

Development and Evaluation of a Chemistry Educational Software for Learning Organic Reactions Using Qualitative Reasoning

Alicia Y. C. Tang, Sharifuddin M. Zain, and Rukaini Abdullah

Abstract—In science education, it is believed that students should understand the qualitative principles that govern the subject including the cause-effect relationships in processes before they are immersed in complex problem solving. Traditional educational programs for teaching organic chemistry do not usually explain or justify an observed chemical phenomenon. These programs do not “explain” simply because the results are obtained through chaining the rules or by searching the reaction routes that have been pre-coded in software. This paper discusses the development techniques, simulation results, and student evaluation of a software tool that aimed to help chemistry students learn organic processes through the study of causal theories in a chemical system. Mastering the causal theories of physical phenomena can help students in answering fundamental questions in science education. The simulation technique used is qualitative reasoning that emphasizes the importance of conceptual knowledge and causal theories in education, particularly concerning predicting and reasoning about system behaviour. The results from a preliminary evaluation showed that the tool is effective in terms of its ability to promote students’ understanding of organic reactions through the inspection of the explanations generated by the software, where students are seen as the recipients of knowledge delivered via the “explanation” pedagogy.

Keywords—Evaluation, explanation, learning, organic reaction, qualitative reasoning.

I. INTRODUCTION

ORGANIC chemistry reaction is a difficult subject to learn. 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 (causal theories) among these processes. If students learn the subject by memorizing the steps and patterns of each reaction, then they may not be able to answer simple questions such as: Why would this reaction go this way? What is favourable about this particular step? Why was the process stopped? This is the educational problem that is being solved,

Y.C. Alicia Tang is with the University of Tenaga Nasional, Selangor, Malaysia (phone: 603-8921-2336; e-mail: aliciat@uniten.edu.my).

S. M. Zain is with the Department of Chemistry, Malaya University, Kuala Lumpur, Malaysia (e-mail: smzain@um.edu.my).

R. Abdullah is with the Department of Artificial Intelligence, Malaya University, Kuala Lumpur, Malaysia (email: rukaini@um.edu.my).

as memorizing formulas is not a good method in any type of learning. In understanding organic reactions, one has to know the many cognitive steps from one chemical reaction to another until a stable product is formed. These cognitive steps (the “mechanisms”) are among the many difficulties chemistry students are facing; such as lacking the skills to analyze the various steps and translate the reactions into the forms that can be used to predict the final product in reasonable and justifiable ways. There has been many strives for innovation in teaching and learning chemistry using computer software. However, most of the chemistry educational software used traditional approach [1]. Traditional chemistry educational software is inadequate to promote understanding such as explaining why and how things happen. These programs do not “explain” simply because the results are obtained through chaining the rules or by searching the reaction routes that have been pre-coded in software. Existing knowledge-based systems for organic chemistry are not using qualitative reasoning as the problem solving technique. Examples of techniques used are Self-Organizing Map (SOM) and Neural Networks and Genetic Algorithms as described in [2].

Qualitative reasoning (QR) which makes causality explicit is of value in education. The potential of this new methodology for building science educational software has been demonstrated by several high cited works such as CyclePad [3], VisiGarp [4]-[6], ALI [7], and Betty’s Brain [8]. The common features of these systems are the ability to predict and explain the behaviour of physical systems in qualitative terms in educational and training setting. The success of the software to promote and induce learning and the birth of articulate software [9]-[10] marked another milestone for further investigation, application, and popularity of qualitative reasoning techniques. Other QR-based systems are: Intelligent tutoring systems for training [11] where the simulation is based on components ontology and QPT, qualitative models in ecology and their use in intelligent tutoring system by Salles & Bredeweg [12] and Salles *et al.* [13], Error-Based Simulation (EBS) to predict the qualitative behaviour of mechanics problems and to generate feedback for learning from mistake [14]-[16], and works on authoring Graph of Microworld (GMW) [17]-[19].

This paper discusses the results of the implementation of the conceptual framework described in previous works [20]-[21].

A tool named QRiOM (Qualitative Reasoning in Organic Mechanism) has been developed. QRiOM is able to simulate (predict the outcome of a reaction) and explain the behaviour of organic reactions “intuitively”. The learning tool consists of nine functional components. Collectively, the components support the tasks of recognizing input substrates, automating the construction of qualitative models, performing the actual simulation and providing both causal and behavioural explanations to justify simulation results. Qualitative Process Theory (QPT) [22] is a type of process-based ontology for qualitative reasoning. Ontology provides a common vocabulary in a defined area (e.g., organic chemistry reactions). It has the potential to facilitate the formation of semantic relationships (e.g., chemical parameter dependency) between various portions of useful information to enhance the learning experience in an educational setting [23]. We have also developed a set of simulation algorithms to “reason” about the models constructed using QPT.

In general, chemistry problems presented in textbooks could be difficult to understand by students because the diagrams and figures are in static form. The educational benefits offered by QRiOM include the ability to take users into environments otherwise inaccessible by conventional face-to-face teaching and the ability to create a dynamic and interactive environment for learning. The tool is similar in idea with some existing systems based on QR technology. However, the software is supported by a two-tier knowledge base, namely the OntoRM reaction mechanism ontology (purely used as a validation tool) and a chemical knowledge base that stores the essential domain knowledge (e.g., basic chemical facts). The QR approach based on QPT described in this work has never been attempted by researchers in the organic chemistry field. The reasoning framework (and the prototype) is able to generate similar result outcomes as the one produced by chemists. Evaluation results showed that the multiple ways of presenting the outputs are effective in promoting one’s conceptual understanding. In specific, students are seen as the recipient of the “explanation” pedagogy embedded in the software.

