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Deriving Causal Explanation from Qualitative Model Reasoning

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***Abstract*—**This paper discusses a qualitative simulator QRiOM that uses Qualitative Reasoning (QR) technique, and a process-based ontology to model, simulate and explain the behaviour of selected organic reactions. Learning organic reactions requires the application of domain knowledge at intuitive level, which is difficult to be programmed using traditional approach. The main objective of QRiOM is to help learners gain a better understanding of the fundamental organic reaction concepts, and to improve their conceptual comprehension on the subject by analyzing the multiple forms of explanation generated by the software. This paper focuses on the generation of explanation based on causal theories to explicate various phenomena in the chemistry subject. QRiOM has been tested with three classes problems related to organic chemistry, with encouraging results. This paper also presents the results of preliminary evaluation of QRiOM that reveal its explanation capability and usefulness.

***Keywords*—**Artificial intelligence, explanation, ontology, organic reactions, qualitative reasoning, QPT.

I. Introduction

QUALITATIVE Reasoning (QR) originates from the field of Artificial Intelligence (AI). The term "qualitative reasoning" pertains to the distinction between reasoning with actual numerical values (and equations) and reasoning with less precise representations. Traditional mathematical and computer modelling languages do not attempt to formalize the notion of causality, and lack of tight coupling between concepts and their embodiment. Traditional chemistry education software is inadequate to promote understanding as the software. In the standard rule-based systems, explanations are generated by tracing all the rules that fired during a search for solution. As such, these systems are incapable of providing behavioural types of explanation on demand, such as explaining why things happen and how they happen. In view of this, the QR approach based on qualitative process theory [1] was investigated. An overview of QR research in education can be found in [2].

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A survey result showed that many chemistry students learn organic reactions by memorizing the steps and formulas of each reaction which can easily be forgotten. They face difficulties in dealing with the principles governing the processes and the cause effect interaction among these processes. Without proper explanation, these observations do not help much in nurturing their understanding of the subject.

We have developed a qualitative simulator, abbreviated QRiOM (Qualitative Reasoning in Organic Mechanism) that helps chemistry students learn organic reactions through the study of parameters functional dependencies and their cause effect interactions. QRiOM is able to construct qualitative models (using the QPT ontology), and to simulate processes (using a set of QR algorithms) such as creating and deleting bonds in order to reproduce the chemical behaviours of organic reactions "intuitively". Specific research questions addressed by this paper are:

- Can qualitative reasoning and simulation be used for generating causal explanation?
- Do students perceive to benefit from using QRiOM?

II. Qualitative Process Theory

Qualitative process theory (QPT) is a process-based ontology that is adequate for representing qualitative knowledge [3]. In QPT, a model can be constructed for a *process*. The *processes* support changes in system behaviour. A *process* is described by five slots: *Individuals, Preconditions, Quantity-conditions, Relations* (statements about functional dependencies among objects' characteristics), and *Direct Influences* (denoted by I+/I–). An important design primitives for describing the relationships between *quantities* is the *Qualitative Proportionalities* that propagate the effects of processes that express unknown monotonic functions (increasing/decreasing/unchanged) between two *Quantities* (e.g., charge, covalent bond, lone-pair electrons, electro-negativity and nucleophilic reactivity). A quantity space is defined by a set of alternating point (e.g., [negative, neutral, positive]). At any given point of time, the charge of any atom is either negative or neutral or positive (see Fig. 1). As to what (new) value a quantity will be assigned is depends on the changing of signs (-1, 0, 1). "-1" means decreasing (i.e. the value on the left side of the space will be taken), "0" is non-changing, and "1" denotes increasing (i.e. the value of the right side will be taken). When a quantity's value is

above or below a specific limit point, some physical phenomena occur. Direct influences are represented as I+/I- (Influences can either be positive or negative). Note that words typed in italics are QPT modelling constructs. Refer to [2] for a complete description of the ontology.

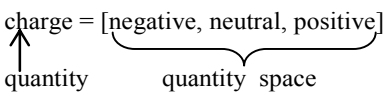


Fig. 1 The "charge" parameter with its values.

