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Use and Design of Analogy-Based Simulations to Teach Abstractions and Abstract Concepts

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Animations, simulations and visualizations are playing an increasingly important role in chemical education. A powerful use of such tools is to give students experience at the particulate level of chemistry by depicting collections of molecules. Here, however, the use of analogy-based simulations is considered as a means to help students learn abstractions that lie at the core of chemical reasoning. Rather than depict atoms and molecules directly, these simulations use a variety of alternate representations. These range from familiar physical systems, such as boxes and steps, to the diagrams employed by expert chemists, such as energy landscapes. Based on a review of analogies and other forms of comparison in educational psychology, abstractions are identified as a core part of expert reasoning in chemistry. Analogy-based simulations help students learn such abstractions by providing multiple representations that clearly illustrate the abstraction's internal relational structure. As examples, analogy-based simulations for the thermodynamic abstractions of thermally-activated processes and entropy-driven reactions are discussed. Based on both the psychological literature and direct experience developing these simulations, design guidelines are developed for analogy-based simulations.

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Introduction

Over the last thirty or so years, analogies have enjoyed increasing attention in both the education and psychology literature. Within the realm of science education, in particular, the study of analogy usage in texts and in classrooms (1–8), as well as advocacy for the use of analogies to teach difficult concepts (9–14) has been significant and influential. Those who specialize in chemistry education have also taken an interest in the use of analogies to teach chemical concepts (15–19). Simultaneously, educational psychologists and cognitive scientists have been building theories of how people use and understand analogies (20–27), which has provided additional guidance to those interested in using analogies in educational contexts. In sum, we now know that when used in appropriate ways in the teaching of well-suited topics, analogies can provide a powerful means to enable students to understand difficult subjects. Furthermore, research is continuing to refine our understanding of which subjects are well-suited to treatment by analogy and how to best present analogies in educational settings.

Over approximately the same span of time as analogies have come to prominence, computer-based visualizations and simulations have also undergone a transition from uncommon to ubiquitous. This has occurred in many fields of science and engineering, though it has been perhaps most pronounced in physics and chemistry. In chemistry education, as computers have become cheaper and increasingly powerful, visualizations have increasingly replaced physical models. Furthermore, the growing body of research in student misconceptions has identified many areas of difficulty that can be traced to deficient understanding of stuctures and processes at the molecular level, providing impetus to create simulations of these structures and processes for students.

Interestingly, in spite of the concurrently increasing popularity of both analogies and simulations, the two have remained largely separate, at least in chemistry education. Here we argue that there are compelling benefits for the marriage of analogy and simulation and we hope that, through this contribution, we will motivate others to think about ways to deepen student understanding through analogy-based simulations.

Analogy-Based Simulations: Why?

What Are Analogies?

Before we discuss analogy-based simulations, it is first necessary to clarify what is meant by the term "analogy". Analogies come in many forms but, fundamentally, they compare one concept or item with another. Vague analogies might take the form "A is like B", where A and B each represent a concept or object. In this case, how exactly A is like B is not specified and remains open to interpretation. A more specific analogy might take the form "A is like B in that…". Such an analogy explains the manner in which A is like B. In the cognitive science literature, stating that two physical objects resemble one another visually is categorized as a statement of "mere appearance", rather than an analogy (20). Analogies, on the other hand, claim similarity between objects on a deeper basis, such as similar relationships between constituent components.

Simple analogies of the form "A:B::C:D" clearly display analogies' focus on relationships. These analogies assert that two pairs of objects or concepts, (A,B) and (C,D), share identical relationships. That is, the relationship that A has to B is the same as the relationship C has to D. These analogies make no claim that any kind of similarity exists between A and C or B and D. Rather, they focus on the similarity of the A-B relationship to the C-D relationship.

While such analogies involve one shared relationship, more useful and powerful analogies typically involve many shared relationships. When drawing an analogy between two concepts or systems of objects, it is unlikely that all internal relationships will be shared; however, good analogies will involve the sharing of many, particularly high-level, relationships (20). A concept or system can be modeled as a group of interconnected nodes, where the nodes represent sub-concepts or objects belonging to the system and the internodal connections represent relationships. Creating an analogy, then, involves aligning the structure of the nodal network of one concept to the structure of another. Gentner (20) coined the terms "structural alignment" and "structure mapping" for this process. In this process, the identity of each node is not important; rather, only the topology of the network and nature of the represented relationships are relevant.

In education, analogies are used to teach students about an unfamiliar concept, system, or process by means of its relationship(s) to a familiar concept, system, or process. In this usage, the unfamiliar concept is typically called the *target*, though some researchers call it the *topic* (5, 28). The familiar concept goes by many different names in the literature, including *base* (20), *source* (29), *analog* (11), and *vehicle* (5, 28). In this chapter, we will use the terms *base* and *target*, respectively.

Analogies And Other Categories of Comparison

Analogy is not the only type of comparison discussed in the literature. Rather, there is a whole spectrum of comparison categories, which are differentiated on the basis of 1) the number of *attributes* (that is, single object descriptors) shared by the compared items and 2) the number of *relationships* (that is, descriptors relating two objects) shared by the compared items (20, 24). These categories are as follow.

