

Preliminary Studies on Embedding Qualitative Reasoning into Qualitative Analysis and Laboratory Simulation

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Abstract

In this paper, we explored the possibilities of embedding Qualitative Reasoning techniques, the Qualitative Process Theory (QPT), and its implementation in the field of inorganic chemistry. The target field of implementation is Qualitative Chemical Analysis and Laboratory Simulation. By embedding such technique in this education software we aim to combine theory and practice into a single package. The system, are able to generate reasoning and explanation based on chemical theories, helping student in mastering basic chemistry knowledge and practical skill as well. We also review the suitability of embedding QPT techniques into chemistry in general, by comparing some examples from both fields.

Keywords:

Qualitative Reasoning; Qualitative Process Theory; Chemistry; Qualitative Analysis; Simulation.

1. Introduction

The objective of the Qualitative Analysis and Simulation Laboratory is to provide chemistry students with a dynamic learning environment by providing interactive graphical interfaces and animations. Such notion aims to overcome the limitations of the traditional laboratory. Simulation Laboratory enables student to observe reactions between two substances and to choose any test of their choice; whereas the Qualitative Analysis laboratory helps students to determine unknown samples from the observations provided, and generate explanation to the conclusion. To accomplish this task, we have employed one of the

qualitative reasoning techniques, the Qualitative Process Theory (QPT) [1]. The QPT is employed as a notion to view the whole chemical processes as a process [1]. A process involves changes of the parameters of the elements' properties, in order to predict possible chemical reactions. Prediction requires detail information of the elements' properties, and basic chemistry knowledge, which is classified here as a commonsense knowledge¹. Some basic chemistry knowledge and problems encounter in Qualitative Analysis laboratory will be explained in Section 2. To accomplish this task, we have employed one of the qualitative reasoning techniques, the Qualitative Process Theory (QPT) [1], which explain in Section 3. The reasoning process, which involves sequential changes of the elements' parameters obeying chemistry theories, will thus enable us to deduce how a particular chemical reaction came about. This will be explained in Section 4 in QPT terms. System strength and design will be explained in Section 5. The advantages, limitations and future work will be discussed in Section 6.

2. Qualitative Analysis in Chemistry

Chemical analysis is defined as a resolution of a chemical compound into its proximate or ultimate parts and the determination of its elements or the foreign substances it may contain [3]. Chemical analysis can be mainly resolved into **qualitative analysis** and **quantitative analysis** [3] as

¹ Refer to [2], many kinds of expertise apparently involve simply a more appropriate way of describing the world, for the purpose at hand. A representation for such expert knowledge would have exactly the same properties as commonsense representation.

shown in Figure 1(a). Quantitative analysis can determine the constituents of a given sample by identifying how much each component or a specified component presented. Before one can perform a specific test on a specific element to determine its amount of the unknown, a test should be performed to determine whether the substances are present

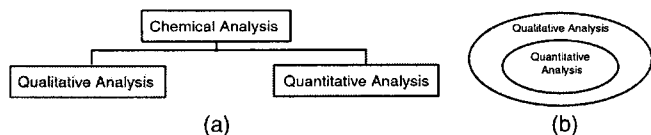


Figure 1 – Classification of Chemical Analysis

in the sample. This lies within the province of **qualitative analysis**. Figure 2(b) is to illustrate a sequential procedure towards determining a specific element by qualitative analysis before a quantitative analysis is performed to determine its amount of present.

In the analytical method of **qualitative analysis**, the element or ion to be detected is converted into some new compound, which have specific properties on the basis that its formation can be elucidated. The chemical change that takes place is known as an **analytical reaction** and the substance causing it is called the **reagent**. For these reactions to occur, there are certain assumptions that we must make and follow. The substance under the test must first be dissolved to form ions. An ion is the simplest form of an element that can be dissolved to form an ionic solution is to do it with water. The presence of certain ions in the solution can be confirmed upon reaction with the reagent where the reaction is almost always accompanied by external effects, which can easily be recognized. These external effects are (a) change in the color of the solution, (b) formation (or dissolution) of a precipitate and (c) evolution of gases. Consider the example iron (II) sulphide below. Given an unknown sample which contain ferrous ions, reaction of ferrous ions and sulphide ions (reagent) will result in the formation of a black precipitate (external effect) of iron(II) sulphide ($FeS\downarrow$) in Equation(1) [4].



