Application Qualitative Process Theory to Qualitative Simulation and Analysis of Inorganic Chemical Reaction

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Abstract

In this paper, we explored the possibilities of embedding Qualitative Reasoning techniques, the Qualitative Process Theory (QPT), and its techniques in the field of inorganic chemistry. The targeted field of implementation is in the Chemical Qualitative Simulation and Qualitative Analysis. The QPT is used to model the chemical reaction, behaviors, properties, principles and commonsense reasoning in chemistry. This has made the learning software more achievable and interactive compared to conventional courseware. We also described the entire phases of the software beginning with recognizing agent, electron configuration engine, molecular formula constructor, individual views constructor and process vocabulary.

1. Introduction

There are two major components in the chemistry syllabus taught in the high schools in Malaysia. Firstly, in qualitative simulation, students are expected to derive and construct molecular formula from a given unknown sample. Secondly, in qualitative analysis, students are required to report observations from the experiments they performed. The QPT is employed as a notion to view the whole chemical processes as a process (Forbus 1986). Earlier work on this application is described in (Jen Sen 2001). A process involves the changes of the parameters of the elements' properties, in order to predict possible chemical reactions. Prediction requires detail information of the elements' properties, and some basic chemistry knowledge, which is classified here as a commonsense knowledge [1]. Some basic chemistry knowledge and problems encountered in qualitative analysis will be explained in Section 2. In section 3, we explain some problems in chemical reaction and the need of qualitative simulation to assist the student in performing reasoning. Section 4 delivers some concepts of application of qualitative reasoning technique into chemistry. 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 5 in QPT terms. In section 6, we describe the qualitative analysis laboratory and some actions in the snapshots. We conclude the strength and drawbacks of our system in section 7.

[1] Refer to (Kuipers 1979), 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 (Vogel 1978a). Chemical analysis can be mainly resolved into **qualitative analysis** and **quantitative analysis** (Vogel 1978a) as shown in Figure 1. 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.

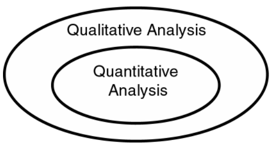


Figure 1 – Classification of Chemical Analysis

This lies the province of **qualitative analysis**. Figure 1 also illustrates a sequential procedure towards determining a specific element by qualitative analysis before a quantitative analysis is performed to determine its amount that present.

In the analytical method of **qualitative analysis**, the element or ion to be detected is converted into some new compound, which has 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 by using 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, the reaction of ferrous ions and sulphide ions (reagent) will result in the formation of a black precipitate (external effect) of iron(II) sulphide (FeS↓[2]) in Equation(1) (Vogel 1978b).

$$Fe^{2+} + H_2S(reagent) \rightarrow FeS\downarrow + 2H^+ \qquad (1)$$

$$H_2S(reagent) \leftrightarrow 2H^+ + S^{2-} \qquad (2)$$

However, student performing this experiment may also encounter a situation where no precipitation occurs although ferrous ion is confirmed to be present. The anomalous behavior is due to the dissolution of H_2S (reagent) in water that produces ion H^+ and ion S^{2-} as shown in chemical equation (2).

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 leads toward 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, H_2S will not dissociate to produce sufficient amount of S^{2-} ion to react with Fe^{2+}, and the 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. These analysis techniques require common sense knowledge (Kuipers 1979) in chemistry; in this case, the knowledge of chemical equilibrium. It is now worth noting that

- qualitative analysis in chemistry does 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. Qualitative Simulation in Chemistry

A chemical reaction is a process. In any process of reaction between reactants, the final product is always accompanied by external effects, e.g. a color precipitate. For example,

A + B → C (black color precipitate) (3)

In the chemical equation (3), A will react with B and the product is C. C is black color precipitate. A chemist will get the same result when he repeats the same reaction under the same condition and environment. The induction process permits the chemist to view this piece of information as facts, and the facts can be used in the future for various purposes. For example, in qualitative analysis, B is used as a reagent to determine the present of A by identifying whether C, a black color precipitation occurs during the reaction. A chemist or student will make a deduction that A is not present if there is no black color precipitate from past experience. However, the deduction of the chemist can be wrong, if the reaction medium changed. Section 2 has clearly illustrated the problem. Therefore, qualitative simulation is performed to model the chemical reaction. In the simulation process, every crucial process of reaction is reported clearly and augmented by explanations to the user. Qualitative simulation requires chemistry theories and facts to generate an explainable result to user. Qualitative reasoning is needed to perform qualitative simulation in the system.