Mere appearance (20) comparisons involve the sharing of many attributes but few relationships. An example of a statement of mere appearance is “Clouds look like pillows.” Clouds and pillows have a similar appearance but they are composed of different substances, behave differently, and have different functions, etc. Their only similiary is in their appearance.

Another type of comparison, known as *literal similarity* (30) involves many shared attributes as well as many shared relationships. An example of a literal similarity is “a Torx wrench is like an Allen wrench.” Both items are similar in size, shape, and color, so they share many attributes. In addition, both are also used by people to tighten and loosen bolts, so they also share person-wrench and wrench-bolt relationships.

The opposite of literal similarity is *anomaly* (31). Anomalies involve few shared attributes and few shared relationships. These are of little utility in science teaching, so we will not consider them further.

From the earlier discussion of *analogies*, it is clear that they involve few shared attributes but many shared relationships. As an example, a common analogy used in physics involves comparing electricity to flowing water (32). Of course, electricity and water are not visually or compositionally similar, so they do not share many attributes. However, the way electricity and water behave is similar, so they share many relationships. For example, they both flow in response to a driving force (voltage gradient, gravitational potential energy gradient) and their flows can be impeded (by a constriction in a pipe, by a resistor), etc.

Finally, a special case of analogy, termed *abstraction*, is similar to analogy in that it involves many shared relationships but few shared attributes. However, it differs from analogy in that one of the compared entities is an “abstract relational structure” (20) rather than a concrete physical object or system of objects. As such, the abstract relational structure simply does not possess many attributes that could be shared. An example of this is “the solar system is a central force system” (33). Central force systems can exist on hugely different length scales (atom vs. solar system) and even the nature of the force (gravitational, electrostatic, magnetic) is not specified. Thus, the notion of a central force system is based on relationships – the forces that objects exert on one another – rather than any attributes. Finally, note the language used in the comparison. While the other categories of comparison use the word "like", with abstractions, we say "is". This indicates that one object is an instance or example of an abstraction.

Although they may appear synonymous, the terms "abstract concept" and "abstraction" are not the same. In the work on thermodynamics discussed below, energy and entropy are two central concepts. These concepts are clearly abstract, since they cannot be observed directly and find broad use across all areas of science. However, they are not abstractions, in the sense described by Gentner (20), since they are not relational. In the work described below on thermodynamics, "thermally-activated processes" and "entropy-driven processes" are abstractions. Just as for the central-force system discussed above, these abstractions apply to situations in which the entities being described have little overlap regarding surface features, but share a common relational structure that leads to a common and powerful mode of reasoning.

What Are Analogy-Based Simulations?

Now that we have considered analogies and abstractions, let us turn our attention to analogy-based simulations. Analogy-based simulations are simulations that do not directly depict atoms or molecules; rather, they simulate a different physical system that relates to a chemical system or concept by analogy. For example, Figure 1 uses (non-interacting) balls bouncing on a vibrating staircase to illustrate how the population of a given state depends upon its energy and the temperature of the system. Table I details the analogical correspondences between features of the staircase system and chemical systems.

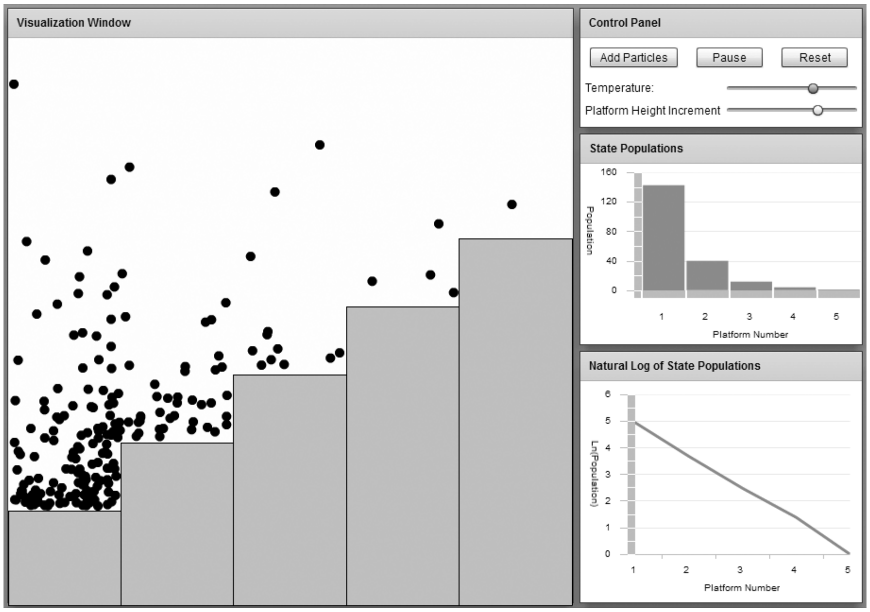

Figure 1: Balls bouncing on a vibrating staircase as an analogy for the population of states in a chemical system.

