Chemistry Modelling and Simulation through Agent Oriented Modelling and Netlogo

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***Abstract*—Education technology is used to enhance students' understanding on science subject. Within the Faculty of Resource Science and Technology (FRST) at Universiti Malaysia Sarawak (UNIMAS) students face difficulty to visualize on the composition of atoms or molecule due to complexity of the topics. Although, students can attend Chemistry labs, the usage of labs are insufficient due to lack of instruments and lab materials. Hence, it is always a challenge to deliver some Chemistry topics and students always feel difficulty on understanding some Chemistry subjects. We believe that simulation can fill this gap. However, how to model the Chemistry theory and develop the Chemistry simulation model is challenging. This paper introduces an Agent Oriented Modelling(AOM) and Netlogo for chemistry modelling and simulation. The AOM is investigated in Chemistry domain and the potential usage is reported. From the finding, the AOM can help the modeller to understand the Chemistry theory and conceptualize the Chemistry theory into agent model and simulation. On the other hand, the agent model (e.g. domain model) has enabling the communication between researchers from two disciplines. Although we have successful model the Chemistry theory, how the simulation can support the Chemistry learning will be explored in the coming periods.**

***Index Terms*—Chemistry Modelling and Simulation; Agent Modelling and Simulation; Methodology**

I. Introduction

Chemistry learning involves understanding the molecules structure, its behaviour and evolution. In university, the concept of chemistry is delivered through theory based, tutorials and experiments. The students are presented with the theory behind certain chemistry concepts and participant in a hand on experiments to further understand the entire chemistry concept. The hands-on experiment is important to allow the students to explore various what if scenario. The students can comprehend the concepts through observation of experiments, discussion among peers and lecturers.

Ideally, the theoretical understanding of chemistry is consolidated with hands-on experiments. Due to limited resources (e.g. lack of instruments, chemical materials and etc), the students may not have the privilege to conduct experiments on every chemistry concept. Hence, the students often demonstrate inadequate understanding on the topics of chemistry subject. Based on the interview with the Chemistry lecturer, fundamental of instrumental techniques such as gas chromatography (GC), Infrared spectroscopy (IR), Ultra-violet visible spectroscopy (UV-Vis) are difficult to be presented in the class. Although computer animation has been used during lectures, students often fail to visualize and apply those concepts. To date, most of the computer animation has failed to deliver the Chemistry concepts. Meanwhile, it is not interactive. We believe that interactive application can fill this gap.

From the review, Chemistry Connect is able to attract the learning of Chemistry among students in US [1]. The Chemistry connect is developed using netlogo in which the entire Chemistry topic is simulated through netlogo. Although various netlogo chemistry model has been shared to public, the simulated chemistry model seems not adequate in addressing the chemistry theory. Hence, there is a need to build a new Chemistry model. We believe that simulation can fill this gap. However, how to model the Chemistry theory and develop the Chemistry simulation model is challenging. There is no clue on how to build the model by people who are coming from different background.

This paper introduces an Agent Oriented Modelling(AOM) as a methodology for chemistry modelling and netlogo simulation, also known as agent oriented chemistry model. The AOM is investigated in Chemistry domain and the potential usage is reported. From the finding, the AOM can help the modeller to understand the Chemistry theory and conceptualize the Chemistry theory into agent model and simulation. On the other hand, the agent model (e.g. domain model) has enabling the communication between researchers from two disciplines. Although we have successful model the Chemistry theory, the working on simulation model through netlogo is still a trivial task in which it is worth to explore in future.

Section II presents the proposed methodology for chemistry modelling and simulation through agent oriented modelling. It covers the steps in modelling a chemistry concept from requirement elicitation, to agent modelling and finally netlogo simulation. The details of a case study for this project is presented in Section III. Section IV presents the walkthrough example of AOM for GC study. A qualitative analysis of the AOM is presented in Section V. This paper is concluded in Section VI.

II. Agent Oriented Modelling for Chemistry Modelling and Simulation

We have adopted the AOM for chemistry modelling and simulation. Agent oriented modelling (AOM) is an agent methodology that is introduced for complex system modelling [2]. The AOM covers three modelling phases. They are conceptual domain modelling (CIM), platform independent design and modelling (PIM) and platform specific design and modelling(PSM).