4. Overview of application of QPT in Chemistry

One of the distinctive characteristic of qualitative reasoning is its ability to produce an explanation of how a dynamic system works, and utilize commonsense knowledge in the problem solving (Werthner 1994). Refer to the problem described in section 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

[2] A down arrow denotes a precipitation.

precipitation (FeS). Therefore, we have to model the chemical reaction between Fe^{2+} ion and H_2S and how the system can generate explanation when the H^+ ion from the environment causes interference in the reaction to yield black precipitation. Figure 2 shows the example of modeling concentration and solubility product for the ions and cations.

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 2 - Quantity type possessed by Fe^{2+}, H^+ and S^{2-} ions are the concentration and solubility product.

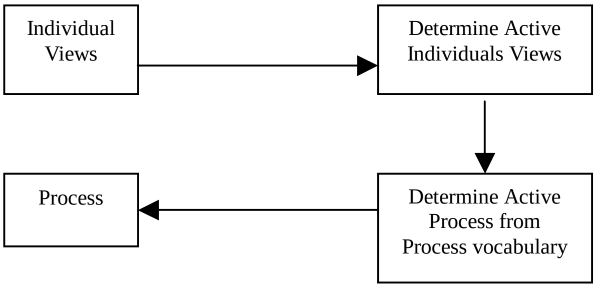


Figure 2a - Quantity type possessed by Fe^{2+}, H

In Figure 2a, *Individual views* describe the situation. Individual views comprise of collection of all objects, assumption made to the state of the objects, inequalities among object's properties and relationships among objects. System constructs the individual views automatically based on user's input. There are active and inactive individual views. Individual views fulfill the assumption and inequalities among object's properties are active, or vice versa. For example, ion H^+, S^{2+} and Fe^{2+} and water are collection of objects. Examples of ion's properties are concentration and solubility product. Assume that the amount of water is constant and all ions dissolve in water, adding of H_2S in the unknown will result to a high concentration of H_2S in water.

Active individual views may result to some possible processes. Types of processes are listed in the process vocabulary. For example, when there is a high concentration of H_2S in water, the possible process is dissociation of substance H_2S into ion H^+ and S^{2-}. On other hand, if there exist ion a high concentration of ion H^+ and S^2 in the water, possible process will be the formation of substance H_2S. In this case, since H_2S exhibits reverse reaction, both dissociation process and formation process are possible.

Process is the description of the process. Process comprise of collection of all objects, assumption made to the state of the objects, inequalities among object's properties and relationships among objects. Besides, *process* has the influence component that describes the direct influence among object's properties.

Process stop when the conditions in the *process* does not hold. For example, dissociation of H_2S may stop before completion due to acidic medium in the solution.

The modeling of chemical simulation required the following phases to be performed. These phases are, (1) Recognizing Agent (2) Electron Configuration (3) Molecular formula Constructor (4) Individuals Views Engine (5) Process Vocabulary and (6) Chemical Equation Constructor.

5. Qualitative Simulation Laboratory

The qualitative simulation lab is designed to familiarize student with the chemical reaction between two reactants. The system provides an extension to conventional wet lab experiments, where students gain flexibility in access to a safe laboratory environment. To facilitate self-study and self-exploration, the system has an agent to recognize the user's input with the right molecular formula instead of predefined sets of chemical substances. The system also allows reaction to be conducted on different medium, e.g. acidic environment, in order to make comparison among various types of reaction. The system has an innate capability in providing intuitive chemical explanation. Explanation is generated based on chemistry theories. The main thrust of the qualitative simulation is the reasoning engine. There are individual views constructor and process vocabulary. Other supportive features are recognizing agent, electron configuration, molecular formula constructor and chemical equation constructor.

The reasoning engine first need to gather information from the databases and the information required are chemical facts and chemical properties with direct and indirect influence to form a causal relationship, namely the chemistry theories. The collection of reactants and reaction medium construct the individual views based on chemistry theories and the system needs to determine the active processes in process vocabulary based in inequalities. The start or stop of a process depends on the ordering of quantity in the quantity space. When a process stops, explanation and chemical equations are generated by the system to explain the chemical process in the reaction. In the case where the reaction does not show as desired, the system will deliver more explanation to clarify the situation. Figure 6 shows user interface for qualitative simulation.