However, student performing this experiment may encounter a problem where no precipitation will occur although ferrous ion is confirmed present. These can be explained through dissolution of H_2S (reagent) in water produces H^+ and S^{2-} ion as shown in Equation (2), until equilibrium is reached between H_2S and both ions.

Since only S^{2-} is used up to react with Fe^{2+} to form precipitation, H^+ ion (which is an ion responsible for acidic environment), remain unused. The accumulation of this H^+ ion towards saturation in the system will hinder the dissolution of H_2S anymore. As the student may perform this experiment under an acidic environment, where the system

is already being saturated by H^+ ion, thus H_2S will not dissociate to produce sufficient amount of S^{2-} ion to react with Fe^{2+} , and precipitation will not be formed.

To understand and explain the problems described above do not require complex equations, unless one wishes to know the exact concentration of S^{2-} that have to react with H_2S . From the above example, reasoning with the qualitative properties gives a less precise but an accurate answer. These analysis techniques also require common sense knowledge [2] in chemistry; in this case, the knowledge of chemical equilibrium. It is now worth noting that

- Qualitative analysis in chemistry do not need complex quantitative equations to model chemical changes, and
- Mastering such laboratory skill requires reasoning with chemistry theories.

In such cases, human intuition is enough to perform the task. In order to adopt human's intuition into the computer system, qualitative reasoning is employed to enable computer to perform reasoning in qualitative manner. Several techniques of qualitative reasoning are available and QPT is chosen for this domain.

3. Concept of Qualitative Reasoning and Qualitative Process Theory

The term qualitative reasoning has been used synonymously with naïve physics, qualitative physics or qualitative simulation [6]. However, it is more general than qualitative simulation, and the application of qualitative reasoning in chemistry is quite new in the sense that the approaches are generally different from qualitative physics.

Objects may move, collide, flow or heat up. These and other that cause changes in objects over time are intuitively characterized by **processes**. Processes are the analog of the differential equations used to describe the dynamics of the system. But the notion of process is richer and more structured than this.

Using the example from [1], it illustrates some of the basic deductions sanctioned by qualitative process theory. Two partially filled containers, C and D are connected by a pipe as illustrated in Figure 2. Initially C contains more water than D, what will happen here?

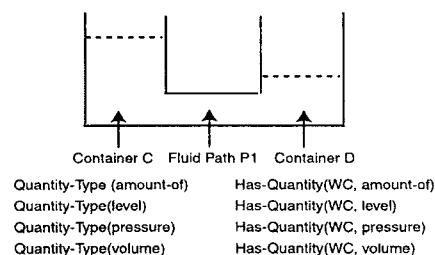


Figure 2 - Two partially filled containers, WC denote water in container C.

² A down arrow denotes a precipitation.

We have no information about the size of both containers or the exact level of fluid in the container C, which is higher than in the container D, nor what is the pressure differences between the two containers. The approximation of what we may make is that the level of fluid in the container C is higher than in the container D, which will induce a fluid-flow process causing the fluid in container C to flow to D through Path P1. The fluid-flow process will stop, when the level of fluid in C and D are the same. The human intuition will have no problem to reason to such conclusion. However, for a computer system to reason to such conclusion, when quantitative information is insufficient or not available in this case, quantitative reasoning is not the first choice.

Qualitative process theory has been developed for this purpose. QPT defines a simple notion of the physical process that appears useful as a language in which to write dynamical theories. However, only some of the basic concepts which is vital to embed the techniques in chemistry will be enumerated. These basic concepts in QPT include *Quantity Space*, *Individual views*, *Process view*, *View Instance*, *Process Instance*, *Functional relationship*, *Process Structure* and *limit analysis*. We will unveil the notion of these QPT terms later and associate it with a situation illustrates in Figure 2.

In Figure 2, processes affect an object through its parameters, and the representation for a parameter is called a *quantity*. The predicate Quantity-Type indicates that a symbol is used as a function that maps objects to quantities. To say that an object has a quantity of a particular type we use the relationship Has-Quantity. In the model of Figure 2, water in the container C and D possess some quantities called level, amount-of, pressure and volume, which is useful in our later reasoning process. A quantity consists of two parts, an *amount* and a *derivative* and the functions A and D map from quantities to amounts and derivatives respectively. Amounts and derivatives are *numbers* and every number has distinguished parts *sign(s)* and *magnitude(m)*. For conciseness, the combination of these functions that select parts of quantities are noted as:

A_m - magnitude of the amount,

A_s - sign of the amount,

D_m - magnitude of the derivative, or rate,

D_s - sign of the derivative.