The remainder of this paper is organized as follows. Section II describes two related systems. Section III provides the background knowledge of this work. Section IV presents the techniques and approaches used in the simulation of organic reactions while the simulation results are discussed in Section V. Section VI discusses the evaluation results of the simulator prototype. Section VII concludes the paper.

II. RELATED WORK

LHASA [24] and QALSIC [25]-[27] are two systems that shared some similarities to our work; in terms of the application domain and the simulation technique used. The former, is an expert system that used database of retro-reactions (called transforms). It has been under development at Harvard since late 1960’s. The knowledge base in LHASA contains “rules” which dictate LHASA’s behaviour towards a target molecule. The transform descriptions are an integral part

of the knowledge base. When LHASA reads a transform entry, it finds instructions (e.g. to build a precursor from the target structure) and acts accordingly. On the contrary our work is to predict and explain the target molecule (i.e. forward planning). LHASA relied heavily on experienced chemists to find and select the best retrosynthetic routes in an interactive and time-consuming manner. There are some associated problems with this approach. For instance, the long-range transforms, which were created based on the expectations of a small group of chemists, took as much as six months to prepare, and the program could easily give cumbersome plans for molecules that contained unusual or unforeseen combinations of functional groups. In the course of development of the LHASA program, the knowledge base organization has become very complex. This will not happen to our system since there is no pre-coded solution or any reaction route kept in the knowledge base, only chemical theories and basic facts required to perform the simulation are stored in the knowledge base. A proprietary language called CHMTRN (CHeMistry TRAnslator) is used for the knowledge base development.

On the other hand, QALSIC is a system that performs inorganic chemistry simulation. QALSIC has managed to break the proof-of-principle question of how inorganic chemistry can be presented in qualitative terms especially in reasoning on its dynamic processes (such as precipitation and dissociation). Although the QALSIC related literatures claimed that the system is able to simulate unknown reactants (substances whose name are not found in knowledge bases), further examination (by rigorous system testing) reveals that the system can make correct prediction only if the chemical equation has the pattern “ $AB + CD \rightarrow AD + CB$ ” (i.e., direct cross-linking of elements is obeyed). In addition, processes and most of the explanations are handcrafted. In contrast, QRiOM is able to construct qualitative models at runtime and provide various forms of explanations on-the-fly.

III. BACKGROUND

This section provides the necessary background for the application domain (organic chemistry reactions) and the modelling formalism (qualitative process theory) used in this work.

A. Organic Reactions

Vast majority of organic reactions take place at functional groups. Functional groups are the structural units responsible for a given molecule’s chemical reactivity. A functional group is a portion of an organic molecule, other than carbon and hydrogen (the normal hydrocarbon framework) or which contain bonds other than C–C and C–H. These units will determine what type of organic process (e.g., “make-bond” or “break-bond”) can be activated. 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. Learning organic reaction mechanism needs some basic skills and these skills are related to the nature of the problem being solved. From an interview,

students' barriers to understanding the organic course were collected as depicted in Fig. 1.

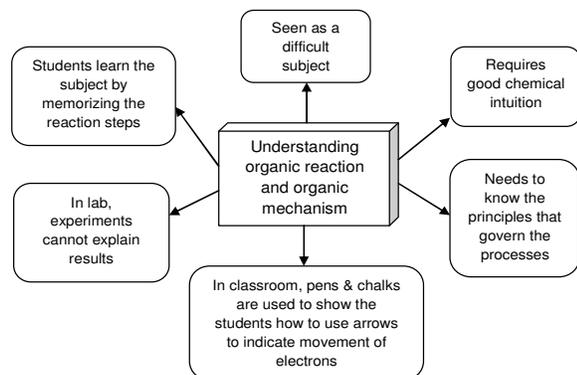


Fig. 1 Students' barriers to understanding the organic chemistry course

Qualitative reasoning is able to make acceptable predictions using only qualitative information. Such qualitative description of domain knowledge is sufficient to understand and explain the underlying chemical principles of organic reactions. Hence, the technique is tested and applied to solving the problem.

B. Representing Chemical Theories Using QPT

QPT is used as the domain knowledge modelling language. The modelling constructs of QPT provides grounds for representing chemical theories qualitatively, with notions of causality which can be used to explain the behaviour of a chemical system. We will now give one example of chemical reaction to show that qualitative description is sufficient to understand the underlying chemical principles. In the example, quantitative data and precise measurement is not at all required. In chemistry class, students are taught that the compound " $(\text{CH}_3)_3\text{C}-\text{OH}_2^+$ " will undergo a "break-bond" process. The cleavage of the carbon-oxygen bond in *tert*-butyloxonium ion ($(\text{CH}_3)_3\text{C}-\text{OH}_2^+$) is due to the unstableness of the oxygen atom since it has three covalent bonds (valency for oxygen is two). Once the bond between the carbon-oxygen is broken, the oxygen will regain its stability. However, the carbon in the main chain of the organic compound will become a positively charged species since one of its valence electron is donated to the oxygen in order to neutralize it. The changes that propagated from a chemical parameter to another can be easily modelled as a few functional dependency statements (called "qualitative proportionalities" in QPT term) as follows. Note that words after the "//" sign are remarks.

```
lone-pair-electron(O) P+- no-of-bond(O)
//decreasing oxygen's covalent bond will increase its lone-pair
electron
charge(O) P-+ lone-pair-electron(O)
//increasing oxygen's lone-pair will decrease the charge on it;
oxygen is being neutralized
charge(C) P+- no-of-bond(C)
//decreasing carbon's covalent bond will increase its charge; carbon
is positively charged
```

As demonstrated above, the formalism of QPT which makes causality explicit is of great value in explaining chemistry phenomena for teaching purposes. Qualitative simulation provides an alternative way for chemist to represent, develop, and implement models.