In chemistry, changes are caused by continuous physical processes. These changes propagate through the system via qualitative proportionalities which indicate causal relationships between quantities. This makes QPT a suitable modelling language for solving organic reaction problem.

III. The Problem Domain: Organic Reaction Mechanism

In organic chemistry, most reactions take place between nucleophiles (electron-rich sites, e.g. "OH" and "Cl-") and electrophiles (electron-poor sites, e.g. "H+"). Organic chemists will identify the electron-poor and electron-rich sites when trying to work out a reaction mechanism through their chemical knowledge and experience. In this work, the organic reaction is either a "make-bond" or a "break-bond" process, as described in [4].

A. Organic Reaction and Mechanism

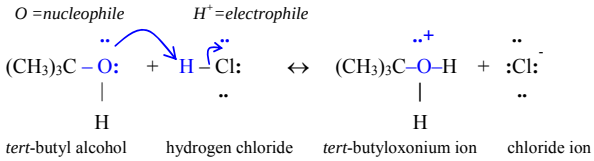
An organic reaction is a chemical reaction involving organic compounds, usually between an electrophilic centre and a nucleophilic group. In any chemical reaction, some bonds are broken and new bonds are made. Often, these changes are too complicated to happen in one simple stage. Thus, usually a reaction may involve a series of small changes one after the other. A reaction mechanism describes this series of changes. Examples of reaction mechanisms are S_N1 (unimolecular nucleophilic substitution) and S_N2 (bimolecular nucleophilic substitution). In this approach, each organic reaction is described as changes made on the chemical parameters (E.g. charge, covalent bond and lone-pair electrons) of the functional groups. These groups are used to determine what type of organic reaction that may occur [5].

B. Nucleophilic Substitution Reaction

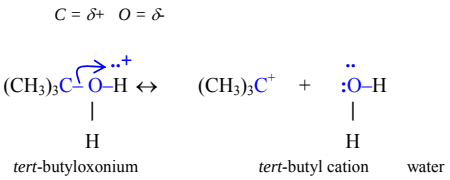
Equation (1) involves "−OH" (Hydroxyl) functional group transformation. The reaction mechanism used in the transformation is S_N1. In (1), A=*tert*-Butyl alcohol, B= Hydrogen chloride, C=*tert*-Butyl chloride, D=Water molecule (H_2O).

$$\underset{A}{(CH_3)_3C{-}OH} + \underset{B}{HCl} \rightarrow \underset{C}{(CH_3)_3C{-}Cl} + \underset{D}{H_2O} \quad (1)$$

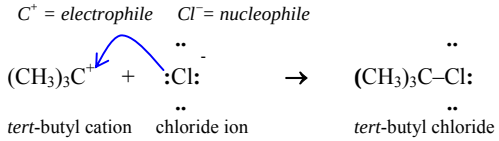
The chemical theories that govern the change of state variables for (1) are depicted in Fig. 2. The entire reaction can be modelled as a series of three chemical processes ("make-bond", "break-bond", and "make-bond" that involved an organic compound – tertiary alcohol). When reasoning is applied to the three organic processes, the behaviour of (1) can be reproduced.



(a) First reaction step. It is a "make-bond" process.



(b) Second reaction step. It is a "break-bond" process.



(c) Third reaction step. It is a "make-bond" process.

Fig. 2 The conversion of a tertiary alcohol to yield alkyl chloride can be described as a series of three small steps. Dots represent the electrons associated with the particular atom in the molecule.

IV. The Qualitative Simulator

Fig. 3 depicts the architecture of QRiOM, while Fig. 4 gives the list of research activities in developing the simulator. The main functions of each component are presented in Table I.

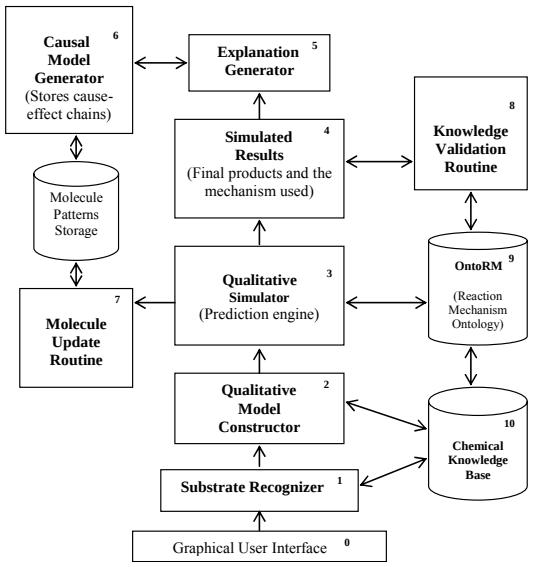


Fig. 3 Main software components of QRiOM.