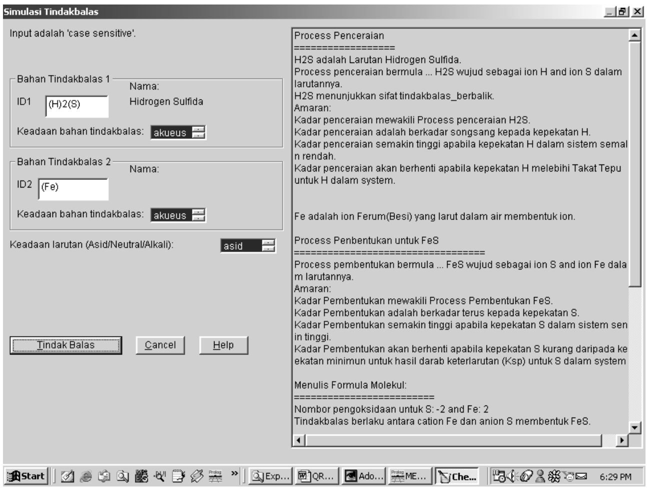


Figure 6 – Qualitative simulation user interface.

5.1 Recognizing Agent

Recognizing agent interprets and translates the user's input reactants to the standard IUPAC's[2] name. Some of the examples are given in Table 1.

The system recognizes H_2S as the aqueous solution, consists of ion H^+ and S^{2-}. Both ions are sent to electron configuration engine to determine its charges, and the charges of both ions will be used by the molecular formula constructor to construct the molecular formula. The molecular formula generated by the system is compared with the user's input of the molecular formula. System will prompt the user if the molecular formula is a wrong one.

Table 1 - IUPAC name, substance and element's state and system's input according to system specification.

IUPAC name	State	User's Input
H_2S	Aqueous	(H)2(S)
NH_3	Gas	(N)(H)3
Fe	Solid	(Fe)

( ) is to separate the two ions.

Recognizing agent is able to verify the state of the element input by user. For example, Fe cannot exist as gas because the boiling temperature for Fe retrieved from the database is 3000°C, which is much higher than the room temperature.

[2] IUPAC has been recognized as the world authority on standardizing chemical terminology and many other critically evaluated data.

5.2 Electron Configuration Engine

The Electron Configuration engine is responsible to figure out the charges of the ions from ion's electron configuration. This is done by assigning the atomic number of element into the orbital, according to two chemistry basic rules and principle, the Hund's rules and Pauli principal (Vogel 1998a). For example, element Fe has the atomic number of 26. The engine then generates the result in a written format of the result. [$1s^2$, $2s^2$, $2p^6$, $3s^2$, $3p^6$, $3d^6$, $4s^2$] represent the electron configuration of ion Ferum. The placement of the electron result in the most outer orbital, $4s^2$, remain 2 electrons, represented by the superscript number. In order to explain why an Iron substance, when it is turned into an ion, has the tendency to lose 2 electrons in its outer orbital requires the component of indirect and direct influences. The formation ion Fe^{2+} was a result of some processes that change the element Fe to an ion Fe^{2+}.

The indirect influence has defined that the Ionization process removes the most loosely held electron from an atom. As the process occurs, and the process is the only source of direct influences, the quantity being direct influences is the Oxidation number. A symbol to represent is I(Q,n), where n is the direct influence on the quantity Q. To clearly stated this situation, we have

I+(oxidation-number(Fe),A[ionization-energy])

Ionization energy is indirectly influenced by atomic radii, which is written as Ionization Energy α_{Q-} Atomic radii is represented in a way that the bigger the atomic radii is, the lesser the ionization energy is needed to eliminate the electron situated at that position. By propagating the relationship of atomic radii, principle quantum number (orbital, n) α_{Q+} is increasing monotonically in its dependence on atomic radii. Therefore, we have reached a conclusion that lesser ionization energy is needed with the removal of the outer electron of an atom in the process of ionization. This explains why ion Fe^{2+} with oxidation number +2 is formed.