While using a simulation to illustrate this concept is not strictly necessary, we believe that it provides a more compelling and memorable learning experience than simply looking at an equation or a graph. Furthermore, many students are not skilled at interrogating an equation or graph in order to construct a general, qualitative understanding of what the graph or equation represents (34). For such students, a simulation of this type may make it easier to construct a qualitative understanding of the important functional relationships that govern system behavior.

Table I: Analogical Correspondences Between Staircase and Chemical Systems

Feature of Chemical System	*Representation in Staircase System*
(sub)System	Ball
State	Step
State energy	Step height
Temperature	Vibration amplitude
State population	Number of balls above a step

While engaging with the simulation shown in Figure 1, students are able to manipulate both the difference in energy between platforms, ΔE, as well as the system temperature, T. As they increase ΔE, they find, as they probably expect, that the number of balls on the highest platorms goes down and a greater fraction of balls occupies lower platforms. This change can be undone by raising the temperature, giving balls the energy that they need to occupy higher platforms.

In addition to the simulation itself, the user interface also provides two further representations of the state populations. Both of these representations are meant to clarify properties of the Boltzmann distribution. The exponential decay associated with the Boltzmann distribution is clearly displayed in the bar graph at top, while the fact that the natural log of an exponential decay takes the form of a downward-sloping line is shown in the line plot at bottom. Thus, in addition to observing that fewer balls occupy higher platforms when ΔE is increased, students may also observe that increasing ΔE causes the slope of the line at bottom to become steeper, while increasing the temperature causes the slope to become shallower.

What Is The Utility of Analogy-Based Simulations?

There are two overarching scenarios in which analogy-based simulations may be used. The first involves using analogies to simulate concepts which are not possible or not feasible to simulate directly with depictions of atoms or molecules, or which could be simulated more clearly by analogy. A good example of such a concept is entropy. As a consequence, many curricula use analogies involving dice (35) or other simple systems (36) to discuss state degeneracy and, by extension, entropy.

The simulation in Figure 1 is another example of a concept that can be treated effectively using analogy. Though it is possible to create simulations of chemical systems that exhibit the Boltzmann distribution, the chemical systems' additional detail can get in the way of understanding. By presenting a very abstract system, which has few attributes to distract students, the core idea and behavior of the Boltzmann distribution can be made clearer.

The second main usage scenario is focused on helping students to understand overarching categories of systems and develop abstract ways of thinking that are similar to those used by experts. We will focus primarily on this mode of usage in this chapter.

Beginning in the 1960's psychologists began to wonder what differentiated experts in a particular domain from novices. This curiosity led to many fascinating and useful discoveries. While there are a number of interesting results, for our purposes in this chapter, the key result is that experts' "knowledge is not simply a list of facts and formulas that are relevant to their domain; instead their knowledge is organized around core concepts or ‘big ideas’ that guide their thinking about their domains” (37). Glaser and Chi (38) elaborate on this by noting that “[e]xperts see and represent a problem in their domain at a deeper (more principled) level than novices.” The fact that experts understand their domain in a deeper, more abstract way than novices has been demonstrated across different domains in a number of studies in which experts and novices were asked to organize problems or representations into categories of their own invention (39–41). In each of these studies, in physics, computer science, and chemistry, respectively, experts were found to create categories on the basis of more abstract, overarching principles that govern the domain, while novices were found to choose categories mainly based on surface features.

Since education concerns itself with turning novices into experts, it is important to consider how we may help this process along with our students. In particular, in light of the above discussion, we may ask how we can help our students to develop domain knowledge that is structured like that of an expert. The purpose of this chapter is not to suggest what the “big ideas” in chemistry are. However, in what follows, we will describe how analogies and analogy-based simulations can help students to understand the “big ideas”, which are sure to be abstract, and to organize their knowledge around them.

First, as discussed earlier, *abstraction* is a special case of analogy, in which the target is an abstract relational structure rather than a concrete object or system (20). Thus, we can help students understand important abstractions by providing them with accessible bases that cleanly map to the features of the abstraction. This is the most direct way of approaching abstractions.

A somewhat less direct approach to abstractions involves creating analogies between different systems that are both instances of the abstraction. In this case, the analogy between the systems captures the important features of the abstraction. That is, while the analogy maps a feature of the base to a feature of the target, in the abstraction, those mapped features are seen as different manifestations of the same abstract entity or phenomenon.

For example, a famous analogy in science is Rutherford’s analogy between the solar system (familiar) and the structure of the atom (at the time, novel). In this analogy, the sun maps onto the atom’s nucleus and the planets map to the atom’s electrons. Of course, an atom’s nucleus does not resemble the sun in any way, nor do electrons resemble planets. Instead, the analogy captures the fact that, like planets orbit the sun, electrons orbit the atom’s nucleus. Gentner (20) fleshes out the analogy by pointing out that, in both systems, a central object is surrounded by other objects that 1) are less massive, 2) revolve around it, 3) attract it, and 4) are attracted by it. This very generic way of describing the systems helps us to understand that, in fact, both the solar system and the atom are instances of a central force system, as mentioned earlier. By analyzing the analogical mappings between these two systems, we can see the key features of the abstraction of which they are both instances. It is worth noting here that what Gentner (20) calls an abstraction has also been called a "superordinate concept" by Glynn (11, 42), and the term "model" is also sometimes used in a similar sense (19), though not always (1).