TABLE I
THE ROLES OF THE MAIN MODULES IN THE QRIOM SIMULATOR

Module	Roles
Module 0 (GUI)	This module provides an interface for the learners to interact with the system.
Module 1 (Substrate Recognizer)	This module checks user selection, and returns the "type" of the input as either a nucleophile or an electrophile.
Module 2 (Model Constructor)	This module automates the construction of QPT specifications (the qualitative models) based on the identity of user input.
Module 3 (Reasoning Engine)	This module does the actual simulation. The main functions are handled by the Quantity Space Analyzer (QSA) and the Molecule Update Routine (MUR).
Module 4 (Simulated Results)	This module will return simulated results based on the selected pair of input. Examples of output include: final products formed, sequence of bond making activities, and the organic mechanism used to predict the output.
Module 5 (Explanation Generator)	This module will generate explanation to justify a simulated result.
Module 6 (Causal Model Generator)	This module constructs causal graph that keep accounts of the system behaviour.
Module 7 (Molecule Update Routine)	This module keeps track of the structural change (pattern) of the substrate, from one organic reaction to another. It also generates reaction route.
Module 8 (Knowledge Validation Routine)	This is a routine that called up by the reasoning engine whenever it needs to use a piece of knowledge to make a decision.
Module 9 (OntoRM)	This is the reaction mechanism ontology.
Module 10 (Chemical Knowledge Base)	This data store contains information such as chemical facts and theories the simulator needed to perform reasoning.

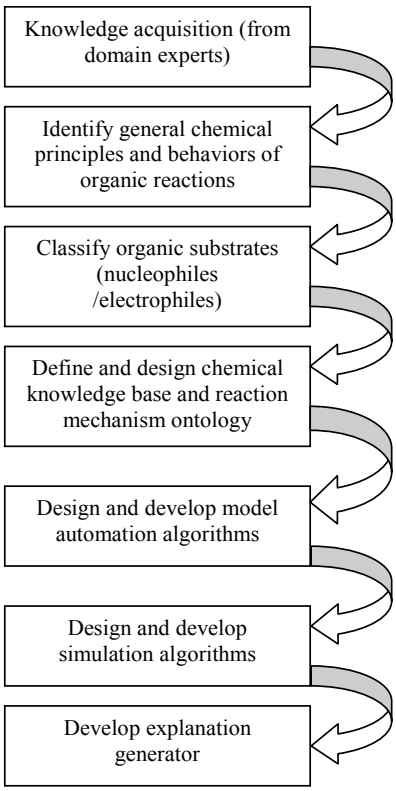


Fig. 4 Research activities in developing the simulator.

A. The Organic Mechanism Ontology: OntoRM

Ontology is a specification of a representational vocabulary for a shared domain of discourse. OntoRM (module 9, Fig. 3) defines chemical knowledge related to reaction mechanism in specific. Samples of the OntoRM can be found in [6]. The reasoning engine will refer to this module to determine what aspects of the domain knowledge should be presented to the qualitative simulator. It can also be used to disambiguate a situation. The roles of OntoRM are summarized as below.

- It is used to describe knowledge, requirements and constraints (no processing).
- It is used for defining special cases and also serves as a bug library.
- It is used as a validation tool (to validate uses of the KB).
- It is used to reject a decision during reasoning or to confirm a prediction before returning the final products.

B. Qualitative Model

Fig. 5 gives a sample QPT model that is used to reproduce the behaviour of the first and third steps of reaction formula (1). Model automation design has been reported in [5]. You may read the right column as "If A and B then C and D". In this case, C and D are qualitatively reasoned by the simulation algorithm (see Fig. 6).

