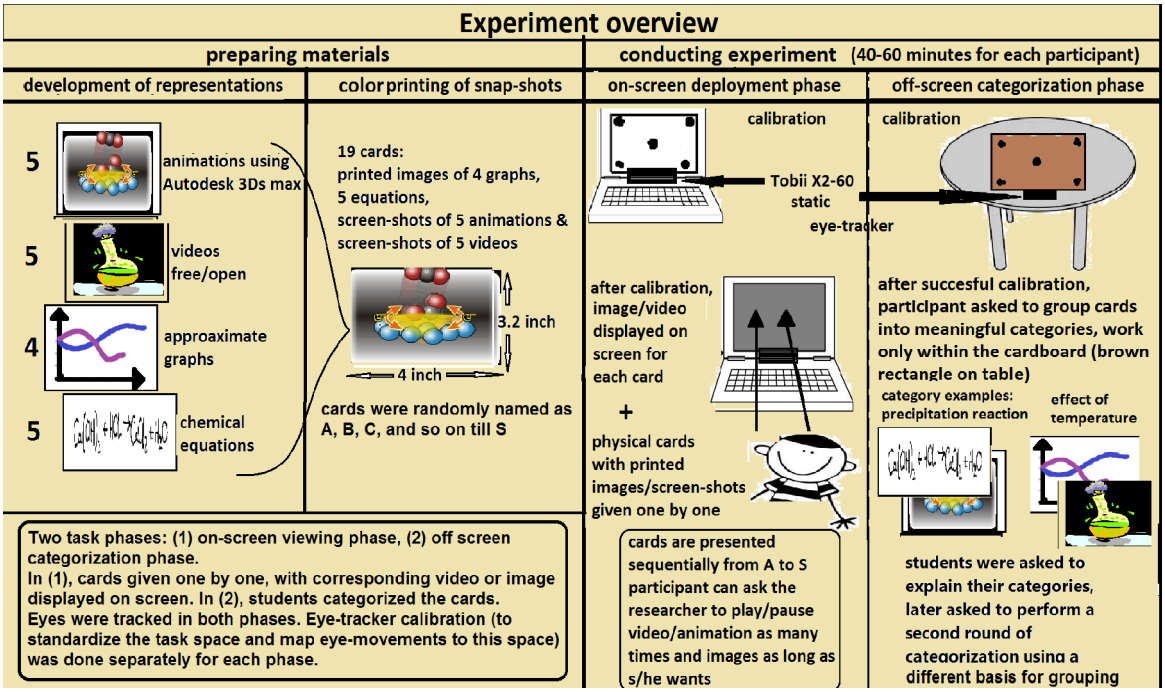

Figure 1. Material development and experimental design details

Six chemistry undergrad students (3 girls) from a nearby college participated in the categorization experiment; each of them performed the task individually.

Sources of data collection: (a) for on-screen phase – dynamic eye-movement and fixation data superimposed on the screen-capture video, (b) for off-screen phase – categories made by the participants, their verbal justifications, dynamic eye-movement and fixation data superimposed on the top-view video of the task-process, and side-view video recording of the categorization and justification sessions. The study session ranged from 40-60 minutes for each participant.

5. Findings and discussion

The number of animations used in chemically meaningful ways, and the explanations of categories (see table 1), suggest students found it difficult to understand animations.

All students, except G2, tended to map surface-features of animations to other MERs. For instance, the heat source in an animation was mapped with 'Δ' (symbol signifying 'heating') in an equation (e.g. equation for effect of temperature on NO_2 equilibrium) and/or with burner shown in videos. Addition of molecules, molecular aggregation, breaking of molecules, illumination of heat source and increase in velocity of the molecules on heating were the most frequently referred-to features in animations. Students often said, '...they (animations) all look alike...' while explaining their categories. None focused on the structure of individual molecules in the animations.

Graphs play a mediating role for linking static (equation) and dynamic (animation) content. An ideal way of examining the graph could be moving across its slope, and imagining the dynamics of the corresponding molecular behavior. None of the students' eye-movements match such a pattern,

nor did any of the students group graphs in chemically meaningful ways, except for B2. However, his eye-movement patterns are not indicative of simulating molecular/reaction behavior from graphs.

Table 1: students' usage of animations in the first round of categorization (each given 5 animations)

Participant	B1	B2	B3	G1	G2	G3
Total animations used (correctly + incorrectly)	5	5	3	5	5	5
Animations used in feature-based + chemically meaningful way	5	3	2	5	4	4
Animations used in only surface-feature-based manned	5	2	2	5	1	4
Animations used in only chemically meaningful manner	0	1	0	0	3	0

G2's results were close to expert-level, so we present brief findings from a preliminary analysis of the task only for G2. She made 4 categories with the 19 representations, placing 4 out of 5 animations with 4 chemical equations (NO_2 equilibrium, precipitation, AgCl-NH_3 equilibrium and aqueous cobalt chloride equilibrium), each animation corresponding to one equation. One pair was incorrect (cobalt chloride equilibrium paired with animation representing neutralization reaction). The remaining animation was grouped with two graphs and two videos (all four representing effect of temperature on equilibrium).

While viewing the animations, G2 tended to follow only one molecule at a time, and was attentive to changes in the number molecules, and their bonding and breaking. G2 did systematic scanning of the equation, looking for molecular formulas and subscripts. Figure 2 shows one segment of G2's gaze sequence, while she viewed an equation. For instance, G2's second fixation (point No. 2) was on the subscript (aq) that denotes aqueous state of KNO_3, at fixation point 3, G2's attention is on subscript (s) that denotes the solid state of PbI_2. Immediate next fixation (point No. 4) occurs on subscript (aq), aqueous state of KI. A similar pattern is observable while G2 viewed other equations. G2 seems to trace the states of elements before and after their displacement. There are both forward (in the direction of the reaction) and backward (opposite to the direction of reactions) eye-movements. Such movements may generally be associated with sequential imagination of reaction dynamics. Her chemically meaningful categories, combining animations and equations, and her gaze pattern, suggests that she imagined the step-wise dynamics of molecular mechanisms, using the symbols in the equations. A detailed analysis of her gaze pattern, and comparison with other participants' gaze patterns, is ongoing. We expect to present details of this analysis at the workshop.

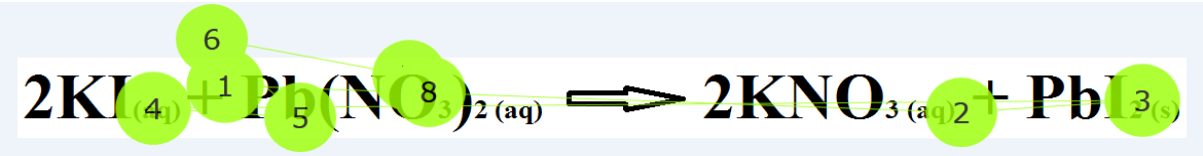

Figure 2. An instance of student G2's eye-gaze sequence

6. Conclusion

Students have difficulties in chemically relating animations to other representations such as graphs and equations. They tend to focus on surface features and ignore important dynamic features in animations. Molecular dynamics are difficult to understand, and integrating them with equations and graphs requires generating dynamic features using static equations and graphs. This imagination of dynamics, and the cognitive mechanisms underlying such imagination, appear critical to the development of RC in chemistry. A preliminary study was done to characterize student difficulties, as a requirements-gathering phase for interaction designs for gaining RC. The study replicated some results from literature, and adds further details about how students move their eyes as they navigate (through) the MERs. Further analysis would help isolate eye-movement and navigation patterns related to RC.

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