So far, we have seen that by directly comparing a base to an abstraction and by comparing a target to a base with the analogy between them capturing an abstraction, we can help students to access abstractions and understand how they encapsulate structural or behavioral relationships shared among superficially different systems. This gets at the heart of an expert's knowledge structure. However, simulations require quite a bit of time and effort to create. What is to be gained by creating an analogy-based simulation, rather than simply presenting and unpacking an analogy with students?

We are not aware of any studies that have compared the efficacy of analogy-based simulations to analogies presented in other ways. Therefore, this is an open research question. However, we believe that analogy-based simulations have a number of advantages over unsimulated analogies, at least for certain use cases.

First of all, since they are interactive and dynamic, analogy-based simulations are likely to be more engaging to students than static, non-interactive presentations of analogies. Since students cannot benefit from an analogy if they do not engage with it, simulations may offer an advantage here.

A further advantage of analogy-based simulations is that they may help to address student misconceptions involving the analogy's base, target or both. Although students may be familiar with a system used as base, they may still hold misconceptions about it (1), which is likely to result in "mismapping" or "failure to map" features of the base to features of the target (43). While a student's misconceptions may be left unchallenged by an analogy involving images and text, the fact that a simulated system behaves according to actual physical principles, and not the student's imagination, means that students may recognize situations in which their intuition conflicts with the simulation. This offers the possibility of conceptual change (44) and improved analogical mapping.

Additionally, a number of authors have described mental models of phenomena and processes as *runnable* (45) or involving mental simulation (46, 47). This implies that many mental models are essentially simulations performed in a person's imagination. We believe that the use of dynamic simulations in instruction can aid students in developing more accurate mental models, which will be useful in future qualitative reasoning and problem solving tasks.

Finally, while analogy-based simulations may offer some benefits for most types of instructional content, we see analogy-based simulations as particularly powerful in situations involving dynamic phenomena, especially those involving emergence. Emergent phenomena are typically very difficult for students to grasp, and though they may think they understand a particular system used as a base, they are likely to have misconceptions around any emergent behavior the system may exhibit (48, 49). By providing them with highly constrained dynamic visualizations of physical systems, students are likely to more fully confront misconceptions about emergent, dynamic phenomena than they are if systems are presented via text or static images.

Analogy-Based Simulations: How?

Now that we have explained the utility of analogy-based simulations, we can turn our attention to the question of how such simulations may be designed. The guidelines we present are a mixture of ideas gleaned from our own experience, as well as relevant guidelines drawn from the literature. Like those whose guidelines we cite, we must emphasize that these guidelines are preliminary and need experimental verification. However, they represent a good starting point for efforts in this area.

Before we can make an analogy-based simulation, we first need an analogy to use. Creating an analogy can be a tricky process and is arguably more like an art than a science. However, below, we present some guidelines for creating an analogy that can form the basis of an analogy-based simulation.

Appropriateness of Chosen Target

As discussed earlier, each analogy consists of two concepts being compared: a familiar one, called the *base*, and an unfamiliar one, called the *target*. If an instructor already has a target in mind, it may seem as though we can immediately move on to choosing a base. However, before attempting to construct an analogy for the chosen target, it is worth considering whether using an analogy to teach the target is a suitable approach.

Else et al.(14) suggest that analogies be "reserved for important or abstract concepts and concepts that are prerequisites to further learning." This is because processing an analogy can be time-consuming (50) and cognitively demanding for students. Furthermore, it is well-documented (1, 7) that analogies can give rise to misconceptions among students, who attempt to carry the analogy too far. Therefore, before choosing analogy as the means to teach a particular target, consider whether the potential upsides of analogies, described earlier, outweigh the possible drawbacks.

If the chosen target is well-suited to treatment by analogy, the next step involves deciding precisely which features of the target should be addressed. Many concepts in chemistry are complex and nuanced. However, for students in high school and most undergraduate courses, addressing all of the complexity and nuance related to a particular concept is unnecessary and unwise. Therefore, the main features that should be addressed need to be identified and the other, more subtle features may be ignored. By simplifying the target, the job of choosing an appropriate base becomes much easier. Furthermore, simplifying the target permits the analogy to be simpler, which appears to aid comprehension (43).

In our work (51–53), we identified entropy and the energy landscape[1] (54, 55) (or potential energy surface) as good candidates for treatment via analogy because of their importance across a number of science and engineering domains, as well as their abstract nature, which makes them difficult to understand directly. While the energy landscape of most systems of chemical interest is of extremely high dimensionality, when only one particular transition on the landscape is considered, it can generally be simplified to two dimensions. We focused on this simplified two-dimensional representation because it is widely used by experts as a tool for problem solving and explanations.