Peocess Slots	Modeling constructs in QP theory	
Individuals	1. H *;represents hydrogen ion* 2. O *;represents the alcohol oxygen*	A
Quantity-Conditions	3. A_m[lone-pair-electron(O)] >= ONE 4. charges(H, positive) 5. electrophile(H, charged) 6. nucleophile(O, neutral) 7. charges(O, neutral)	B
Influences	8. I_- (no-of-bond(O), A_m[bond-activity]) 9. I_+ (no-of-bond(H), A_m[bond-activity])	C
Relations	10. D_s[charges(H)]= -1 11. D_s[charges(O)]= 1 12. lone-pair-electron(O) P^+_- no-of-bond(O) 13. charges(O) P^-_+ lone-pair-electron (O) 14. lone-pair-electron(H) P no-of-bond(H) 15. charges(H) P^+_- no-of-bond(H)	D

Fig. 5 A "make-bond" model fragment represented in QPT. This model is used to reproduce the behaviour of the first reaction step of "$(CH_3)_3COH + HCl$", using the S_N1 mechanism.

C. Reasoning Algorithm

The behaviour of a chemistry system can be described as a sequence of qualitative states occurring over a particular span of time. Changes are caused by continuous chemical processes, which provide the notion of mechanism for causality. Since QPT only can represent the domain knowledge, we have developed a set of algorithms to "reason" or "apply" the knowledge. Fig. 6 gives the algorithm that explains the qualitative simulation steps used by module 3 of Fig. 3.

QPT-BASED SIMULATION ALGORITHM

Q_Simulation(substrate, reagent, OUTPUT)
1. Recognizing substrate and reagent entered by the user
2. Determine a chemical process based on the recognized units
3. Construct QPT process model
4. Perform process reasoning
   4.1 Store the process's entry conditions
   4.2 Store the directly influenced process's quantity
   4.3 Perform quantity space analysis (by QSA module)
5. If process_stopping_condition = true Then
   Store propagated effects in data structures
   Collect and store new individual
   End
6. Update the substrate's molecular structure (by MUR module)
7. If View_Instance_Structure <> EMPTY Then
   Go to step 2
   Else
   Store final products and mechanism in OUTPUT
   End If
8. Return OUTPUT

Fig. 6 Reasoning algorithm based on QPT.

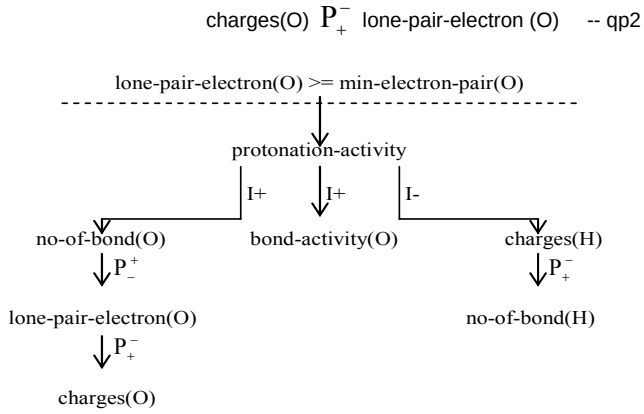
Simulation for the first reaction step works as follows. Initially, there are 3 species: a proton, the chlorine ion, and the alcohol substrate. The "make-bond" process (Fig. 5) is activated in order to simulate the chemical behaviours of the first step of the reaction formula "$(CH_3)_3COH + HCl \rightarrow (CH_3)_3CCl + H_2O$". It is the candidate process because the statements in quantity-conditions also satisfied (Lines 3 – 7), which speak for "the process needs a proton and alcohol oxygen with at least one pair of non-bonded electron to be donated to the proton in order to make a bond". As the process occurs, the quantity being directly influenced is the number of covalent bond, which is defined as two direct influence statements using the I+/I- notation of the QPT; as shown in Line 8 and Line 9. These effects will propagate to other dependent quantities. For example, the oxygen's lone-pair electrons will decrease when more covalent bonds are made on the "O" via the inverse qualitative proportionality defined in Line 12. When the lone-pair electron on "O" decreases, its charges will increase (Line 13). This will make the "O" a positively charged species with three covalent bonds (hence it is unstable). When this is done, the "H" is no longer positively charged (derived from Line 15), thus violating the statement in the quantity-conditions slot. The new quantity created by this process is the oxonium ion, and it will be inserted into the View Instance Structure (VIS). All values assigned to each individual are taken from the quantity spaces by the Quantity Space Analyzer (QSA) that keeps track of the current values of each quantity and the direction of change (increase/decrease). Each state change is recorded in special purpose data structures, and the contents of these structures form the basis for the causal explanation approach used in this work.