5.3 Molecular formula Constructor

Molecular formula constructor plays a role to interpret user's input reactant and convert into IUPAC standardize molecular formula; and to construct a molecular formula according to ion's charges. User is required to put the symbol ( ) around the substances which involved more than one molecule in the constituent of the substance's molecular formula. The molecular formula is also designed to construct molecular formula according to the ion's charges obtained from the electron configuration engine.

5.4 Individual Views Constructor

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

$$K_s = [Fe^{2+}]\ [S^{2-}] \quad (4)$$

If the solubility product exceeds certain level, then precipitation may occur. A brief description of the collection of objects is illustrated in Figure 3.

Individual is the collection of all objects. *Preconditions* and *Quantity conditions* stated that all of these reactants can exist as an ion, and the concentration is more than ZERO. Symbolic representation of *p, p1 and p2* in *Relations* is to represent ions Fe^{2+}, H_2S and H_E, respectively and have their location stated to indicate that all have their surfaces contacted to each other, where a reaction is possible to occur. As Ferum can exist in two different states, an ion state on a solid as illustrated in Figure 3(b). However, no particular piece cannot exist 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").

Individual View Reactant(p)

Individuals
W water
Fe Fe^{2+} ion
H_2S solution
H_E H^+ ion initially in the environment
Preconditions
Can-Dissolved-In(Fe, W)
Can-Dissolved-In(H_E, W)
Quantity Conditions
A[concentration-of(Fe,W)] > ZERO
A[concentration-of(H_E,W)] > ZERO
A[concentration-of(H_2S)] > ZERO
Relations
There is p, p1,p2 ∈ piece-of-stuff
inside(W)=location(p)
Fe=made-of(p)
inside(W)=location(p1)
H_2S=made-of(p1)
inside(W)=location(p2)
H_E=made-of(p3)

(a)

Individual View Solid(p)

Individuals
p ∈ piece-of-stuff
Quantity Conditions
~ ion(p)

Individual View Ion(p)

Individuals
p ∈ piece-of-stuff
Quantity Conditions
~ solid(p)
Relations:
K_S(p) α_{Q+}concentration-of(p)

(b)

Figure 3 - (a) describes the condition under which pieces of stuff are dissolved in the water. Figure (b) describes the states of substances under different conditions and relationships with other properties.

If the experiment is done in an acidic environment, which H_E presents besides Fe^{2+} and the reactant H_2S, then VI in Figure 3 should be set to active.

5.5 Process Vocabulary

Processes start and stop when ordering of the quantity space change. In the quantity space of concentration, there are two elements [ZERO, saturated] exist as landmark value. When the H_2S solution is added, it is the nature that H_2S solution starts to dissociate into ion S^{2-} and H^+. Process dissociation occurs because Am[concentration-of(H)] > ZERO and Am[concentration-of(S)] > ZERO, represent a process will start or stop when the quantity of both ions pass through landmark values. The process of dissociation of H_2S is illustrated in Figure 4(a).

As stated in quantity condition, process will start when there is a 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+}. Its amount maps value information (inequalities) from one quantity space to another via α_{Q+}. A typical example taken from (Forbus 1986), 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 5(a); if the length of the band described above is greater than its rest length, the internal force is greater than zero.

Process Dissociation of H_2S

Individuals
H dissolved ion
S dissolved ion
W fluid that dissolve ion
Preconditions
Ds[amount-of(w)] = 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(H_2S) α_{Q-} concentration-of(H)
dissociation-rate(H_2S) α_{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+(amount-of(H), Am[dissociation-rate(H_2S)])
I+(amount-of(S), Am[dissociation-rate(H_2S)])

(a)

Process Precipitate formation of FeS

Individuals
Fe dissolved ion
S dissolved ion
W 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
; Let formation-rate be a quantity
K α_{Q+}concentration-of(Fe)
K α_{Q+}concentration-of(S)
Am[formation-rate] α_{Q+}concentration-of(S)
;K = [Fe] * [S]
Correspondence((amount-of(FeS), ZERO), (min-solubility-product(S), ZERO))
Influences
I+(amount-of(FeS), Am[formation-rate(FeS)])

(b)

Figure 4 - Process involves dissociation of H_2S and precipitation of FeS and ';' denotes comment.