While powerful, this abstract representation of the energy landscape presents a number of difficulties for students. First, in some cases the *y*-axis represents potential energy, while, in others, it represents Gibbs free energy. The *x*-axis represents an abstract quantity called the *reaction coordinate*, which is created by abstracting the large number of system parameters involved in an actual, high dimensionality energy landscape down to a single variable. Understanding this axis alone represents a significant challenge for novices. Finally, the temperature is not represented in this representation at all. These three issues taken together make the representation of the energy landscape commonly used by experts very difficult for novices to interpret or use for reasoning qualitatively.

[1]In this chapter, we sometimes refer to the energy landscape as an abstraction. We should note, however, that every chemical system has an energy landscape – a function that specifies its potential energy in terms of all relevant system parameters. In this sense, a system's actual energy landscape is not an abstraction; it is simply a complex attribute of the system. However, among experts, two dimensional energy landscape diagrams are used to represent as qualitatively similar many systems that do not possess even remotely similar sets of relevant system parameters. By examining these qualitatively similar diagrams, we see that, in fact, the two dimensional energy landscape drawn by experts is an abstract relational structure, possessing three states in specific relationship to one another: a low energy stable state, a medium energy metastable state, and a high energy activated state situated between the stable and metastable states. Therefore, though a system's energy landscape itself is not an abstraction, the representation of it used by experts is.

Choosing a Base

Once the target has been established, the next step in creating the analogy is choosing the base. The overriding concern at this stage is that the base and the target possesses *structural parallelism,* which Gentner and Holyoak (56) describe as "consistent, one-to-one correspondences between mapped elements". That is, in order for students to understand the key features of the target, there must be a clear correspondence between them and features of the base. This can be seen in Table I, where each important feature of the chemical system (the target) is "mapped" to a feature in the simulation (the base).

Beyond the requirement of structural parallelism, the literature contains a number of additional guidelines that should be taken into consideration when choosing a base. The most fundamental of these is that the base should already be *familiar* to students (1, 57). Indeed, throughout this chapter, we have described the target as the unfamiliar part of the analogy, while the base is the familiar part. Without structural parallelism there is no analogy and without the base being familiar, the analogy is of little didactic value. So, these two requirements can be seen as the most fundamental when creating an analogy.

In the case that a number of potential bases are found that satisfy both structural parallelism and student familiarity, a number of additional selection criteria may be applied.

Harrison (58) found that using an *interesting* base can have a motivating effect on students, causing them to engage with the analogy. Conversely, a base that students found uninteresting caused students to lose focus and not engage with the analogy. A reasonable extension to this suggestion is that the modes of interaction provided to the student in order to manipulate the simulation should be interesting, as well as the base.

Work by Else et al. (43) suggests that simpler analogies, involving fewer mapped relationships, can be easier to understand. Unfortunately, the number of features that need to be mapped is largely a feature of the target and is not something that can be controlled solely through choice of base. However, in situations involving complex, multi-faceted targets, Spiro et al. (59) present the use of multiple bases (multiple analogies) as an alternative to oversimplifying the target to fit a single base. In this approach, each base maps to a subset of features possessed by the target. The analogy made with any one base is incomplete; however, when all bases are considered together, they provide a complete analogy, mapping to all of the target's features.

Finally, for the purposes of creating an analogy-based simulation, it is necessary that the chosen base can be visualized in some way. Educational simulations are inherently visual, so, while a base that cannot be visualized could be of use in a textbook or in a lecture, such a base is inappropriate for a simulation.

In our work with the energy landscape we used a couple of different bases to illustrate the key relationships embodied by the abstraction of it that experts use. This abstract representational form involves a stable state, a metastable state, and an activated state, with the activated state (or energy barrier) lying in between the stable and metastable states. Thus, we needed to find a base that had features that could map to these states. The simplest and most familiar base we used for this was a cardboard box resting on a platform, depicted at bottom in Figure 2. In the curriculum that accompanied the simulations, we also provided 1,2 dichloroethylene as a simple example of a chemical system with states that qualitatively map to this energy landscape.

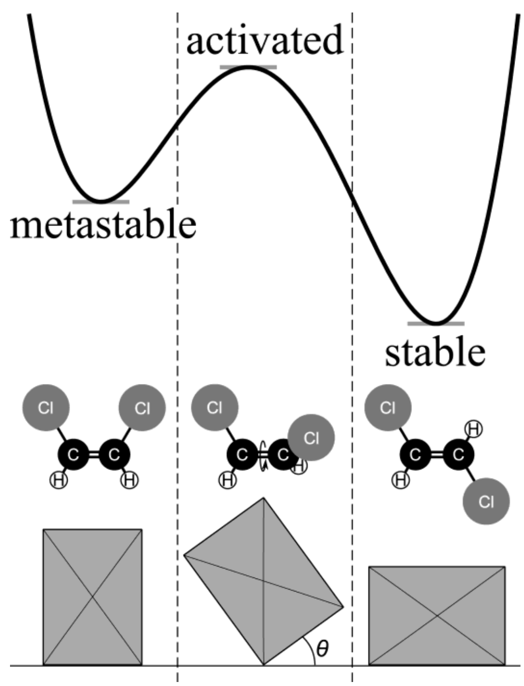

Figure 2: Correspondence of cardboard box and 1,2 dichloroethylene to the states in a schematic energy landscape.