The CIM layer constitutes a high-level motivation layer of the system. It provides a description at the level that allows a non-technical person to understand the requirements for the system. Furthermore, it is not dedicated to any specific platform or architecture. The PIM layer corresponds to the designer view of the system in which system design is decided and represented. However, the design descriptions presented at this layer are not related to any implementation platform or language. The design layer instead provides a description that can be turned into a implementation at the next layer. The PSM layer is the lowest level of the system design. The design description at this layer allows the system to be deployed and executed in a environment like specific platform, hardware, technology, and architecture.

In this project, we propose the chemistry modelling and simulation by extending the AOM based on the following steps.

Step 1: Sketching on the simulation of chemistry subject

The sketching is conducted through elicitation requirement. In this case, the modeller will ask the domain expert to sketch on the chemistry simulation model. As both stakeholders are difficult to communicate due to different domain, competency questions are introduced to guide the sketching process. The competency questions are adopted through HOMER. Within the Melbourne University AgentLab, HOMER is practiced modelling the goal model and role model from the discovered requirement. HOMER is used to elicit client requirements through elicitation questions [3]. From the elicited answer, the discovered requirement can be easily translating into the agent models. The HOMER is based on the organization metaphor-hire a staff in which to hire a staff, one might understand the role of the staff, the interaction with the others, the constraints, responsibilities of the staff; the resources to be used by the staff to fulfil their position.

1. If you were to simulate the subject domain, which concept do you need to understand?
2. For each subject topic, we need to collect a “concept description” of chemistry model:
   a. What is the purpose of the simulation model? What aspects of the concept will this simulate use for?
   b. Which entities are involving in the Chemistry model?
   c. For each entity that is required:
      i. What are the tasks required in the model?
      ii. What are the constraints for the entity?
      iii. How does this entity is interacting with the chemistry graph?
   d. What parameters (e.g. domain entities) do we need to provide to students?
   e. What knowledge of chemistry will student person require to correctly perform the simulation?
3. What parameters must be observed by the students in related to the model?
4. What other rules of chemistry must need to understand for this model?

Step 2: Goal modelling for chemistry study

Goal model describes the purpose of the system (e.g. system functionality) at a higher level of abstraction. The notion of goal provides an overview of the functionalities that should be achieved by an agent system. Goals can be divided into sub-goals. For example, in GC the main goal is to separate of component. Achieving a goal consumes resources and a goal is related to a role which indicates the actor or agent that is involved in achieving the goal.

Step 3: Role modelling for chemistry study

A role model describes the role played within an organization. In the chemistry context, the role model will model the structure of molecules and constraint that are required for the entire molecules. A role model is represented as a role schema which consists of the following elements: role name, role description, responsibilities, and constraints.

Step 4: Domain modelling for chemistry study

The domain model represents the information that is handled by the system as a set of domain entities and the relationships between them.

Step 5: Interaction modelling for chemistry study

An interaction model models the social influence between agents. In this model, interactions between agents are represented through message passing. The interaction model models the content and order of the messages to be exchanged.

Step 6: Behaviour modelling for chemistry study

A behaviour model indicates what individual agents of a type do [2]. It enables both proactive and reactive behaviour to be modelled. An agent achieves a goal through performing activities. The sequence of activities is modelled by means of control flows. A rule is the basic behaviour modelling construct. The triggering of a rule happens due to an activity start event, conditions that have been fulfilled, or an action event caused by external agents. The execution of a activity is modelled by triggering a rule to update the agent’s mental state and/or send the message or perform an action of another type by an individual agent. An agent is proactive if its mental state can trigger an activity. An agent reacts due to the perception received through a communication action or physical action by a human agent. A communication action involves exchanging messages between agents. A physical action involves a direct command by a human, which normally occurs through a graphical user interface.

Step 7: Transform into netlogo construct

A transformation guideline is introduced to transform the agent models into netlogo construct. NetLogo[2] is a multi-agent simulation platform for simulating complex phenomena. NetLogo is suitable for modeling evolution of complex systems over time. Modelers can program these “agents” to operate autonomously and interact with each other. The modeler can explore connections between micro-level behaviors of individuals and macro-level patterns that emerge from their interactions. NetLogo teaches model and simulation programming concept in the form of turtles, patches, links and the observer. Turtles are of which “agent” is referred to. Patches are the ground (the grid) which the turtles move on. The links are what connects two turtles. The observer “observes” and “oversee” the world by giving the command to the patches or turtles (i.e. sets the color of patches or specific turtle).