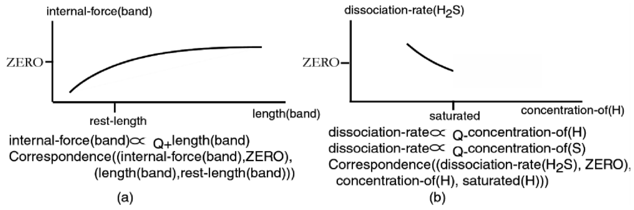


Figure 5 - The rough shape of the graph is determined by the α_{Q+}, the equality between the two points of correspondence.

As stated in quantity condition, a process will start or stop when there exists the substance H_2S, and both the ion H^+ and ion S^{2-} are not saturated. As dissociation rate is inversely proportional to the concentration of ion H^+ and ion S^{2-}, dissociation process should continue towards completion as implied by the function α_{Q+}. Process dissociation will stop when there is no more substance H_2S exist in the system. However, in an acidic environment, ion H^+ initially exists in the system. Dissociation process that yields ion H^+ and ion S^{2-} quickly saturats the system with the ion H^+ before dissociation process completed. When another landmark value [saturated] met, this processes will stop. Correspondence is another kind of information that can be specified about the function implied by α_Q.

Correspondence((dissociation-rate(H_2S),ZERO), (concentration(H),saturated(H)))

The correspondence statement means that if the concentration of ion H^+ is greater than the saturated, no dissociation should occur, the dissociation process should cease. The shape of the graph is shown in Figure 5(b). The system is now saturated with ion H^+, but due to incomplete dissociation, concentration of ion S^{2-} would be negligible.

A reaction will occur between ion Fe^{2+} and ion S^{2-} to form black precipitation of FeS. Figure 4(b) illustrates the formation of precipitation process. The formation rate of FeS is proportional to the concentration of S^{2-}.

Correspondence((formation-rate(FeS),ZERO), (concentration(S),min-solubility_product(S)))

The solubility product of FeS is 4.0×10^{-19}moll^{-1} under the room temperature. If the concentration of FeS does not exceed the solubility product, then the substance will not be precipitated. Therefore, 4.0×10^{-19}moll^{-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 4(b) in the correspondence section. As the concentration of S^{2-} is insufficient to meet the requirement of solubility product of FeS due to an incomplete dissociation process, therefore, the black precipitation of FeS will not be formed in an acidic environment.

5.6 Chemical Equation Constructor

Chemical equation constructor is responsible to construct chemical equation to describe the chemical reaction. The constructor is able to balance off chemical equation. For example,

$$Fe^{2+} + H_2S \rightarrow FeS + 2H^+$$

Balancing off chemical equation is often the problem faced by the student as it involves technical skill to balance the number of element and substance in both side to balance the charges and to write proper molecular formula.

6. Qualitative Analysis Laboratory

Qualitative Analysis Lab provides users with a virtual laboratory environment of an upper secondary school level. The system will give the explanation and results in the text and graphical form after the users had chosen the test and started the experiment. The system provides 12 individual common tests and 58 specific tests for testing purpose. 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. Figure 7 is the user interface for the student to input their observation after the student performed the test with ammonia aqueous.

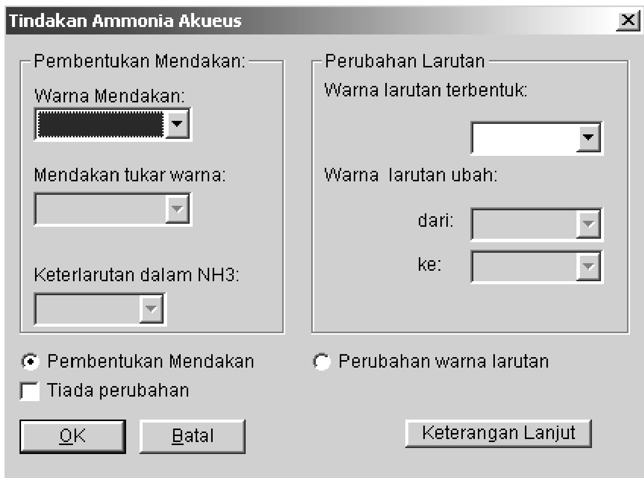


Figure 7 – Dialog box for the student to input observation when the student performing ammonia test to the unknown.