Initially, water level in C is higher than in D, but we have no idea of whether water in C is higher or lower than the height of container D. If we are about to order the quantity level according to water level, this collection of partially ordered quantity is called *quantity space*. A graphical notation for a quantity space is illustrated in Figure 3.

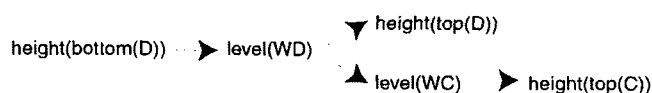


Figure 3 - WC and WD are the pieces of liquid in containers C and D respectively. The arrow indicates that the quantity at the head is greater than the quantity at the tail.

As seen, the level(WC) and height top(D) are unordered. We presume that both containers are aligned at the bottom, thus the height of the bottom(C) and bottom (D) are the same. To model such situation at initial, QPT suggested a qualitative representation called *Individual views*. Individual views are introduced to describe both the contingent existence of objects and object properties that change drastically with time. Individual views consist of four parts, the *individuals*, *preconditions*, *quantity conditions*, *relations*. The *individuals* include the object container and liquid (substance inside the container), which is simplified to con and sub. *Preconditions* contain statement that cannot be predicted within a purely physical theory. *Quantity conditions* concern the inequalities between quantities of the individuals. In this case, quantity conditions must be stated that the water must exist in the container, and the preconditions is that the container must be able to hold the water inside there. Finally, it must have a collection of *relations*, statements that are true whenever the view is true.

For the collection of objects (the fluid and the container) that satisfies the description of the individuals for a particular type of individual view, there is a *view instance*, VI. Whenever the preconditions and quantity conditions for a VI hold, we say its status is Active, and Inactive otherwise. In the example in Figure 4, we have one VI (there exist two containers, a fluid path, and water level in container C is more than in container D, and water level in container D is not empty), and the VI is active because both the preconditions and quantity conditions hold. However, if the initial situation begins with all the fluid is in the container C, and the amount-of fluid in D is ZERO, then another VI should be set to active.

So far our description of the model has been static. However, things might change. Water level in both containers may vary from time to time, but the means by which changes actually occur is not provided. The ways in which things changes are intuitively characterized are known as processes. A physical process is something that acts through time to change the parameters of objects in a situation.

Processes usually start and stop when orderings between quantities in quantity space change. However, conclusion cannot be made which only depends on the ordering of quantity space of level. In fact, all assumption, quantities involved and their relationship must be put together to model the changes of a situation. A process is specified by five parts, the *individuals* it applies to, *preconditions*, *quantity conditions*, *relations* and influences. Basically, a process is just like an individual views, it is a

time-dependent thing, except that it has something we called *influences*. *Influences* contains statements about the direct influences of process to the parameter of the objects. For instance, the rate of the fluid-flow process may induce a negative effect of the water level of container C. Influences can be resolved into direct and indirect influences. Direct influences of the number n on the quantity Q can be written as:

$$\begin{array}{ccc}
 I+(Q,n) & I-(Q,n) & I\pm(Q,n) \\
 (a) & (b) & (c)
 \end{array}$$

According to whether its influences is positive (a), negative (b) or unspecified (c). For example, the flow-rate will decrease the amount-of water in source container (src), and increases the amount-of water in the destination container (dst).

Influences: $I+(\text{amount-of}(\text{dst}), \text{Am}[\text{flow-rate}])$
 $I-(\text{amount-of}(\text{src}), \text{Am}[\text{flow-rate}])$

If one parameter is being influenced by more than one parameter in a situation of individual views, this will induce functional dependencies between the parameters of a situation. For example, the quantity level is being indirectly influenced by the quantities amount-of, pressure and volume individually. To represent the indirect influences, QPT provides the notion of *qualitatively proportional* (α_Q). We would thus express the fact that

$$\text{level}(\text{WC}) \alpha_Q \text{ amount-of}(\text{WC})$$

Sign + and - denotes whether the function is increasing or decreasing monotonic in its dependence of level(WC).