IV. METHODS

Fig. 2 relates the use of qualitative reasoning, simulation and explanation within the context of this work. The relationships among these terms form the basis for the development of the simulator prototype described in this paper.

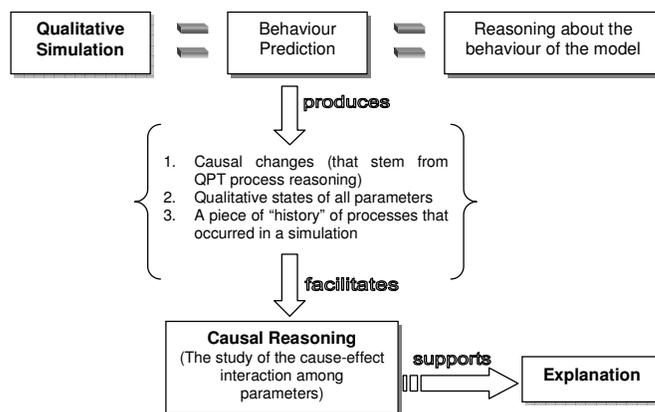


Fig. 2 The use of qualitative reasoning, simulation and explanation within the context of this work

A. Qualitative Reasoning as the Simulation Technique

This research began by conducting an empirical study on chemical reactions involving alcohols and alkyl halides. From the study, "make-bond" and "break-bond" were identified as two generic processes in the simulation of organic reactions involving two groups of substrates (alcohols and alkyl halides). The two processes are the reusable models in the framework to support multiple reactions simulation. From analysis of various chemical reactions occurring under S_N1 and S_N2 mechanisms, the common set of chemical theories and behaviour have been identified for the two processes; from which the model automation logics are formulated [20].

A set of QR algorithms used for reaction simulation is developed to "reason" about the QPT models [21]. The issue of lack of explanation in chemistry software was addressed by embedding a causal explanation generator that produces explanation in various forms (texts and diagrams). The generator justifies and explains a simulated result by tracing the chains of causality that stem from model reasoning.

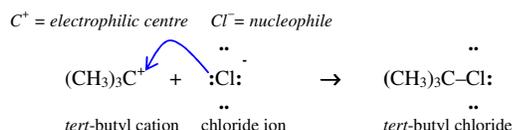
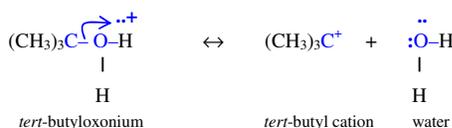
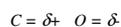
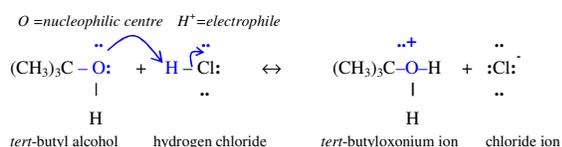
B. Thought Processes as Simulation Task

In this work, " $A + B \rightarrow C + D$ " is named as a chemical equation; " $A + B$ " is an organic reaction (where "A" is an organic substrate). Before a simulation can begin, the reaction steps of a chemical equation must first be identified. As an example, (1) can be described as a series of processes that

occurs and these processes will be used to explain how the product is formed (i.e. the “mechanism” used). Overall, the reaction will convert the starting material ((CH₃)₃COH, a tertiary alcohol) to final product ((CH₃)₃CCl, alkyl halide).



The “thought processes” for the chemical equation “(CH₃)₃COH + HCl → (CH₃)₃CCl + H₂O” is depicted in Fig. 3 as a series of the small reaction steps. Each small step is represented as a QPT process model (an example is presented in Fig. 4). The QR algorithm will then be applied to the QPT model to predict the outcome of the reaction as well as reproducing the behaviour of an organic reaction. Note that double dots represent the electrons associated with the particular atom in the molecule.



Name of the chemical process	Reactant 1	Reactant 2
Protonation (“make-bond”)	(CH ₃) ₃ COH (nucleophile)	H ⁺ (electrophile)
Dissociation (“break-bond”)	(CH ₃) ₃ C-OH ₂ ⁺	
Capturing of anion by carbocation (“make-bond”)	(CH ₃) ₃ C ⁺ (electrophile)	Cl ⁻ (nucleophile)

(d) Reactants and their associated chemical processes

Fig. 3. The conversion of a tertiary alcohol to yield alkyl chloride can be described as a series of three small steps

C. Chemical Process Reasoning

Fig. 4 is a QPT model that captures the general chemical behaviour of an organic process that adds a covalent bond between a nucleophile and an electrophile. The QPT model is similar to the mental model constructed by chemists when solving the same problem. The models people use in reasoning about physical world are called mental models [28]. The QPT model represents the first reaction step presented in Fig. 3(a).