V. Causal Explanation

Traditional systems that use pre-coded rules and search routes tend to generate explanation by returning the rules being fired when attempting to draw (or reach) a conclusion. We solicited from the students in an earlier survey that causal account is of help and meaningful to them. As such our approach stresses on the causal theories. Such approach produces results based on reasoning from these qualitative models represented by the QPT formalism. To achieve this aim, a chain of effect propagation represented as functional dependency among chemical parameters will be constructed during runtime by QSA routine (in order to produce the causal graphs). A causal graph depicts the set of causal relationships between quantities occurring in the simulation. A sketch of one such cause-effect relationships is depicted in Fig. 7.

In Fig. 7, the inequality statement shown above the dotted line represents the quantity-condition that must be true for the protonation process to start. Effects are then propagated via the direct (I) and indirect (P) influences of QPT ontology. The process's quantity is protonation-activity. This quantity directly influences no-of-bond for "O" and "H". In other words, after the protonation process "O" will have an extra covalent bond. The effects will propagate to other dependent quantities shown in the diagram. For example, the number of lone-pair electron will decrease when more covalent bonds are made at "O" atom via the inverse qualitative proportionality defined in qp1. In qp2, when the lone-pair electron on "O" decreases, the charges for "O" will increase. Besides, qp2 also explains why "O" is positively charged (loosing of electron to make a covalent bond). Causal graph generation and interpretation have been discussed in [5].

lone-pair-electron (O) P^+_- no-of-bond(O) -- qp1



Legends: I = Influences, and P = Proportionalities.

Fig. 7 A sketch of the causal model for the "protonation" process. The process begins due to having a nucleophile and a proton in the solution.

VI. Simulation Results

A. QRiOM: Problem Solving Model

The problem solving model when running the QRiOM simulator prototype is given in Fig. 8. The alphabets "A" to "H" correspond to the labels in Fig. 9.

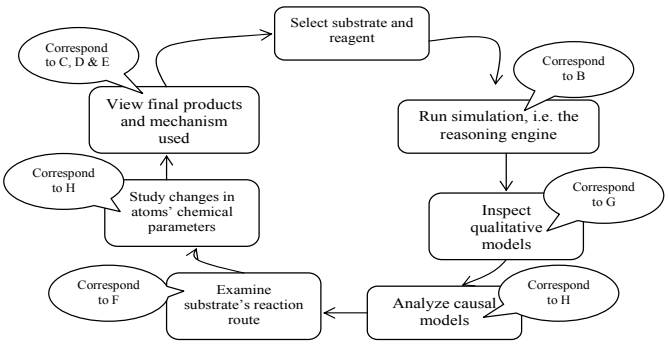


Fig. 8 Problem solving model.

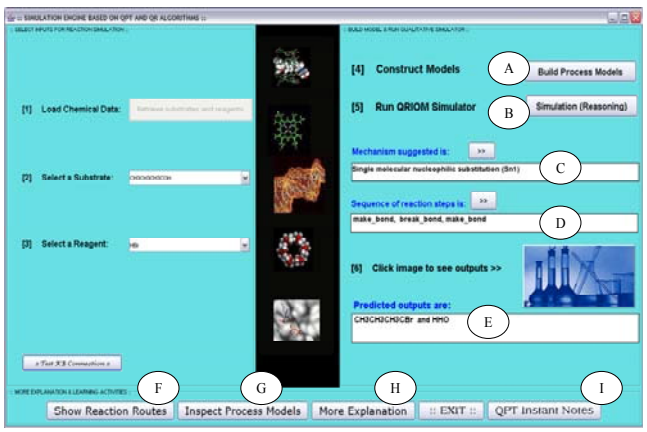


Fig. 9 Main interface of QRiOM.