To recapitulate, for every collection of objects that satisfy the individuals specification for a particular type of process, there is a process instance (PI) that relates them. PI's status is set to active when preconditions and quantity conditions hold. In other words, the PI represents the potential processes that can occur between a set of individuals. With this situation so far, there are only two PI, one corresponding to flow from WC to WD, and the other corresponding to flow from WD to WC. The collection of active PIs is called the *Process Structure* (PS) of the situation, to mean "what's happening" to the individuals in a particular situation. Since pressure WC is higher relative to WD as water level of WC is higher relative to WD, status of PI representing fluid flow from WC to WD is set to active, and now the PS is set to Fluid-flow(WC,WD,PI). Fluid-flow is the process that directly influence the amount-of WC and WD (decreases the amount-of (WC),

$D_s[\text{amount-of}(\text{WC})]=-1$, where -1 denotes decrease and D_s denotes the changes of water level over time), and the quantity amount-of in turn influences (decreases) volume, ($D_s[\text{volume}(\text{WC})]=-1$), level ($D_s[\text{level}(\text{WC})]=-1$), and pressure ($D_s[\text{pressure}(\text{WC})]=-1$). However, quantities liked heat and temperature remain unchanged, ($D_s[\text{heat}(\text{WC})]=0$, $D_s[\text{temperature}(\text{WC})]=0$). Changes in quantities are summarized in Figure 4.

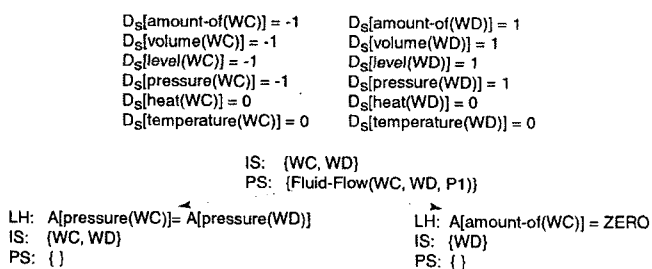


Figure 4 – Resolved influences and limit analysis. The individuals in the situation are labeled IS, the process structure by PS, and limit hypotheses by LH.

Changes in quantities can result in process and view structure themselves changing. Determining these changes is called *limit analysis*; when quantities change, ordering in the quantity space will change correspondingly. For example, when the level of WC is equal to WD, another *view structure* (VS) and *process structure* (PS) will be set to be active. Thus, we must find the points in the quantity space responsible for the collection of objects to exhibit distinctive behavior. For example, in the heating process, 100°C is called a limit point in the quantity space of temperature corresponding to the boiling process. In the quantity space of WC, level of WD is the limit point. Thus, the limit analysis here is rather simple. When the level of WC equals to WD, the pressure will eventually be equaled, which means the fluid flow will stop, and the result is summarized in Figure 4. Initially, it begins with one IS (individual structure) and one PS (process structure). Considering quantity conditions in the PS, the fluid will flow from container C to container D, yield two limit hypothesis, where water pressure of in container C is equal to water pressure in container D, or container C become empty, thus ending WC's existence (although it is not possible in the particular drawing shown). PS: {} in both cases denotes there exist no further possible situation to be considered.

4. Embedding Qualitative Reasoning in Chemistry

Why do we need to use qualitative reasoning in our qualitative analysis of chemical reactions? There are two main reasons. First, the descriptive behavior of chemical changes in the form of equations, or detailed quantitative information is inadequate, or not available. Example in

Equation (1) and Equation (2) has illustrated this problem. Second, human beings do not react to specific situations based on complex equations. In the case of chemical problem of Equation (1) and Equation (2), resolving such problem requires only concepts of chemical equilibrium - qualitative reasoning is adequate. Other distinctive characteristic of qualitative reasoning is its ability to produce an explanation of how it works, and utilize commonsense knowledge in the problem solving [5].