Table 1 shows an example of mapping the behaviour model into netlogo construct. Here, the agent activities type is mapped to netlogo procedures; the agent interaction is mapped to netlogo syntax “-here”; and the agent decision is mapped to netlogo syntax if-else.

Table 1
Mapping of behaviour model into netlogo construct

Behavior Model		
Model contexts	NetLogo construct	Examples of NetLogo syntax
Agent *activities type* (i.e. move, bite and feed, infect human)	Procedures	ask mosquito[move bite-and-feed] to bite-and-feed if is-infectious? [ask human-here with [is-susceptible?] get-bitten-acquire-disease] end
Agent *interaction* activity (*i.e. infect human)*	The syntax "-here" in procedure	ask human-here with [is-susceptible?] get-bitten-acquire-disease]
Rule and *condition* (i.e. *for allowing mosquito to infect human*)	The "if" or "ifelse" control flow and logic operator	if is-infectious? […..etc]

III. Case Study

A case study of Chemistry study is presented in this section. The case study is used as a walkthrough example to validate and evaluate the proposed agent oriented chemistry modelling and simulation. In this case study, the concept of gas chromatography (GC) is elaborated. GC is the fundamental knowledge that is delivered among the first year Chemistry students in Faculty of Resource Science and Technology (FRST), UNIMAS.

GC is used to separate components of a sample. The sample is injected into the system and is carried under the flow of a gas serving as mobile phase through a column containing stationary phase where separation takes place. Fundamentally, the separation occurs as a result of different affinities between components of samples and the stationary phase based on the rule of like-dissolves-like. A component that interacts stronger with the stationary phase will be retained longer in the column hence more time is taken to be eluted and detected. For example, a sample containing component A, B and C with increasing polarity is injected into the GC system equipped with a polar column. Essentially, component C will interact stronger with the stationary phase followed by B and A. The resultant chromatogram will illustrate 3 peaks with the first peak representing the component with the lowest polarity, A.

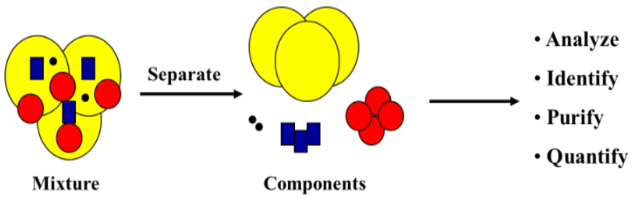

Figure 1: The concept of GC

IV. Walkthrough Example of GC through AOM

In the previous section, the GC concept is elaborated. A walkthrough example of GC through AOM is described in this section. As mentioned before, the AOM starts with requirement elicitation. From the elicitation, a paper based model is presented. This is followed by agent modelling and netlogo simulation.

Three interview sessions are conducted among the project team members which consists of Chemistry lecturer, FRST, and lecturer from Faculty of Computer Science & IT. The aim of the interview session is to understand the GC concept. Guided by HOMER extension, the elicitation questions are used to identify the concept of GC among the team member. Table 2 shows a partial elicitated answers based on the interview session with Chemistry lecturer, FRST. It presents the details of one entity, gas molecule, its tasks, constraints.

Table 2
Elicitated answer for GC study

Question	Answer
2c) For each entity that is required: *i. What are the tasks required in the model?*	For Gas Molecule, Tasks: Gas molecules move around the surrounding Subtasks: There is no subtask for this role
ii. What are the constraints for the entity?	• If the size of the gas molecule is bigger, it will take longer time to pass through the porous medium. • The higher the polarity of the gas molecule, the shorter the time taken to pass through the non-polar porous medium. • The bigger the amount of the gas molecule, it takes longer time for all gas molecule to pass through porous medium.
iii.How does this entity is interacting with the chemistry graph?	The entity will update to the chemistry graph.

A. *Goal model for GC*

Figure 2 presents the goal model for GC. Here, the purpose of GC is to separate components. The main goal for the GC is 'handle separation' in which it involves sub-goals of 'handle concentration' and 'handle stickiness'.