At the end of a simulation, the following outputs are returned via various interface pages:

- A causal graph that depicts the cause effect chain of chemical parameters in the simulation.
- The whole set of the parametric values taken by each chemical parameter in the reaction simulation. This is called a piece of "history" (see Fig. 10 and Fig. 12).
- The reaction route taken by the input substrate. This result helps explain why certain atom leaves (or approaches) a given compound. The result permits learners to study how a substrate's molecular structure is changed from one process to another (see Fig. 11).
- The pair of reacting species used in each reaction step, and the intermediates produced (Fig. 13).
- The organic process (represented using QPT template) used in predicting the final product of a reaction.

B. Learning from System's Explanation

This section shows how the explanation generated by QRiOM can help nurtures one's conceptual understanding. Much of the explanation used by QRiOM is achieved by tracing the effects propagated through ontological modelling constructs. Inspecting parameter dependency and their direction of change can help a learner to pick up the underlying concepts much better than merely memorizing the reaction steps or formulas.

As mentioned earlier, the state change of each chemical parameter during simulation is recorded for future retrieval (see Fig. 10). The results can then be used for producing the necessary reaction route. An example of the reaction route generated by QRiOM is depicted in Fig. 11, in which the step-by-step changes of the molecular structure of an organic substrate are shown. The system can explain not only the steps it takes during the reasoning process, but also the reasons for following these steps. When Fig. 10 is used in conjunction with Fig. 11, the structure of the final product can be easily drawn. For example, when the charge on "C" is positive (A1, Fig. 10), then a positive sign is assigned next to the "C" atom (B1, Fig. 11). Likewise, in A2 of Fig. 10 (under "After step 3" heading), the "C' regained its stability, and this change is reflected in B2 of Fig. 11.

Learners can also browse the behavioural change of parameters belonging to each reacting species (Fig. 12). User may select a species (from a pull down list), and the whole happening of the selected atom can be viewed.

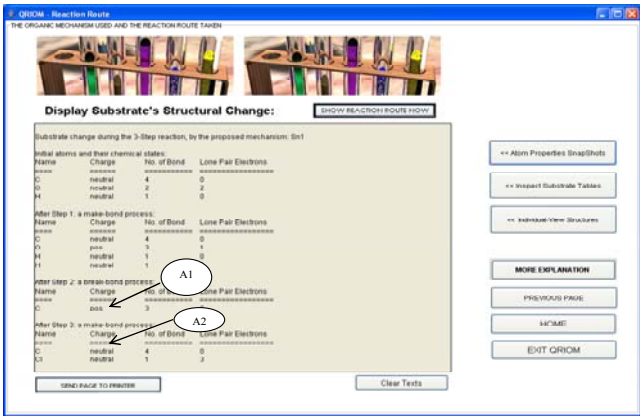


Fig. 10 Main parameters of an atom and the associated values are recorded for further inspection.

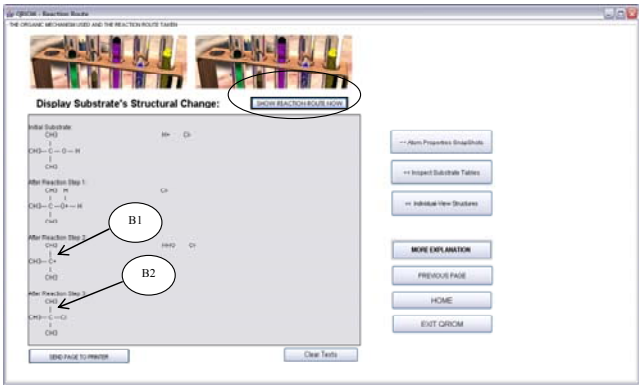


Fig. 11 A substrate's structural change is presented in 2D format. The diagram corresponds to the series of three small reaction steps shown in Fig. 2.