Qualitative reasoning attempts to model the knowledge of how and why we do something. Every testing method in qualitative analysis involves a reaction between the reactant and an unknown sample. The goal of this simulation is to generate the chemical reaction between these two reactants, and whether this reaction totally based on their chemical properties. This is prerequisite for a system to know 'why', when it knows 'how' something comes about. If the system does not know 'how' the black precipitation come about, or 'why' the dissociation of excess ion H^+ would hinder the formation of black precipitation, then the system would not provide any further explanation to the student, rather than only suggest to repeat only certain due to procedural error, which is not correct in this case. Without using complex equations, it is clear that model building has to neglect aspects and attributes of reality and that simplification and approximation are the inherent features of mapping the "infinity of reality" to a finite description [4]. While neglecting some of the irrelevant features such as the temperature and the exact concentration of the unknown ion, we only concentrate on the substances or elements involved constrained by some prior assumption (as stated in Section 2).

Refer to the problem in Equation (1) and Equation (2); qualitative analysis has to be performed on an unknown sample to determine the ion presence in the sample. Among the reagents used, only H_2S gives positive result, which is the black precipitation (FeS). Therefore, we have to model the chemical reaction between Fe^{2+} ion and H_2S and how can the system generate explanation when the H^+ ion from the environment causes interference in the reaction to yield black precipitation.

Quantity-Type(concentration)	Has-Quantity(Fe , concentration)
	Has-Quantity(S , concentration)
	Has-Quantity(H concentration)
Quantity-Type(solubility-product)	Has-Quantity(FeS , solubility-product)

Figure 5 - Quantity type possesses Fe^{2+} , H^+ and S^{2-} ions are concentration and solubility product.

Fe^{2+} , H^+ and S^{2-} exist in water as dissolved ion. The quantity type they possess among others, is concentration (represented by "[]"), which denotes amount of quantity per liter of water. Another quantity type is solubility product, K_s , which denotes multiplication of two ions' concentration under reaction. For example,

$$K_s = [Fe^{2+}] [S^{2-}] \quad (3)$$

If the solubility product exceeds certain level, then precipitation may occur. A brief description of the collection of objects is illustrated in Figure 6.

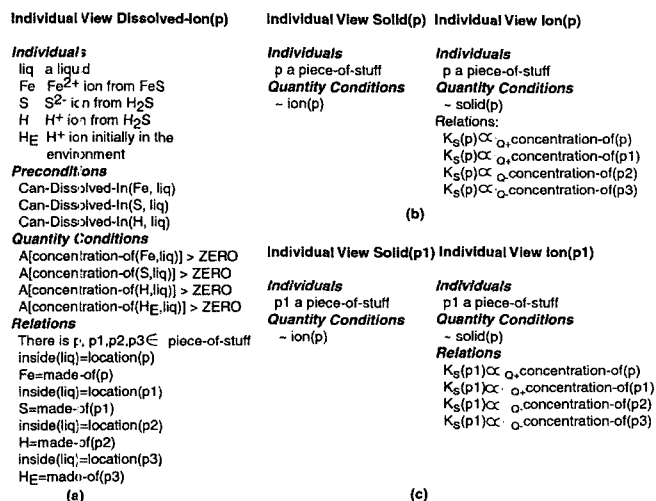


Figure 6 - (a) describes the condition under which pieces of stuff are dissolved in the water. Figure (b) and (c) describe the states of substances under different conditions and relationships with other properties.

Figure 6(a) clearly stated four types of ions exist in the reaction in *Individuals*, they are Fe^{2+} , S^{2-} , H^+ (from dissociation of H_2S) and H^+ (from acid, H_E to represent). *Preconditions* and *Quantity conditions* stated that all these reactant can exist in ion form, and the concentration is more than ZERO. Symbolic representation of p , $p1$, $p2$ and $p3$ in *Relations* is to represent ions Fe^{2+} , S^{2-} , H^+ and H_E , and have their location stated to indicate that all have surface contact to each other, where reaction is possible to occur. As Ferum can exist in two different state, an ion state and a solid as illustrated in Figure 6(b), so as to Sulfur in Figure 6(c), where that a particular piece cannot be in both states at once. No state description for H^+ ion since it is impossible for H^+ ion to exist as solid or liquid individually under normal condition ("~" denote "not").

If experiment is done in an acidic environment, which H_E is present besides Fe^{2+} and the reactant H_2S , then VI in Figure 6 should set to active.

Processes start and stop when ordering of the quantity space change. When the reactant, H_2S is added to the unknown sample, H_2S will start to dissociate and exist as ion H^+ and S^{2-} individually. The process of dissociation of H_2S is illustrated in Figure 7(a).

