

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

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, is 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. 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 3 in QPT terms. The advantages, limitations and future work will be discussed in Section 5.

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.

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 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 in the sample. This lies within the province of **qualitative analysis**. Figure 1(b) illustrates a sequential procedure towards determining a specific element by qualitative analysis before a quantitative analysis is performed to determine its amount of present.

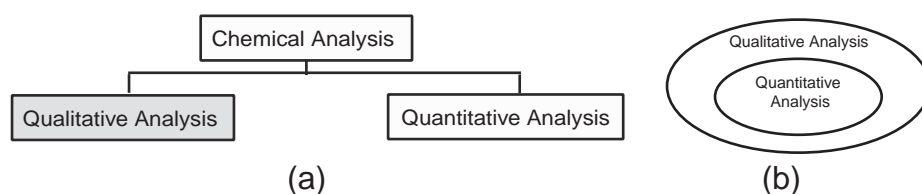
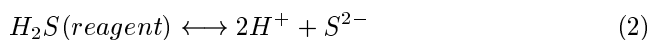


Fig. 1. Classification of Chemical Analysis.

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 colour 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 ($\text{FeS} \downarrow$) (Eq.1) [4].



² A downarrow denotes a precipitation

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 (Eq.2), until an 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 its 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 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 behaviour of chemical changes in the form of equations, or detailed quantitative information is inadequate, or not available. Example in Eq.1 and Eq.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 Eq.1 and Eq.2, resolving such problem require 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 utilizes 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 come 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 [5]. 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 Eq.1 and 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^+ ions 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)

Fig. 2. 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. If the solubility product exceeds certain level, then precipitation may occur. A brief description of the collection of objects is illustrated in Figure 3. Figure 3(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 others, where reaction is possible to occur. As Ferum can exist in two different state, an ion state and a solid as illustrated in Figure 3(b), so as to Sulfur in Figure 3(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 (\sim 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 3 should set to active.

<p>Individual View Dissolved-Ion(p)</p> <p>Individuals liq a liquid Fe Fe²⁺ ion from FeS S S²⁻ ion from H₂S H H⁺ ion from H₂S H_E H⁺ ion initially in the environment</p> <p>Preconditions Can-Dissolved-In(Fe, liq) Can-Dissolved-In(S, liq) Can-Dissolved-In(H, liq)</p> <p>Quantity Conditions A[concentration-of(Fe,liq)] > ZERO A[concentration-of(S,liq)] > ZERO A[concentration-of(H,liq)] > ZERO A[concentration-of(H_E,liq)] > ZERO</p> <p>Relations There is p, p1,p2,p3 ∈ piece-of-stuff inside(liq)=location(p) Fe=made-of(p) inside(liq)=location(p1) S=made-of(p1) inside(liq)=location(p2) H=made-of(p2) inside(liq)=location(p3) H_E=made-of(p3)</p> <p style="text-align: center;">(a)</p>	<p>Individual View Solid(p)</p> <p>Individuals p a piece-of-stuff</p> <p>Quantity Conditions ~ ion(p)</p> <p style="text-align: center;">(b)</p> <p>Individual View Solid(p1)</p> <p>Individuals p1 a piece-of-stuff</p> <p>Quantity Conditions ~ ion(p)</p> <p style="text-align: center;">(c)</p>	<p>Individual View Ion(p)</p> <p>Individuals p a piece-of-stuff</p> <p>Quantity Conditions ~ solid(p)</p> <p>Relations: K_S(p) ∝ Q₊concentration-of(p) K_S(p) ∝ Q₊concentration-of(p1) K_S(p) ∝ Q₋concentration-of(p2) K_S(p) ∝ Q₋concentration-of(p3)</p> <p>Individual View Ion(p1)</p> <p>Individuals p1 a piece-of-stuff</p> <p>Quantity Conditions ~ solid(p)</p> <p>Relations K_S(p1) ∝ Q₊concentration-of(p) K_S(p1) ∝ Q₊concentration-of(p1) K_S(p1) ∝ Q₋concentration-of(p2) K_S(p1) ∝ Q₋concentration-of(p3)</p>
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Fig. 3. Figure 3(a) describes the condition under which pieces of stuff are dissolved in the water. Figure 3(b) and (c) describe the states of substances under different conditions and relationships with other properties.

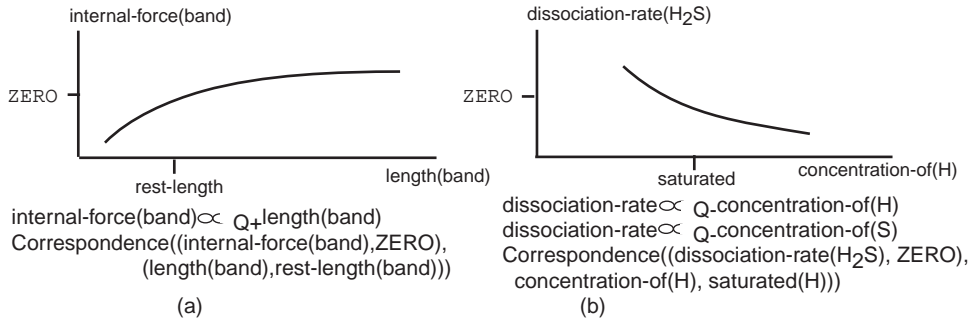


Fig. 4. The rough shape of the graph is determined by the α_{Q+} , the equality between the two points of correspondence.

Process Dissociation of H_2S

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 H_2S be a quantity
Am[amount-of(H_2S)] > 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(H_2S), ZERO),
concentration-of(H), saturated(H))
Correspondence((dissociation-rate(H_2S), 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)

Fig. 5. Process involve dissociation of H_2S and precipitation of FeS and ‘;’ denotes comment.

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 5(a). As stated in quantity condition, process will start when there is the substance H_2S , and both the ion H^+ and S^{2-} 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 4(a); if the length of the band described above is greater than its rest length, the internal force is greater than zero.

In Figure 4 (b), the correspondence statement means that if the concentration of H^+ or S^{2-} 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 $4.0 \times 10^{-19} \text{moll}^{-1}$ [4] under room temperature. If the concentration of FeS exceeds the solubility product, then the

substance will be precipitated. Therefore, $4.0 \times 10^{-19} \text{ mol l}^{-1}$ is defined as one of the limit points in the quantity space of solubility product of FeS , and is defined as ZERO in Figure 5(b) in the correspondence section.

$$K_s = [Fe^{2+}][S^{2-}]$$

The reasoning process therefore involves two processes, the Process Dissociation and Process Precipitate Formation. Since concentration of Fe^{2+} is excess in amount, only S^{2-} indirectly influences K_s according to the K_s equation above. However, the concentration of S^{2-} is determined by the process dissociation. Process Dissociation is set to be active only when the amount of H_2S is more than ZERO and the concentration of ion H^+ or ion S^{2-} is not saturated as in Figure 5(a). In an acidic environment, where there exist 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 S^{2-} 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 S^{2-} 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 S^{2-} again. However, it is clearly stated in Figure 5, 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 S^{2-} . As a consequence, the process will stop because there is no S^{2-} ion for the quantity formation-rate to occur.

4 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 subsystem, a user can choose one cation, one anion and one test from the provided list as in Table 1.

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

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

Simulation Lab and Qualitative Analysis			For Simulation Lab only
Cations	Anions	Reagents (Tests)	Reagents (Tests)
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)			

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.

5 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 [8], 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 [9], 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.

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