Figure 2 illustrates the fact that the box and 1,2 dichloroethylene could be used in an analogy as base and target, respectively, with the key relationships of the energy landscape captured by the analogy. Table II provides the mappings between the box and a general chemical system.

Finally, it is important to note that the connection between the energy landscape and the cardboard box is only valid as long as the box remains in contact with the platform (53). If the box-as-base is to work, it cannot function exactly like a normal cardboard box, which could be kicked off the platform, into the air. Once the box leaves the platform, the analogy breaks and loses its didactic power. Fortunately, it is possible to add these types of constraints to the simulation in order to preserve the analogy. In the design of analogies or analogy-based simulations, it is important to watch for issues of this type.

Table II: Analogical correspondences between chemical system and box on platform system

Feature of Chemical System	*Representation in Box System*
State	Box orientation
Stable state	Box resting on longest face
Metastable state	Box standing on shortest face
Activated State	Box standing on corner
State energy	Box center of mass height
Reaction coordinate	Rotation angle

Using The Analogy

Once the target and the base have been chosen and the list of desired mappings is complete, we can move on to designing the simulation that will make use of the analogy. A number of authors have made suggestions for how to use analogies in educational texts or classroom settings (10, 12, 42, 60, 61). For our purposes, the key recommendations found in these suggested modes of analogy use are 1) clearly identify the features that are mapped from the base to the target and 2) clearly identify the features of the base that should *not* be mapped to the target. In order for the analogy to be valuable, students need to clearly understand the correspondences between features of the base and features of the target. In addition, they need to understand where the analogy breaks down, so as to avoid forming misconceptions through “overmapping” (43).

Simulation Design and Multiple External Representations

Creating a simulation is a complex and multi-faceted task. However, while research from fields such as human-computer interaction or user interface design could be helpful, we will limit our attention to the representations of the simulated systems. Furthermore, since analogies necessarily involve the comparison of two items or systems (the target and base), we will focus on the use of multiple external representations (62). In this usage, "external" simply refers to the fact that the representations are outside of a person's mind, represented in a concrete form on a real, physical object like paper or a computer screen.

Before addressing the roles of multiple external representations, let us first consider the roles that a single external representation might play. Scaife and Rogers (63) indicate that external representations may play three distinct roles: 1) *computational offloading*, 2) *re-representation*, and 3) *graphical constraining*. In the first role, representing information outside of one's head, for example, by drawing a diagram, frees up memory that would otherwise be needed to retain the information. This makes solving problems easier.

The term *re-representation* acknowledges that not all representations are equally helpful for certain tasks. An unhelpful representation can be transformed into a more helpful representation, that, for example, enables a user to more easily solve a problem or identify a pattern. As an example, most subway maps are highly simplified in order to clearly communicate the interconnectivity of stations and make route planning easier. This simplification, however, may make them less useful for other tasks, like determining the precise location at which a subway tunnel passes underneath a particular street.

Finally, *graphical constraining* indicates that graphics are often more precise than text, meaning that potential interpretations about the represented object or system that might be made from reading a passage of text can be ruled out through the greater specificity of a graphic. Dynamic representations are even more fully constrained, in that they provide concrete information, not only about the configuration of a system at a given point in time, but also about how the system changes as time advances.

Given the principle roles of single representations, we can move on to multiple representations. According to Ainsworth (64), there are three overarching categories of functions that multiple external represention can serve: they can 1) play *complementary roles*, 2) *constrain interpretation*, and 3) *construct deeper meaning*. Multiple representations can play complementary roles by either representing the same information in different ways or representing different, but complementary information. For the purposes of analogy-based simulations, we are primarily concerned with multiple representations' abilities to constrain interpretation and construct deeper meaning.

Ainsworth's concept of *constraining interpretation* is very much like visual analogy. The idea is that by using one familiar representation and one unfamiliar representation, it is possible to help students to build an understanding of the unfamiliar via the constraints imposed by the familiar. In our work using the cardboard box as the base and energy landscape as target, we used linked representations of the box and its energy landscape as seen in Figure 3.

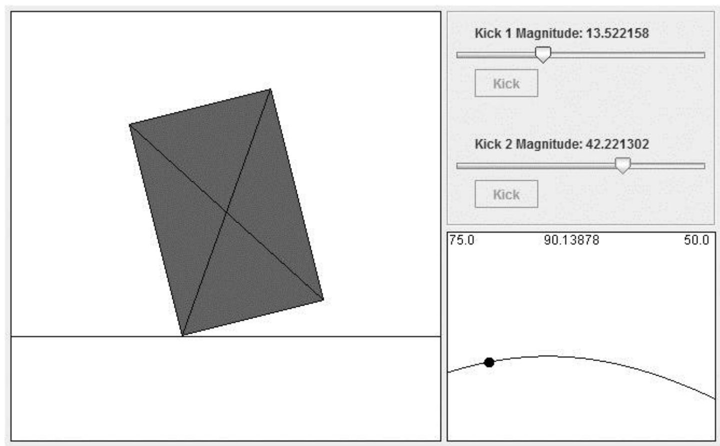

Figure 3: Visualization of a cardboard box on a platform along with a plot of its energy landscape, which is its potential energy as a function of rotation angle.