Process Dissociation of H₂S

Individuals
 H dissolved ion
 S dissolved ion
 liq fluid that dissolve ion

Preconditions
 Ds[amount-of(liq)] = 0
 ; amount of fluid should be constant

Quantity Conditions
 ; Let H₂S be a quantity
 Am[amount-of(H₂S)] > ZERO
 ~ saturated(H)
 ~ saturated(S)

Relations
 ; Let dissociation-rate be a quantity
 dissociation-rate \propto Q₋ concentration-of(H)
 dissociation-rate \propto Q₋ concentration-of(S)
 Correspondence((dissociation-rate(H₂S), ZERO),
 concentration-of(H), saturated(H))
 Correspondence((dissociation-rate(H₂S), ZERO),
 concentration-of(S), saturated(S))

Influences
 I+(concentration-of(H), Am[dissociation-rate])
 I+(concentration-of(S), Am[dissociation-rate])

(a)

Process Precipitate formation of FeS

Individuals
 Fe dissolved ion
 S dissolved ion
 liq fluid that dissolve ion

Preconditions
 Ds[amount-of(liq)] = 0
 ; amount of fluid should be constant

Quantity Conditions
 Am[amount-of(S)] > ZERO
 Am[amount-of(Fe)] > ZERO

Relations
 ; Let K be a quantity
 K \propto Q₊ concentration-of(Fe)
 K \propto Q₊ concentration-of(S)
 Am[formation-rate] \propto Q₊ concentration-of(S)
 ; K = [Fe] * [S]
 Correspondence((amount-of(FeS), ZERO),
 (K(FeS), ZERO))

Influences
 ; Let formation-rate be a quantity
 I+(amount-of(FeS), Am[formation-rate])

(b)

Figure 7 - Process involve dissociation of H₂S and precipitation of FeS and ‘;’ denotes comment.

As stated in quantity condition, process will start when there is the substance H₂S, and both the ion H⁺ and S²⁻ are not saturated. **Correspondence** is another kind of information that can be specified about the function implied by α_{Q+} . It amount to mapping value information (inequalities) from one quantity space to another via α_{Q+} . An typical example taken from [1], illustrating the movement of an elastic spring involves two parameters, the internal forces and the length of the spring, plotting against each others in Figure 8(a); if the length of the band described above is greater than its rest length, the internal force is greater than zero.

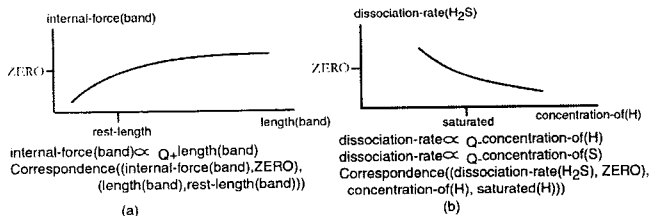


Figure 8 - The rough shape of the graph is determined by the α_{Q+} , the equality between the two points of correspondence.

In Figure 8 (b), the correspondence statement means that if the concentration of H⁺ or S²⁻ is greater than the saturated, no dissociation should occur, and process dissociation should then cease.

Since many of the quantities involved have been ignored, such as temperature changes, then there is only one process that is in our interest - the **precipitate formation process**. The ordering of quantity space of solubility product (K_s) plays a vital role. The solubility product of FeS is 4.0X10⁻¹⁹ mol^l⁻¹ [4] under room temperature. If the concentration of FeS exceeds the solubility product, then the substance will be precipitated. Therefore, 4.0X10⁻¹⁹ mol^l⁻¹ is defined as one of the limit points in the quantity space of solubility product of FeS, and is defined as ZERO in Figure 7(b) in the **correspondence** section.

The reasoning process therefore involves two processes, the **Process Dissociation** and **Process Precipitate Formation**. Since concentration of Fe²⁺ is excess in amount, only S²⁻ indirectly influences K_s according to the K_s equation above. However, the concentration of S²⁻ is determined by the **process dissociation**. **Process Dissociation** is set to be active only when the amount of H₂S is more than ZERO and the concentration of ion H⁺ or ion S²⁻ is not saturated as in Figure 7(a). In an acidic environment, where there exists ion H⁺ initially in large amount, saturation of ion H⁺ will be reached before the dissociation is completed. As a consequence, the **quantity conditions** of **process dissociation** will not be hold, the process will stop before the process dissociation completes, and therefore reduces the concentration of ion S²⁻ also.