In the figure, you may read the right column as “If (A and B) Then (C and D)”. In this case, C and D are qualitatively reasoned. Our work follows with the notion of “processes” defined in [22], in which “processes” are the agent of change in a chemical system. Influences contain statements that specify what can cause a quantity to change, through direct influence imposed by the process (label C). As the process occurs, bond-activity is a direct influence’s process quantity and it has a positive influence (I+) on the no-of-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. Other propagation of effect is defined in Relation-slot (label D). It is propagated via a set of qualitative proportionalities defined in the QPT process model. In this case, the number of covalent bond the “O” possesses is directly influenced by the process. These effects will propagate to other dependent quantities. 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. Decreasing lone pair electron on “O”, will cause and increase in its charge (Line 13). This will make the “O” a positively charged species with three covalent bonds (hence it is unstable). When “O” is protonated, it is no longer neutral (given in Line 13) thus violating the statement in the quantity-conditions slot.

Process Slots	Modelling constructs in QPT	
<i>Individuals</i>	1. H ;represents hydrogen 2. O ;represents the alcohol oxygen	A
<i>Quantity-Conditions</i>	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
<i>Direct Influences</i>	8. I ₊ (no-of-bond(O), A _m [bond-activity]) 9. I ₊ (no-of-bond(H), A _m [bond-activity])	C
<i>Relations</i>	10. D _S [charges(H)] = -1 ;decreasing sign 11. D _S [charges(O)] = 1 ;increasing sign 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. 4. A “make-bond” model fragment represented using QPT. This model fragment is used to reproduce the behaviour of the first reaction step for “(CH₃)₃C-OH + HCl” reaction

Along with the reasoning, the running states of all the chemical parameters are kept in special purpose data structures (e.g., 2D arrays). The contents of these structures are used for generating causal graphs (see below). These graphs will then be used for explaining and justifying the simulation results produced by QRiOM.

D. Causal Explanation

Earlier we solicited from the chemistry students that causal account is of help and meaningful to them. Since one of the objectives of this work is to prepare and generate explanations in a language (and format) understandable to the learners, as such our approach stresses on the causal theories. The

procedures for generating causal graphs have been reported in [29]. A causal graph depicts the set of causal relationships between quantities occurring in the simulation. A hand-instantiated version is presented in Fig. 5. The computer generated version can be found in Fig. 8. Tracing and interpreting a causal graph are the basis of the causal explanation generation approach used in this work.

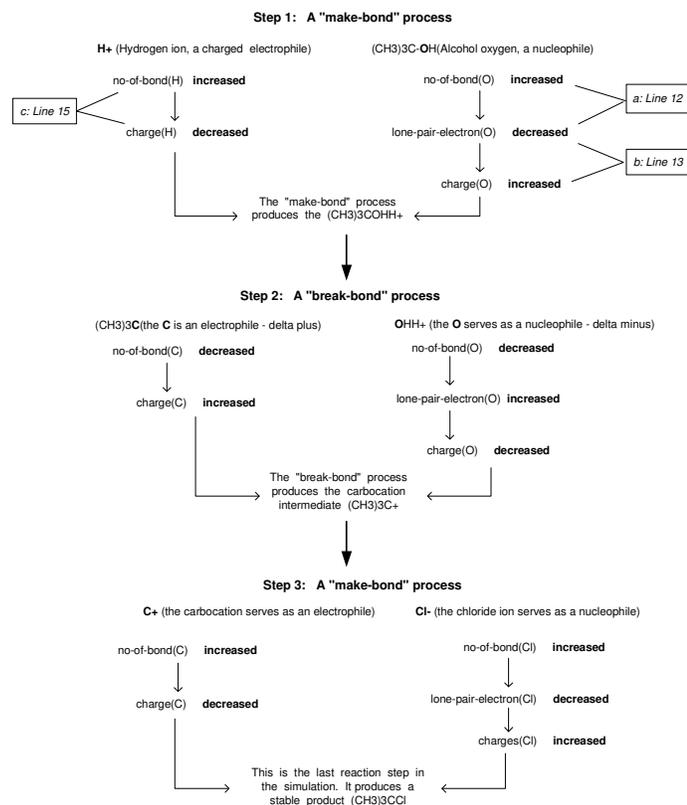


Fig. 5. A causal graph showing cause-effect relationship of chemical parameters during the simulation of “(CH₃)₃C–OH + HCl” reaction

For cross checking purposes, label “a” in Step 1 of Fig. 5 represents Line 12 (lone-pair-electron(O) P₋ no-of-bond(O)) of the “make-bond” process depicted in Fig. 4. Similarly, from the same graph, label “b” is derived from Line 13 (charges(O) P₊ lone-pair-electron(O)) and label “c” represents Line 15 (charges(H) P₊ no-of-bond(H)) from the same model.

V. SIMULATION RESULTS

At the end of a simulation, QRiOM will return the final product formed as well as the following simulation results:

- The entire reaction route. This output helps explain why certain atom leaves (or approaches) a given organic compound. Such result permits learners to study how a substrate’s molecular structure is changed from one process to another (Fig. 6).
- The QPT model representing the behaviour of an organic process (Fig. 7).
- A causal graph that depicts the reacting species used; the

intermediates produced, and the cause-effect chain of chemical parameters in the simulation (Fig. 8).

- The whole set of the parameter state histories. This is called a piece of “history” in QPT.
- The atom property table that contains the chemical states possessed by each reacting unit during simulation (Fig. 9a).

As far as the simulation results are concerned, they matched those written in textbooks. Table I presents a summary of the computer screenshots together with the objectives they serve and the questionnaire used to test it. Survey results are presented in the following section.