In this simulation, students can "kick" the box and see how it responds. In the curriculum, they are asked to find the minimum kick magnitude that is sufficient to cause the box to transition from lying down (stable) to standing up (metastable) and vice versa. When the box is kicked, a dot moves on the energy landscape, showing how the box's current position maps to the energy landscape representation. Thus, using a familiar and accessible system, they gain an understanding of the key attributes of the energy landscape: the activated state or energy barrier, which must be overcome when transitioning from one state to the other; the stable state, from which a larger kick is necessary to overcome the barrier; and the metastable state, which, by virtue of its higher energy, requires a smaller kick to cross the energy barrier.

Finally, both analogies and multiple external representations share the ability to help students *construct deeper meaning*. As discussed earlier, the comparison of multiple examples and use of analogies can lead students to create abstract categories of systems that function in similar or analogous manners. As we noted, the possession of these abstract categories and the organization of specific knowledge around them is a characteristic of an expert knowledge structure. Multiple external representations (MERs) can facilitate the construction of abstractions as "[l]earners can construct references across MERs that then expose the underlying structure of the domain represented" (64).

In our work, in order to strengthen and deepen students' understanding of the energy landscape, we introduced another base involving balls bouncing on vibrating platforms, similar to the system in Figure 1. In this case however, the platforms map directly to states on the energy landscape, as seen in Figure 4.

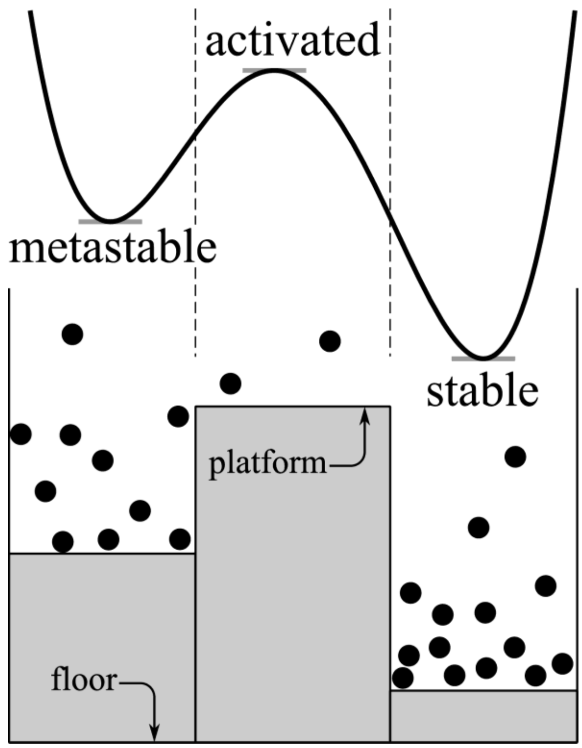

Figure 4: Analogical model of balls bouncing on a set of vibrating platforms and its correspondence to the energy landscape abstraction

Like Figure 1, this base was used to help students easily visualize and understand equilibrium state populations as a function of temperature. However, later in the curriculum, it was placed alongside a large group of cardboard boxes like the one in Figure 3, this time also on vibrating platforms, to demonstrate that, in spite of very different surface features, the two systems exhibit the same behavior, with equivalent populations of states at equivalent temperatures. The simulation, shown in Figure 5, creates an analogy between the two simulated systems and enables students to construct a deeper, more abstract understanding of the energy landscape that underlies both systems.

In this section, we have seen two variants of analogy-based simulations. In Figure 3, we presented a system that, from an analogy perspective, maps a simple, accessible base to a target abstraction and, from a multiple representations perspective, uses the familiar representation of a cardboard box to *constrain the interpretation* of the energy landscape. In Figure 5, we presented a simulation that, from an analogy perspective, creates an analogy between two systems with different surface features but common deep features, and, from a multiple representations perspective, seeks to *deepen understanding* of an abstraction by comparing two systems, the analogy between which captures the important features of the abstraction.

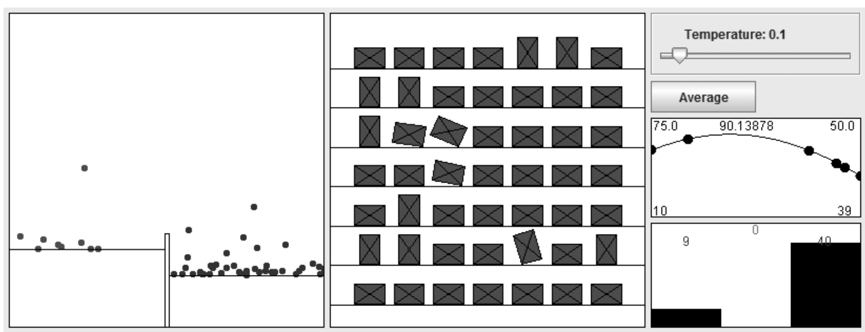

Figure 5: Two different bases set in analogy to one another in order to deepen understanding of the energy landscape