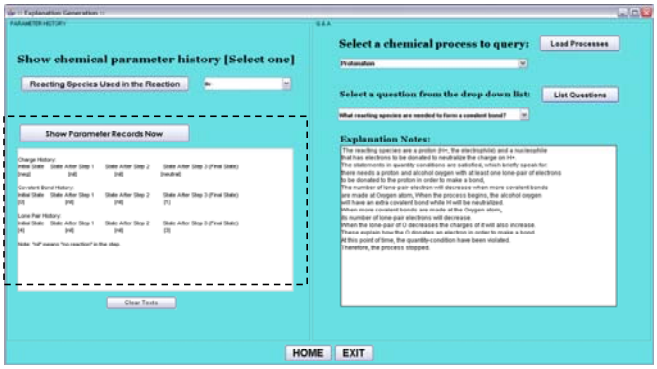


Fig. 12 Chemical parameter state of each reacting species involved in a simulation task can be examined in greater detail.

Since majority of the chemistry students have difficulties in identifying the right view pairs for processes activation, the tool will generate the whole set of view pairs used in the simulation (Fig. 13), thus informing the learner of the type of functional units that activated a given process. For instance, "H+" and "CH3CH3CH3COH" are the reacting species (an electrophile and a nucleophile respectively) that activated the "make-bond" process. The process also generated an intermediate called "CH3CH3CH3CO+H2" (see "After Step 1" heading).

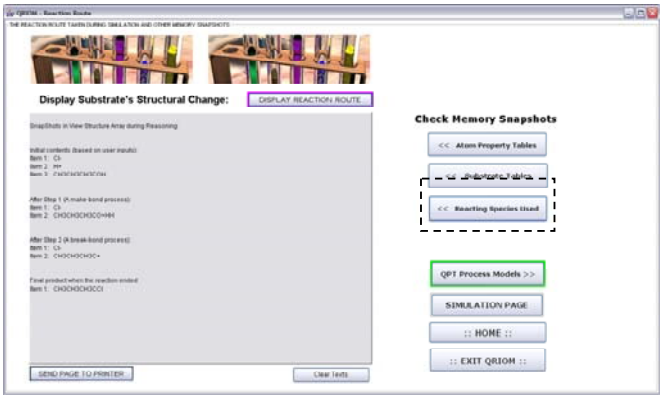


Fig. 13 The choice of reacting species for each reaction step, and the intermediates produced are displayed.

VII. User Feedback

A survey comprised of questionnaire and hands-on was conducted as soon as the completion of the first prototype. The procedures used in shown in Fig. 14. The survey abided two objectives. First, it was designed to collect the students' attitude and receptive towards using a software tool. Second, the survey was to find out how far the prediction and explanation generated by the QR/QPT approach can benefit the chemistry students (i.e. to test the "usefulness" when using QRiOM). There is a positive response as far as the student evaluation is concerned.

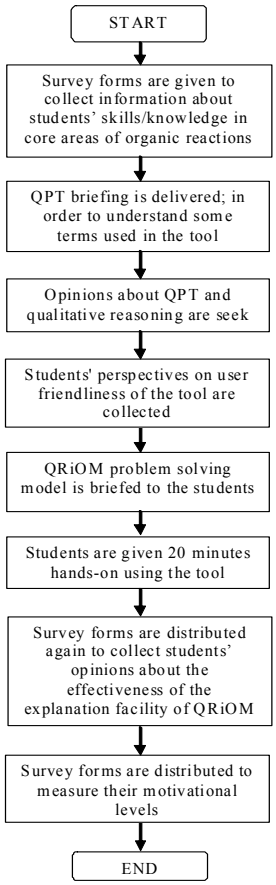


Fig. 14 Flowchart of the QRiOM evaluation exercise.

A. Evaluation Context

For this preliminary survey, a purposive sampling method was used to select the students. The study recruited a small group of chemistry students (with different academic standing) enrolled in an introductory chemistry class. The first set of the survey was meant to find out whether they could do better in solving new problems in terms of achieving better understanding of the subject. To achieve this aim, the survey starts by having the participants to answer the "*Before using the simulation tool...*" part of the questionnaire. This particular questionnaire is to assess their skills in core areas of organic reactions before using the tool. After that, they were given having some hands-on. Then, the same set of questionnaire was used again to seek if their levels of understanding of the core areas have been increased.

