Embedding explanation facility in chemistry educational software: Towards the qualitative reasoning approach

Alicia Tang Y.C.[a], Sharifuddin Mohd. Zain[b], Noorsaadah Abd. Rahman[b], Rukaini Abdullah[c]

[a]*College of Information Technology, University of Tenaga Nasional, Malaysia*
[b]*Chemistry Department, University of Malaya, Malaysia*
[c]*Artificial Intelligence Department, University of Malaya, Malaysia*
aliciat@uniten.edu.my

Abstract: This work discusses the explanation facility of a tool called QRIOM for providing support to teaching and learning in the area of organic reactions. The approach is to use Qualitative Reasoning (QR), in particular, Qualitative Process Theory (QPT). This paper will focus on the reasoning engine and the explanation modules that served as embedded intelligence in the software tool. Explanation generated by the software can help learners to pick up the underlying concept better than merely memorizing the basic facts or the reaction steps. The main finding of this work is that when the domain knowledge is represented using QPT, the coupling between concepts and their embodiment in software are tightened. This type of conceptual embodiment may facilitate the acquisition of the fundamental principles of organic reactions in that a learner's cognitive capability is improved.

Keywords: Qualitative reasoning, qualitative process theory, organic reactions, explanation

1. Introduction

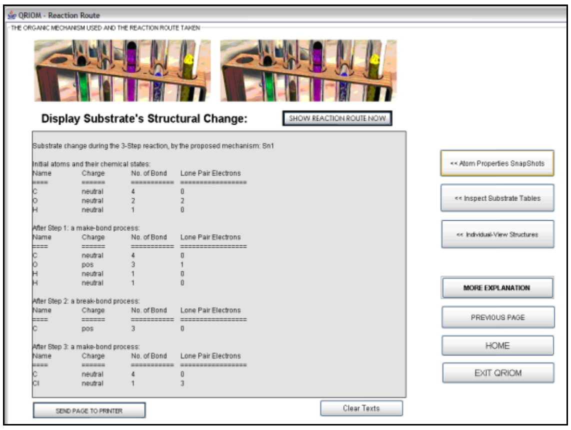
Systems based on Qualitative Reasoning (QR) have the ability to predict and explain the behavior of physical systems in qualitative terms; without involving any mathematical equations. Learning organic reaction requires the application of domain knowledge at intuitive level, which is difficult to be programmed using traditional approach. There have been many strives for innovation in teaching and learning chemistry using software. However, most of the chemistry educational software used traditional approach [1]. In the standard rule-based systems, explanations are generated by tracing all the rules that are fired during processing. As a result, these approaches are incapable of providing explanation such as explaining why things happen and how they happen. Many chemistry students learn organic reactions by memorizing the reaction steps and formulas of each reaction which are easily forgotten. This paper discusses a new technology for constructing a tool (QRIOM) that uses "knowledge articulation" as the learning pedagogy for learning organic reactions. The tool is able to construct qualitative models and to simulate processes such as creating and deleting bonds, and to explain the underlying principles of various chemical phenomena.

2. Domain Knowledge Modeling and Reasoning

Domain knowledge is modeled using Qualitative Process Theory (QPT) ontology [2]. The ontology provides good means for describing notions of causality which are important to explain behavior of chemical systems. In QRIOM, models construction stage is automated. A set of QR algorithms has been developed to keep track of the chemical state changes via the functional dependency constructs of the ontology that represent the cause-effect interaction of the chemical parameters. The top-level design of the simulation steps is given in Fig. 1 (a). In (b), a simulated result showing the different chemical states is presented.

```
QUALITATIVE SIMULATION ALGORITHM
Q_Simulation(substrate, reagent, OUTPUT)
1. Recognizing substrate
2. Suggesting a chemical process
3. Constructing QPT models
4. Processes reasoning
      Initialize multiple data structures
      Perform quantity space analysis
      Check qualitative proportionalities in Relation-slot
      Refer to quantity spaces for each view used in the process
      Store propagated effects in data structures
      Store new individuals (intermediates) that produced
      Update  all affected data structures
5. If view_structure <> EMPTY Then
              Go to step 2
    Else
              Suggest mechanism used in the simulation
              Show overall reaction route
              Display final products
    End If
6. Generating explanations based on users' queries
```

(a)



(b)

Fig. 1: (a) Main steps in QPT-based reasoning (b) Chemical parameter can be examined in greater detail. The values help explain why certain atom leaves (or approaches) a given compound.

3. Explanation Generation

In QRIOM, an explanation is supported by showing four scenarios, namely, (1) The whole set of the parametric values taken by each chemical parameter that involved in the reactions. (2) The updated list of reacting species (before and after each chemical process) within the entire reaction. (3) The entire reaction route taken during conversion of the substrate to the final products. (4) The constructed qualitative models. All of the above are generated based on the set of QR algorithms as outlined in Fig. 1 (b). Causal reasoning is one of the methods used for providing explanation. For example, when given '*P* causes *Q*', we believe that if we want to obtain *Q* we would bring about *P*. As such, when we observe *Q* we will think that *P* might be the reason for it. In QRIOM, this simple notion is represented as causal diagrams (pictorial representation of cause-effect chain of parameters in a reaction).

4. Conclusion

The combined use of QR and QPT gives a promising representational and computational technique to explain phenomena in science subjects such as chemistry. The approach encourages a learner to think deeply about the causal and behavioral aspects of a reaction, as the means to nurture the learner's reasoning ability.

References

[1] Cartwright, Hugh M. (1993). *Application of Artificial intelligence in Chemistry*. Oxford Science publications, Oxford University Press Inc., New York.

[2] Forbus, K. (1984). Qualitative Process Theory. *Artificial Intelligence*, 24, 85–125.