TABLE I
COMPUTER SCREENSHOTS, OBJECTIVES AND THE QUESTIONNAIRES USED

Computer screenshots	Educational objectives	Questionnaires that test the achievement of the objectives
Reaction route (Fig. 6)	<ul style="list-style-type: none"> • Promote conceptual understanding • Able to articulate various aspects of a reaction 	<ul style="list-style-type: none"> • “Effectiveness of the explanation of QRiOM” survey form • From an interview
QPT model (Fig. 7)	<ul style="list-style-type: none"> • Able to articulate various aspects of a reaction 	<ul style="list-style-type: none"> • “Usefulness and Helpfulness of QRiOM” survey form • “Effectiveness of the explanation of QRiOM” survey form • From an interview
Causal graph (Fig. 8)	<ul style="list-style-type: none"> • Promote conceptual understanding • Able to articulate various aspects of a reaction 	<ul style="list-style-type: none"> • “Effectiveness of the explanation of QRiOM” survey form • “Usefulness and Helpfulness of QRiOM” survey form • From an interview
Parameter state histories	<ul style="list-style-type: none"> • Promote conceptual understanding 	<ul style="list-style-type: none"> • “Usefulness and Helpfulness of QRiOM” survey form
Atom property table (Fig. 9a)	<ul style="list-style-type: none"> • Promote conceptual understanding 	<ul style="list-style-type: none"> • “Effectiveness of the explanation of QRiOM” survey form

Reaction route: In QRiOM, a substrate’s structural change is represented in 2D format, resulting in the so-called “reaction route” of a simulation. An example of reaction route generated by QRiOM is depicted in Fig. 6. Reaction route gives the step-by-step change of the molecular structure of an organic substrate. When organic reactions are described in this way, the product of an organic reaction can be readily predicted, without recourse to memorization. Inspecting such a 2D representation can help promote the conceptual understanding of a student.

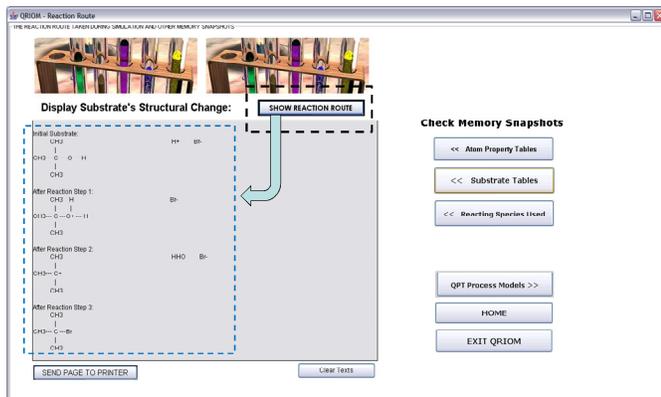


Fig. 6. Step-by-step change of the molecular structure of an organic substrate

QPT models: There are different ways in which learners can acquire knowledge. Inspecting ready-made simulations is one; another approach is to engage learners in building models as a way to acquire knowledge. Model construction activity is not included in our implementation. Instead, qualitative models are automated for their inspection. This is because it does not suit the learners' background of this work. When inspecting a model, students have to articulate relationships between entities and dependencies. This can help improve their reasoning ability. A screenshot of model inspection page is shown in Fig. 7. The main reason for letting students to inspect qualitative model is that they can articulate ideas behind the design of the various slots in a QPT model. For example, the "quantity-condition" can be used to justify why would a process start/stop? Students typically have problems in describing the chemical parameters needed to solve the problem. This is due to lack of the necessary chemical intuition, especially on how to relate the parameters within a deficiency.

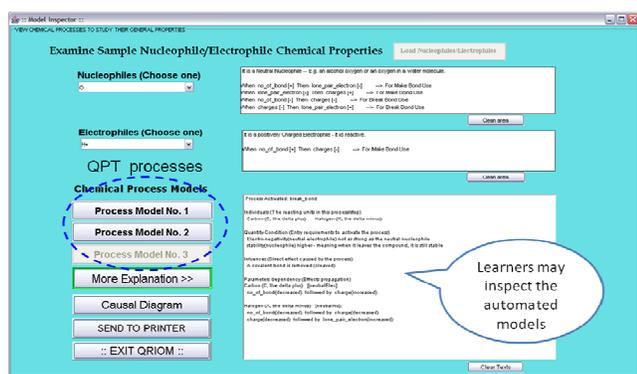


Fig. 7. A QPT model generated by the tool

Causal graphs: Much of the explanation used by QRiOM is achieved by tracing the effect propagation through ontological modelling constructs of QPT. During each reaction simulation, a causal graph (Fig. 8) is generated that shows the use of the qualitative proportionality statements in the QPT models. Inspecting a causal model helps learners to rationalize why a

particular process occurred. This can lead to a deeper understanding of chemical processes.