In the real reaction, both processes often happen simultaneously. However, for explanation, we might assume that process of precipitate formation occurs after the process dissociation has stopped. The **Process Precipitate Formation** is active because there exist the ion S²⁻ in insignificant amount. The yield of this process is the black precipitation of FeS, which means the process is directly influencing the quantity **amount-of(FeS)**. Initially, we might assume that precipitation occurs in the first loop of this process in a negligible amount. The formation of FeS will also reduce the concentration of ion S²⁻ again. However, it is clearly stated in Figure 7, that precipitation will not exist if the quantity K is less than ZERO (K_s) in the statement **correspondence**, and the quantity K is qualitatively proportional to the concentration of S²⁻. As a consequence, the process will stop because there is no S²⁻ ion for the quantity **formation-rate** to occur.

5. Simulation Laboratory and Qualitative Analysis Laboratory

The simulation Lab is designed to help students familiarize themselves with the procedures of running specific tests and recording of the results. In this sub-system, a user can choose one cation, one anion and one test from the provided list as in Table 1.

Table 1 – List of Cations, Anions and Reagent (Tests) available for Simulation Lab and Qualitative Analysis

Simulation Lab and Qualitative Analysis			Simulation Lab
Cations	Anions	Reagents	Reagents
Sodium	Carbonate	Sodium Hydroxide	Sodium Chloride
Ammonium	Sulfate	Ammonia aqueous	Sodium Sulfate
Calcium	Chloride	Dilute Nitric Acid	Sodium Carbonate

Magnesium	Nitrate	Acidic Barium Chloride	Potassium Iodide
Lead(II)		Acidic Silver Nitrate	Potassium Ferrocyanide
Iron(II)		Brown Ring test	Potassium Ferricyanide
Copper(II)			Potassium permanganate
Zinc(II)			
Aluminum			
Iron(III)			

Upon user selection, the simulator then calls an executable program to show the results of the chemical reaction by identifying the original color of the ionic solution, the test name and the result of the reaction.

Qualitative Analysis Lab provides users a Chemistry lab environment of a upper secondary school level. The system will give the explanation and results in the text and graphical form after users had chosen the test and started the experiment. The system limits the number of species to 10 cations, 4 anions and 6 reagents. See Table 1 for details of cations, anions and reagents available for testing.

Users must provide results for the six tests and the system will analyze the unknown chemical and provides explanation of the simulator's results in an intuitive and causal form. The Qualitative Analysis Laboratory module gives qualitative ideas of the substances that might be present in an unknown sample. Students are then able to compare the actual laboratory results with the simulated results and confirm the presence of specific ionic species in the sample.

6. Discussion

Qualitative Analysis and Simulation Laboratory is an example of the application of artificial intelligence techniques in chemistry. Simulating a real laboratory environment in a computer is by no means a substitute for traditional teaching method, rather, it is meant to enhance learning efficiency. This work, which utilizes the concept of qualitative process theory and process based ontology of Kenneth D. Forbus proves applicable to the field of chemistry. The system combines theory and practice into a single package. The system is not comparable to CyclePad [7], an articulate software that helps engineering undergraduates to learn principles of thermodynamics. However, virtual lab inherits the notion of CyclePad to capture a significant aspect of inorganic chemistry, which helps student in mastering the skill of qualitative analysis laboratory work and chemistry principles at the same time. The goal of this system is to introduce qualitative reasoning techniques namely the qualitative process theory into the

field of chemistry. Although the technique was not meant to capture student's learning behavior as with the STEAMER project [8], explanation can be generated to resolve common questions asked by students based on chemistry principles.

The biggest hindering factor to the expansion of the existing system is the organization and construction of the knowledge representation of chemistry in QPT terms. Since the application of QPT in chemistry is still in its infancy, scarce amount of literature can be reviewed. Notwithstanding the current limitations, the application of this ontology in chemistry is waiting to be explored to the extent that qualitative analysis in chemistry can, in the future, cover a wider range of ions and elements or even encompass other fields of chemistry.

Acknowledgments

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