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.

6.1 Database

Databases are needed to store chemical facts and the quantity type of chemical substances. Facts and quantity type are stored in the most fragmented format. The fragmented format is to ensure an extensible knowledge base. Additional chemistry facts and quantity type can be added in anytime without affecting the system operation. Chemical facts are useful to disambiguate possibilities resulted from envisioning. Chemical facts are those properties that will not change over time. The database classified the chemical facts into (1) color of precipitation (2) testing of gas (3) gaseous (4) color of aqueous and (5) chemical compound that display reverse reaction. User is able to amend, modify and extend the facts in the database through the user interface without having to posses programming skill.

Table 2 – List of some quantity type posses by ion.

State of Element	Quantity Type
Ion	concentration
ion	solubility product
ion	saturated

Table 3 – Functional relationships

The database that contains quantity type of chemical are classified into (1) quantity component (2) direct and indirect influences component and (3) correspondence component. Table 2 displayed some of the quantity types possesed by the ions.

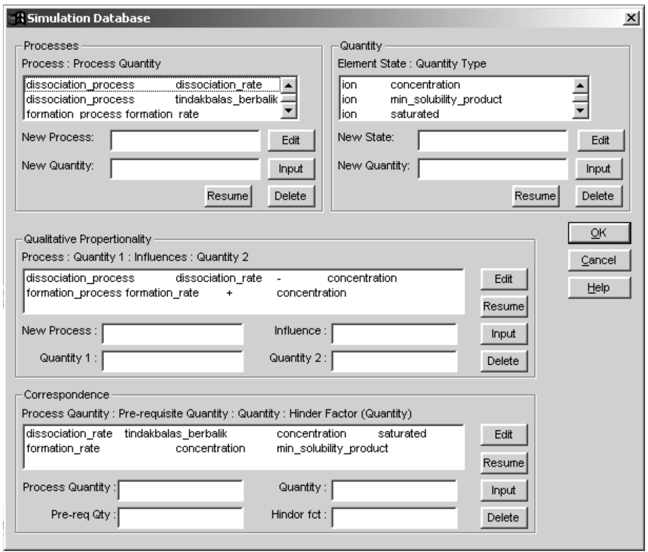
Process	Quantity 1	Functional dependencies	Quantity 2
dissociation process	dissociation rate	-	concentration
formation process	formation rate	+	concentration

Table 4 – Correspondences specific the prerequisite factor of the reaction, the quantity type and the hinder factor of the process.

Process	Quantity 1	Functional dependencies	Quantity 2
dissociation rate	reverse reaction	concentration	saturated
formation rate	-	concentration	solubility product

All the information in Table 2, 3 and 4 are interrelated, together construct the chemistry theories and to be used in the reasoning process. However, information is stored in the most fragmented format, simplifies maintenance and provides scalability.

Figure 6 – a user interface enable instructor to modify, delete or extend the information stated in Table 2, 3 and 4.



6.3 Articulate Software

According to Forbus in his article (Forbus 2000), Articulate software should have the properties of (1) fluent, (2) supportive, (3) generative and (4) customizable. The qualitative simulation and qualitative analysis laboratory have fluency property, because the system is able to understand the chemistry domain by linking all chemistry properties to perform the reasoning. The system is also able to provide explanation if the user's goal is not achieved. Explanation is provided thru what the system understand of the chemistry knowledge. Electron configuration engine is the example of supportive properties. The engine shows the student the procedure of filling electron into the orbital according to the chemistry principle. This will help the student to understand chemistry concept from the fundamental approach and to develop chemical intuition. The software is generative because the software is designed to handle situation within its understanding of chemistry knowledge. The software is customizable such that the instructor is able to modify, update and extend the database of chemical facts and the chemistry theories in order to enhance the reasoning abilities of the system. Maintenance is accessible instructor through user friendly interface, without any amendment to the programming.

7. Discussion

Qualitative Analysis and Qualitative Simulation Laboratory are examples of the applications of artificial intelligence techniques in chemistry. Simulating a real laboratory environment in a computer is by no means a substituting the 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 applicability to the field of chemistry. The system combines the theory and practice into a single package. The system is not comparable to CyclePad (Forbus et. Al. 1998), 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 (Clancey 1992), explanation can be generated to resolve common questions asked by the 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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