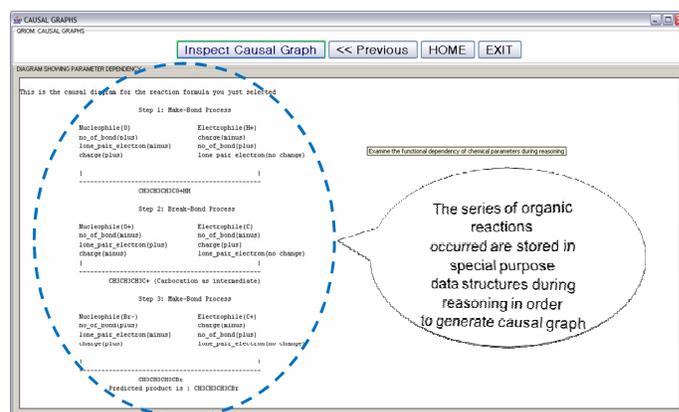


Fig. 8. A causal graph generated by QRiOM that enables learners to examine the cause-effect relationships of chemical parameters during reasoning

The values assigned to the chemical parameters during simulation are recorded in special purpose data structures for future retrieval. One such structure is the atom property table (Fig. 9a). These results can then be used to generate the necessary reaction route (Fig. 9b). The structure of the final product can be easily drawn from Fig. 9a. For example, when the charge on "C" is positive (A1, Fig. 9a), then a positive sign is assigned next to the "C" atom (B1, Fig. 9b). Likewise, in A2 of Fig. 9 (under "After step 3" heading), the "C" regained its stability and this change is reflected in B2 of Fig.9b.

Display Substrate's Structural Change: DISPLAY REACTION ROUTE

Substrate change during the 3-Step reaction, by the proposed mechanism: Snt

Initial atoms and their chemical states:

Name	Charge	No. of Bond	Lone Pair Electrons
C	neutral	4	0
Br	neutral	1	3

After Step 1: a break-bond process:

Name	Charge	No. of Bond	Lone Pair Electrons
C	pos	3	0

After Step 2: a make-bond process:

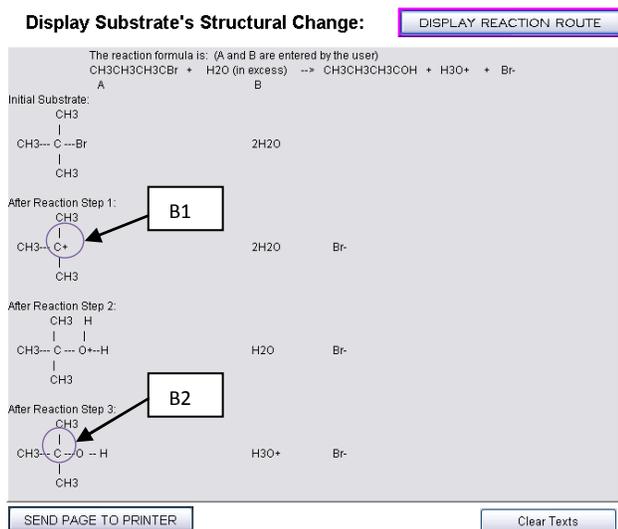
Name	Charge	No. of Bond	Lone Pair Electrons
C	neutral	4	0
H2O	pos	3	0

After Step 3: a break-bond process:

Name	Charge	No. of Bond	Lone Pair Electrons
C	neutral	4	0
OH	neutral	2	2

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(a)



(b)

Fig. 9. (a) The chemical states possessed by each reacting unit during simulation are stored in atom property table, (b) A reaction route drawn from using the data values in atom property table

This work produced better explanation (in terms of less technical in its presentation) as compared to LHASA and QALSIC. LHASA presented a bunch of equations and very complex molecular structures while QALSIC does not give any explanation. Apart from this, QRiOM prototype is able to handle new cases since only general chemical principles of organic reaction are stored and not the specific reaction routes that produce the final product.

VI. PROTOTYPE EVALUATION

An evaluation was conducted upon the completion of the QRiOM prototype. Only a small group of chemistry students enrolled in an introductory chemistry class was recruited, as QRiOM currently has the status of a prototype. The survey comprised questionnaire distribution, interviews and QRiOM hands-on. The results of the evaluation suggest that QRiOM is effective in terms of its ability to promote understanding in learning organic processes through the inspection of the various forms of explanation generated by the tool.

A. Procedure Used

The evaluation includes a lecture on the QPT ontology and a tutorial on QRiOM, particularly focusing on some common ontological modelling constructs and the notion of qualitative causal graphs. After introducing the modelling language and a walkthrough on QRiOM, time limited hands-on sessions began. At the end of each session, students are given a survey form. Fig. 10 shows the procedures used in conducting the system evaluation while Table II summarizes all the questionnaires and the associated educational objectives that each achieved.

