

Chemistry Modelling and Simulation through Agent Oriented Modelling and Netlogo

Cheah WaiShiang¹, Shane Nissom¹, Sim Siong Fong² and Muhammad Asyraf b Khairuddin¹

¹Faculty of Computer Science & Information Technology.

²Faculty of Science and Resource Technology.

wscheah@unimas.my

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