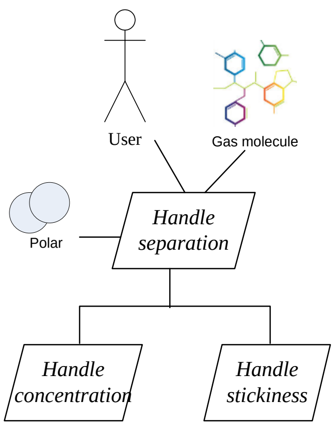

Figure 2: Goal model for GC study

B. Role model for GC

Table 3 shows the role model for GC. They are three role models in GC study. They are gasMolecule, user and polarColumn. The user is a person or student who is using or simulate the model. Here, it presents the tasks of the user and the constraint which is the pre-requirement knowledge prior using the model. The GasMolecule and PolarColumn are the entities for GC. In this case, the GasMolecule is designed to receive input from the user (e.g. stickiness and concetration); move towards polar column; coordinate movement. Meanwhile, the responsibility of the PolarColumn is to set the size of the column.

Table 3
The role model for GC

Role	Responsibilities	Constraints
Gas molecule	Move towards polar column Receive level of stickiness Receive level of concentration Coordinate and set the movement	The movement is controlled based on the level of stickiness.
Polar	Set the polar column	-
User	Setup Run the simulation Set the level of stickiness Set the level of concentration	Chemistry pre-knowledge

C. Domain model for GC

Figure 3 shows the domain model for GC. It can be interpreted that the GC consists of gas molecule which will move towards polar column. The gas molecule has concentration and move according to the level of stickiness.

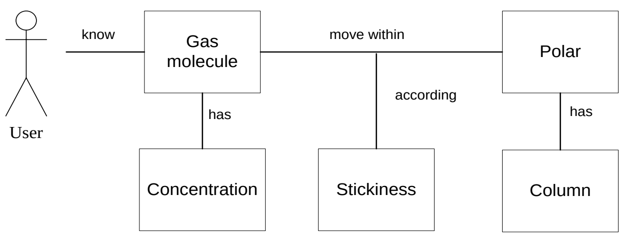

Figure 3: Domain model for GC study

D. Behaviour model for GC

Figure 4 shows the behaviour model for GC study. They are three agents involved in GC, user, gasMoleculeAgent and PolarAgent. The GC involves the knowledge items of 'Molecule' and 'Polar Column'. The knowledge item of molecule is owned by the gasMoleculeAgent while the 'Polar Column' is shared among the 'gasMoleculeAgent and PolarAgent.

In the behaviour model, first the user will assign the number of concentration and number of stickiness to the gasMoleculeAgent. Upon the setup, the PolarAgent will set the environment for the gas molecule to pass through. This happens through running the activity type of 'set polar column' by PolarAgent. Meanwhile, the 'gasMoleculeAgent' will perform the activity type of 'set concentration' by creating a new knowledge item, 'molecule'. The 'set concentration' involves the sub-activity to spawn individual agent. In other words, the activity involve cloning with a new gasMoleculeAgent. During the cloning, a new knowledge item of 'molecule' is created and be updated with molecule type. Then, the gasMoleculeAgent will heading towards the polar column. In GC, the separation of component is modelled as a movement pattern of gasMoleculeAgents. In this case, each type of gasMolecureAgent will move through the polar column based on the level of stickiness. The level of stickiness will determine the waiting time of the entire agent type. For example, if the level of stickiness is 1 for agent type 1 and the level of stickiness is 2, the agent type 1 will start to move instead of agent type2. This simulate the separation of component in GC. Finally, the movement of the agents will continue until the agent leave the polar column or exit from the polar. This showcase the ending of the separation in GC.

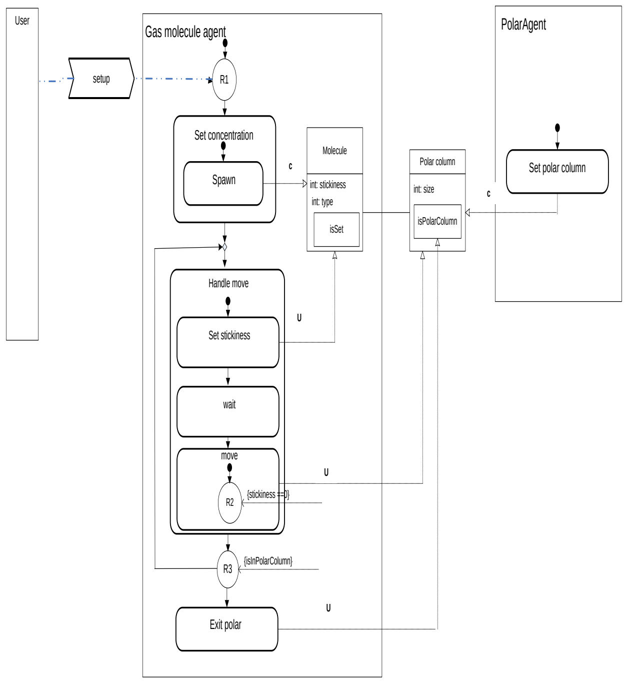

Figure 4: Behaviour model for GC study

We present the agent modelling for GC model in the previous description. The simulation model of GC is developed and presented in the following section.