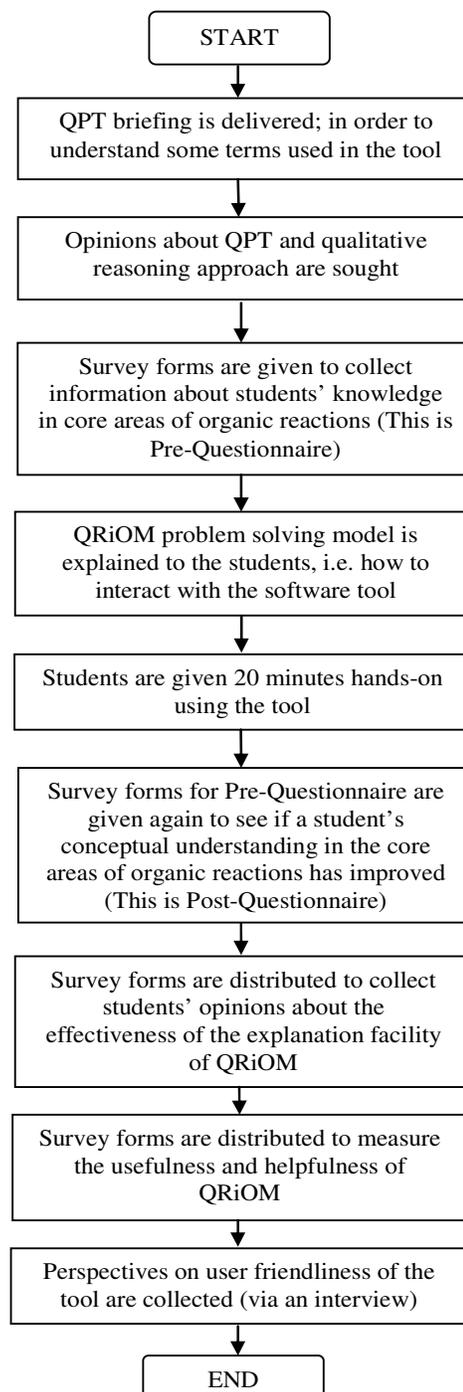


Fig 10. Flowchart of the QRiOM evaluation exercise

TABLE II
QUESTIONNAIRES AND THE FULFILMENT OF RESPECTIVE EDUCATIONAL OBJECTIVE

Questionnaire	Educational objectives	Survey Results
1. "Pre-Questionnaire" survey form	<ul style="list-style-type: none"> Improve in conceptual understanding There is a positive mental change (high scores were given in post-test evaluation) 	Fig. 12
2. "Post-Questionnaire" survey form		
3. "Effectiveness of the explanation of QRiOM" survey form	<ul style="list-style-type: none"> Improve in conceptual understanding (especially in behavioural and causal aspects of a reaction) Able to articulate (can provide longer answers) 	Fig 14
4. "Usefulness and Helpfulness of QRiOM" survey form	<ul style="list-style-type: none"> There is a positive mental change (more confidence in attempting new problems) Able to articulate 	Fig. 15

B. Evaluation Results and Discussion

Assessment of students' skill in core areas of organic reaction: Participants were asked to answer the "Before using the simulation tool..." questionnaire (Fig. 11). It is termed as Pre-Questionnaire. This questionnaire is to assess student skill and knowledge in core areas of organic reactions before using the tool. These set of questionnaires were distributed twice to observe the pre- and post- differences; once was before the students were exposed to the tool and once after they had the hands-on session.

Skill-Set Area	Poor	Fair	Good	Expert
1. Fundamental principle of organic reactions				
2. S_N1 and S_N2 mechanisms				
3. "Make-bond" and "break-bond" processes				
4. Parameters dependency in an organic reaction				
5. Use of reacting species in "make-bond" and "break-bond" organic processes				
6. Classifying structural units as nucleophiles or electrophiles				
7. Chemical theories that support an organic reactions				
8. Rule-of-thumb use in predicting final product(s)				

Fig. 11. The survey form for course competency assessment distributed before/after using the simulator

Participants were then briefed with the problem solving model of QRiOM. After that, the students were exposed to the tool and then they were asked to rate their competencies for several technical skills stated in "After a number of hands-on..." questionnaire. This survey aims at collecting the opinions from the students to observe if there is a mental change/shift experienced after using the tool. It is also to find out if the students can do better in solving new problems. The same set of questionnaire is used as in Pre-Questionnaire. The chemistry students are observed to learn better in terms of their

conceptual understanding of the reactions. Based on the feedback, it can be concluded that they could do better in solving new problems (e.g., when given a new set of reactants) as a result of acquiring skills in knowledge articulation (Fig. 12).

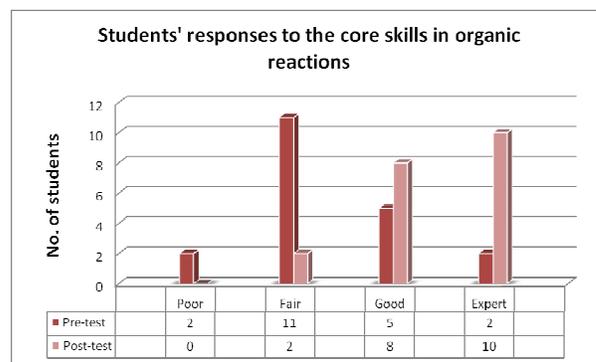


Fig. 12. Student pre-test and post-test responses to the core skills

Assessment of Effectiveness of QRiOM's Explanation Facility: After answering the "before-and-after" sets of questionnaire, they were told to continue with the questions that aimed at assessing the effectiveness of the explanation facility of QRiOM. The set of questionnaire shown in Fig. 13 was meant to solicit the students' responses towards the explanation generation capability of QRiOM. This survey enables us to assess if chemistry students are able to articulate knowledge after analyzing the various ways of presenting the results of a simulation.

Knowledge aspects	Not at all	To a limited extent	To a moderate extent	To a great extent
1. The conditions to start/stop a chemical process				
2. The proper identification of nucleophile and electrophile to activate a chemical process				
3. Cause-effect propagation among chemical parameters				
4. Behavioural change of a substrate (in terms of its charge, lone pair changes)				
5. The production of an intermediate: the why and how?				
6. Fundamental concepts of S_N1 and S_N2				
7. Fundamental concepts of "make-bond" and "break-bond" processes				

Fig. 13. Sample questions for the measure of explanation-based learning in skills reinforcement

Fig. 14 indicates the overall results for each rating score presented in Fig. 13. Particularly, majority of the respondents felt that their knowledge on the two aspects as described in Q3 and Q4 has been improved to a great extent. 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. They have never thought of using a causal graph or even the reaction route to express the overall behavioural change of substrates.