Second set of the questionnaires was distributed after the students were exposed to the simulator tool. They were asked to give comments on some Graphic User Interface (GUI) design criteria, such as clarity of interface (80%), interface consistency (70%), and meaning of commands (60%). Percentage in bracket indicates the satisfaction level. Attitudes toward using the software have also been measured, including several affective components, for example, "I like it" or "I dislike it". The result demonstrated that, (1) Students with positive attitude outperformed those with negative attitude, (2) Most of them reported being very pleased of the hands-on they had done, and (3) Many felt that there was too much emphasis on the QPT terms and suggested more lectures should be given to them. The responses collected seem very encouraging given that this is the first time the chemistry students had tried a qualitative simulator. We will take the third comment of the students to improve on the software tool, such as to convert most of the QPT terms into layman's words.

The third set of questionnaire was meant to solicit the students' responses towards the explanation generation capability of QRiOM. Some results are presented in the following section.

B. Survey Results

Overall, there was general understanding that the new means of learning through qualitative simulation had proved valuable. The data indicated that slightly less than half of the students, representing 40%, felt that they underwent a change of reasoning (thinking), as the explanation does reveal the intuition behind the design. They have never thought of using a state graph or causal graph or even the reaction route to express the overall behavioural change of substrates. More than 70% of the respondents strongly agreed on question 2 and question 3 in the questionnaire. Namely, students seemed to find analyzing the reaction route the cause-effect demonstration helpful in learning how an organic process takes place, and the overall changes undergone by the organic substrate. Fig 15 shows the students' opinions in the selected skill sets before and after using the simulator. In Fig. 16, the students' responses reveal that most students were motivated while using the tool. The tool motivates the student to learn, especially in several areas such as the following:

- They can repeatedly run the same reaction equation.
- They are allowed to choose different combination of <substrate, reagent> pair.
- The tool offers certain degree of interactivity.
- The tool provides adequate coaching.

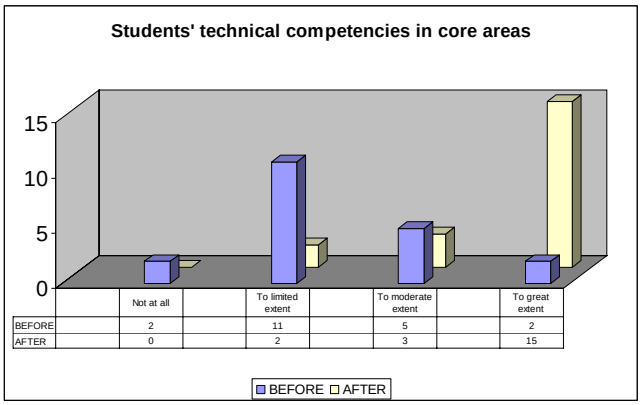


Fig. 15 Student pre-test and post-test responses to the core skills.

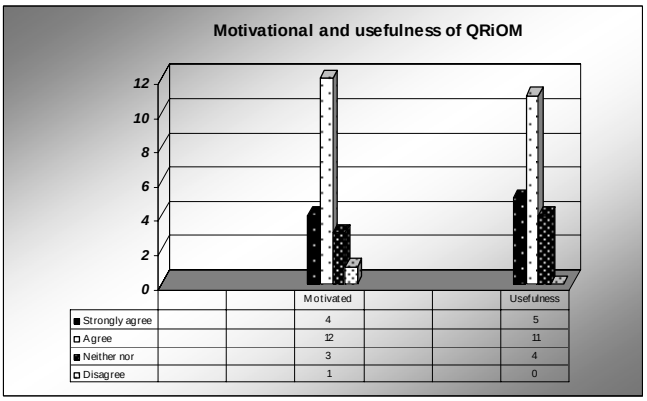


Fig. 16 Students' feedbacks on motivational and usefulness aspects.

VIII. Conclusion

The dynamic explanation generation capability of QRiOM has been discussed. This reasoning framework appears to be a viable alternative for implementing learning software for chemistry education. The hybrid use of qualitative reasoning based on QPT ontology can explain various phenomena in the subject. Although QRiOM was not meant to capture student's learning behaviour, the explanation provided by QRiOM can resolve common questions asked by the students based on organic chemistry principles. After being developed the prototype and tested our QR algorithms, we anticipate a fully usable system that can assist the chemistry students not only in understanding the subject, but engaging them in building simple models as a mean to acquire knowledge.

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