E. Chemistry simulation in Netlogo

The GC simulation model is shown in Figure 5. It models the separation of the gas molecules after passing through the polar column. The left-hand side of the Figure, presents the setting corner. Here, the student can set various concentration of gas molecule as well as the polarity of the molecule. The separation of component/gas will simulate after the run button is activated. During the simulation, a chromatogram will plot. It presents the abundance value vs retention time of the entire gas molecule.

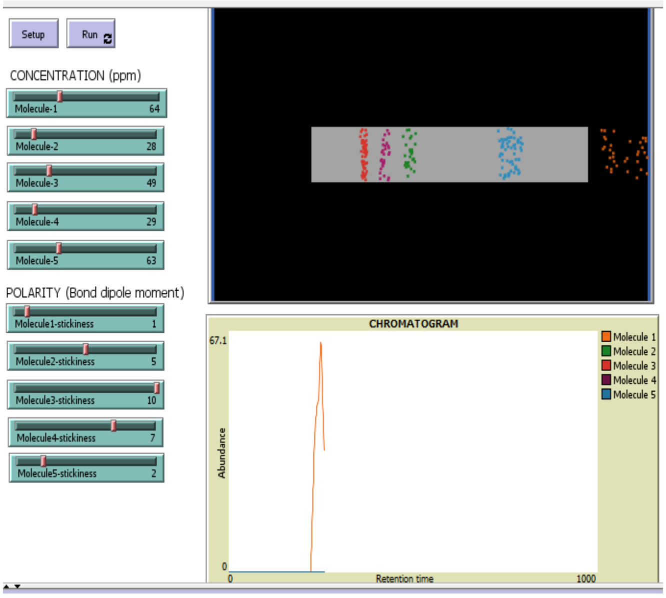

Figure 5: Simulation of GC model

V. Lesson Learnt

In general, the Chemistry model and simulation can produce an interesting learning platform to students. We further claim that this cannot achieve without a good methodology. The methodology should enable the communication between the team members that are coming from different discipline.

The AOM can bridge the communication gaps between the team members. It is enabling a person who has the computer science background to understand the chemistry concept and use the elicitation answers to model the agent oriented chemistry model. Meanwhile, a proper documentation is produced and the modeller can use the document to further expand the model in which more to explore in future. For example, the current GC model has not fully utilized the agent interaction; and the polar agent is not fully modelled and implemented. These can be further expanding for more advanced version of GC.

Although we have successful model the chemistry concept through agent models, working on a right simulation model is challenging. For example, how to model a vibration behaviour in FTIR, and continuous update the vibration in the plot? How to keep track of the students behaviour during the simulation? How to model a behaviour with a calculation of 185.5 as stated in UV?

VI. Related Works

Chemistry modelling and simulation is introduced to promote chemistry learning among students in US. From the review, most of the literature are concentrated on the experiment results of chemistry simulation. Although the Chemistry models are publicly accessible, some models are inadequate for our local context. Perhaps the models are developed by non-chemistry experts. As a result, there is a need of a mechanism to validate and verify the Chemistry model. Meanwhile, the current documentation for chemistry model is text based. This lead to disambiguous of some requirements and some requirements are implicit.

Agent oriented modelling has been investigated in the domain like collaborative learning [4], environmental modelling[7], rural ICT4D[6], sustainability engineering[9], 3D virtual characters[8], intelligent human detection in video surveillance[5]. The potential of AOM is promising. However, more to explore to validate the usage of AOM in various domain. The validation is important towards promoting the methodology to a wider audience.

VII. Conclusion

In sum, this paper presents an agent oriented modelling for chemistry modelling and simulation. From the case study, the proposed modelling can mediate the communication among team members who are coming from different disciplines. On the other hand, the model is successful developed through netlogo. In future, more works are needed to investigate the AOM in other chemistry topics. Also, empirical study will be conducted to measure the effectiveness of the AOM in chemistry modelling and simulation. The empirical study involves conducting a workshop to understand how chemistry experts and computer scientist can use AOM in chemistry modelling and simulation.

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