Finally, we should note that if the representations developed for use in a given analogy-based simulation faithfully capture the desired deep features, then those representations may be useful for related abstractions. The above representations were designed around the mappings in Tables I and II, where the focus is on state energies and populations. During the design process, we discovered that only small extensions were needed to use these representations to address the related abstraction of entropy-driven reactions, as seen in Figure Figure 6. In the platform representation at left, a number of microstates (individual platforms) can be grouped into single macroscopic thermodynamic state (the set of platforms with a given height). The number of platforms is the degeneracy of the thermodynamic state. In the three-dimensional box representation, the degeneracy of the states corresponds to the number of faces on which the box can rest with a given gravitational potential energy. Each box in Figure 6 has four ways to stand up and two ways to lie down. Thus, although the stable state is energetically favored, the metastable state's greater degeneracy makes it entropically favored. In the platform representation, it is especially clear why the four higher-energy states have a higher population than the two lower-energy states at high temperature. This can then be mapped over to the box representation. These representations expose the key qualitative aspects of an entropy-driven process, clearly demonstrating that, at low temperature, low energy states are favored while, at high temperature, high entropy states are favored. These representations also motivate the use of free energy in chemistry, by showing how the population between two states is influenced by both the energy difference and the degeneracy (entropy) difference.

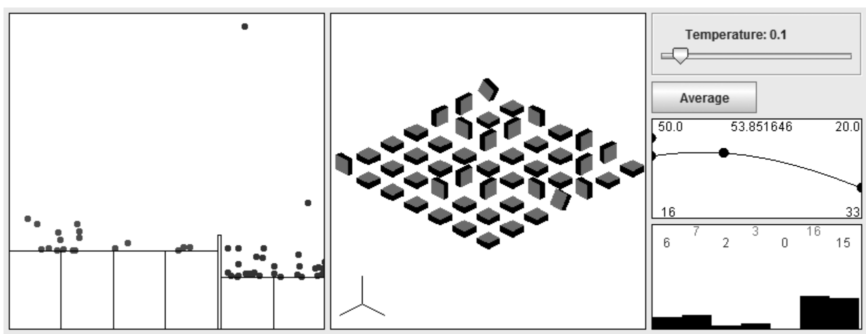

Figure 6: Three-dimensional boxes and balls bouncing on platforms corresponding to the boxes' faces.

Practical Considerations in Simulation Design

While the overall design of the simulation can be guided by the role its multiple representations are intended to play (constrain interpretation, deepen understanding), there are a number of important issues to consider in the design of the individual representations and the connection between them.

In designing simulations, it is wise to limit the number of distinct representations as much as possible (64) and keep each representation as simple and as clear as possible. Thus, it is important to adequately identify key features necessary for students to understand the correspondences between representations. However, it is also necessary to avoid including too much information in any one representation. Certainly, extraneous elements like "chartjunk" (65) should be omitted. In an effort to balance proper identification with visual clarity, the simulations in Figure 3, Figure 5, and Figure 6 do not include many labels. Instead, prior to the use of each simulation, the curriculum provided students with an image of the simulation in which all salient features were labeled.

In both types of simulations described in the preceding section, it is important that students understand the connection between the two representations. In order to accomplish this, the simulation in Figure 3 uses a technique known as “dyna-linking” (64), in which action in one representation produces results in another. Correspondences can also be made clear via static visual cues, such as consistent colors across representations (64). Dyna-linking and color coding can be useful but they should be used judiciously. In attempting to deepen understanding, it is critical students be able to understand the mapping between the representations. However, making the mapping too obvious “may not encourage users to reflect upon the nature of the connection and could in turn lead learners to fail to construct the required deep understanding” (64). For example, while we could have dyna-linked the two main representations in Figure 5, we chose not to, in order to prompt students to link the representations themselves.

Conclusion

We have presented a brief overview of analogy and how analogy can be used as the basis for simulations. Like analogy alone, analogy-based simulations have the power to help students understand difficult and abstract concepts starting from familiar concepts and to enable students to understand and construct abstract categories like experts.

Here we would like to take the opportunity to stress that we are not arguing for the replacement of simulations involving direct depictions of atoms with analogy-based simulations. Rather, we are arguing for the use of analogy-based simulations in areas that cannot be addressed using direct simulations of atoms or as a way to directly address the abstractions used by experts. That is, we are advocating for analogy-based simulations as a *complement* to particulate simulations.

In order to accommodate others who may now be interested in developing their own analogy-based simulations, we have presented a rough outline of a design process on the basis of our own work and suggestions in the literature. It is our hope that such simulations will become a common feature in chemistry curricula, enabling students to better grasp difficult concepts and useful abstractions. Futhermore, we hope other researchers will join us in developing and testing analogy-based simulations in order to better understand how to they may be effectively used to help students understand difficult concepts and organize their knowledge like experts.

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