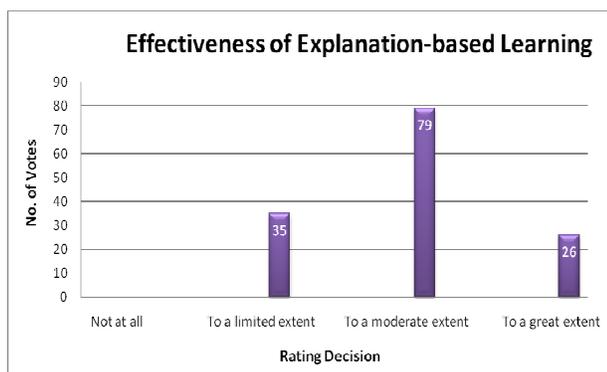


Fig. 14. Students' feedbacks on the extent to which the tool improves one's knowledge in terms of skill reinforcement through explanation-based learning.

After answering the questionnaire for measuring "effectiveness of explanation facility", they were told to continue with the questions that aimed at assessing the usefulness and helpfulness of the tool. The main objective of the survey is to determine if the tool is useful (e.g., students are more confident in answering new questions) and helpful (e.g., the materials presented motivate the student to learn). In Fig. 15 majority of the students agreed that the tool is useful (in terms of the confidence gained) in their learning process. On the other hand, helpfulness covers the value of the materials presented as well as the ease with which a user can operate the application. Students gave very high score to the tool on this aspect. They found the tool helpful because it motivates the student to learn, especially in several areas such as:

- They are allowed to choose different combinations of <substrate, reagent> pair.
- The tool offers certain degree of interactivity.
- The tool provides adequate coaching.

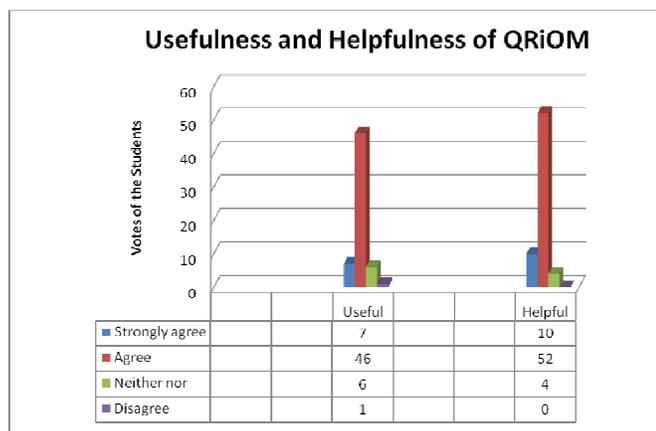


Fig. 15 Students' feedbacks on helpfulness (motivated) and usefulness (gain more confidence) of QRiOM.

In an interview, slightly less than half of the students representing 40% felt that they underwent a change of reasoning (thinking), as the explanation provided by the software does reveal the chemical intuition needed to solve the organic reaction problems.

VII. CONCLUSION AND FUTURE WORK

A simulator named QRiOM based on qualitative reasoning approach has been developed. QRiOM is able to construct qualitative models (using QPT ontology) and to simulate organic processes (using a set of QR algorithms) such as adding and deleting bonds in order to reproduce the chemical behaviours of organic reactions "intuitively". The tool has been evaluated in terms of its usefulness, helpfulness and effectiveness in explaining chemical phenomena related to the fundamentals of organic reactions. Overall, the results are promising as students commented that the tool generally enhanced their knowledge. QRiOM is also viewed as useful and helpful where most of the student underwent mental change when exposed to the software. In specific, use of the tool can help oneself to discover his mental change, such as realizing or knowing own reasoning ability. The achievement of these learning objectives is due to the "explanation" pedagogy that is embedded in QRiOM that assists chemistry students to learn organic reactions through the study of parameters' functional dependencies and the causality chain. The authors believe that this research provides a good foundation for future works in the application of QR technology in other subfields of the organic chemistry. So far the prototype does not support much student-initiated exploration. After developing and testing the prototype, we anticipate a full version learning software by embedding user modelling module and an assessment system. A problem ontology that handles user queries much like the work described in [30] is also the direction of our future work. The main purpose of having the problem ontology is to deal more accurately with questions that may be asked by the learners.

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Alicia Tang obtained her Master of Science from Manchester University, United Kingdom. She is a senior lecturer at the University of Tenaga Nasional. Her research fields include Qualitative Reasoning, Prediction Engine Design for Organic Chemistry Reactions, Computer Based Learning, and Data Mining. She is a member of APSCE, QRAM, IEEE, and IEEE Computer Society.

Sharifuddin Mohd. Zain received his Ph.D. in 1995 from Imperial College, London, United Kingdom. He is a Professor in the Department of Chemistry at University of Malaya. His research interests include Computational Chemistry, Application of Computers in Chemical Research and Education, Artificial Intelligence in Chemistry, Chemometrics, and Environmental and water quality data analysis and modelling. Prof. Sharifuddin is also a Regional Editor for the Journal of Global Environmental Engineering.

Rukaini Abdullah obtained her Ph.D. from University of Leeds, United Kingdom. She is attached to the Faculty of Computer Science and IT, University of Malaya. Her research interests are Natural Language Processing, AI in Education, Information Retrieval, and Computer Based Learning.