Project Deliverable D-Conceptual Design

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Group 4

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Abstract

Students in organic chemistry have trouble visualizing the dynamic nature of molecules. A VR environment will help demonstrate the connection between molecular and macroscopic views of molecular chemistry. In this deliverable our design team compiled a list of possible solutions for the design concept of our VR environment. Our goal is to provide the users with a better understanding of the connection between macroscopic and microscopic levels of chemical reactions. Ideas for the design of the surrounding environment of the VR and storylines were discussed, as well as ideas of different reactions that could be fun and helpful for first year organic chemistry students. We compared the different design concepts through multiple stages of benchmarking and group discussions to choose the final solution for the design of our final project.

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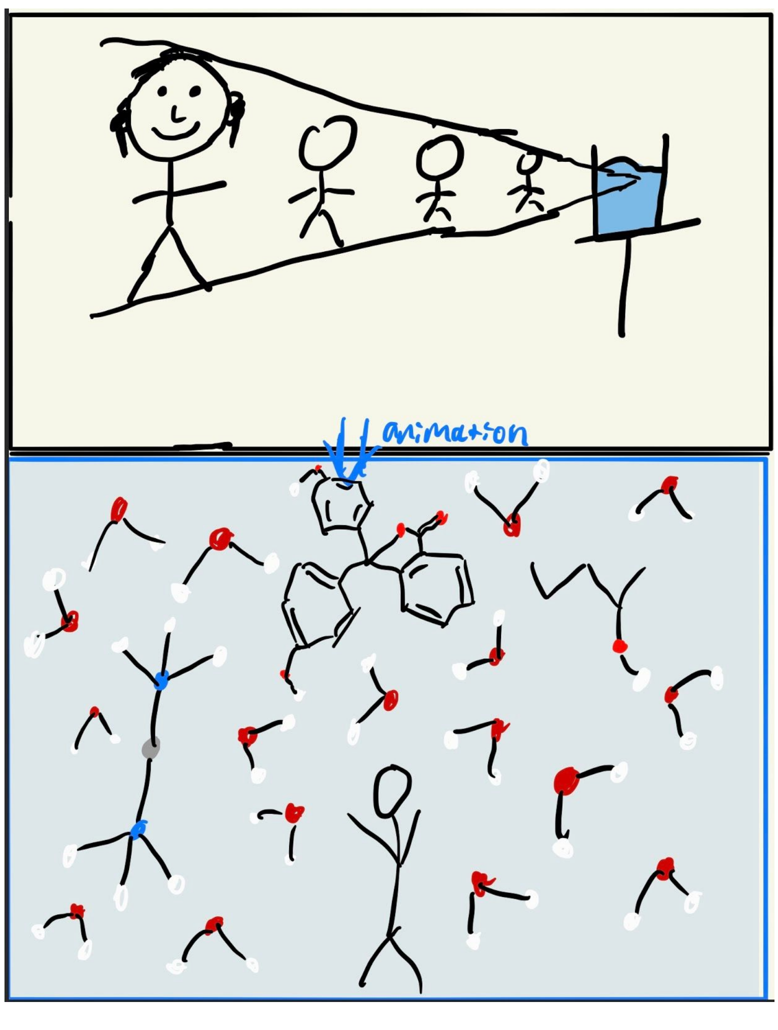
1. Environment setup options

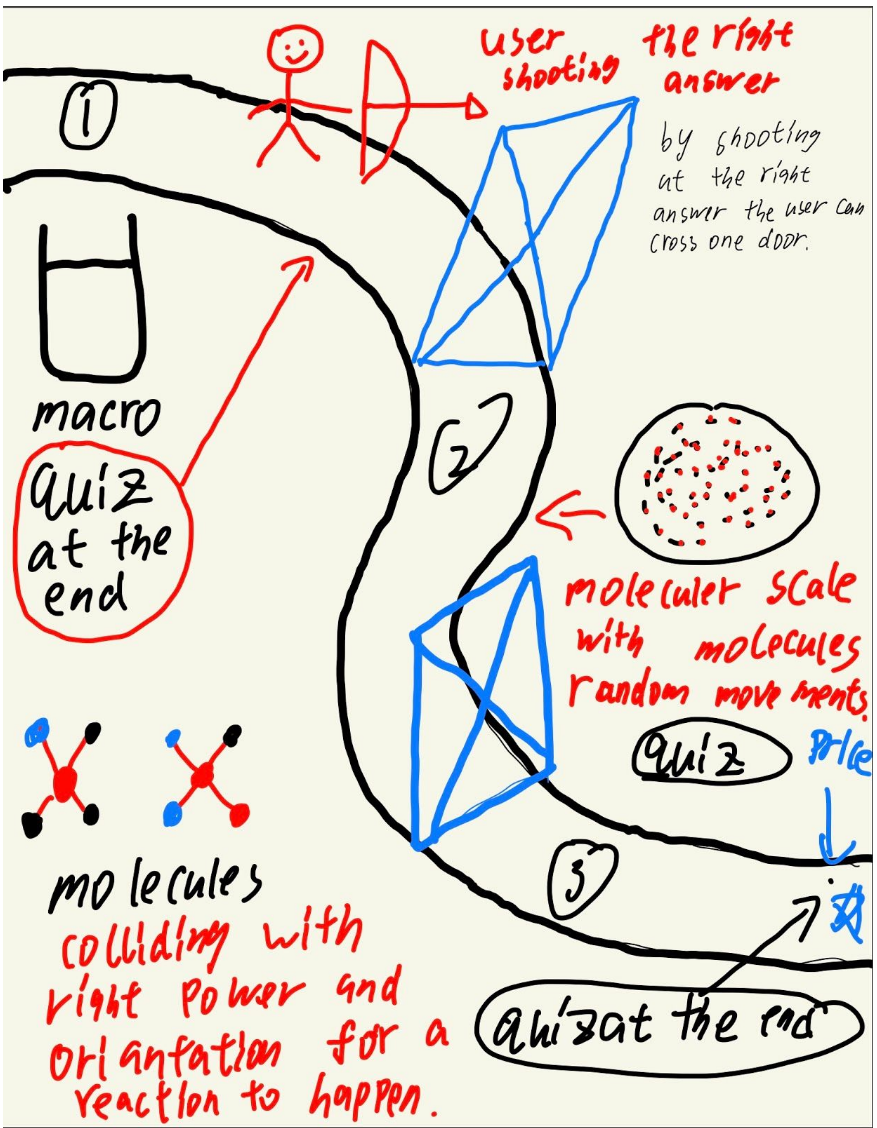
1.1 Jumping in

In this scenario, the environment starts with the user present in an environment that is scaled in real life. There is only a table present with beakers on top of it, each containing a different reactant in their aqueous states. The user is able to "jump into" each beaker and observe the microscopic level, being surrounded by the molecules. The user is also capable of going back and forth between both levels. While on the macroscopic level, the user can grab a beaker and pour its contents into another one to make them react. Visible changes from the reaction can be observed on this level. If the user teletransports into the microscopic level, it is possible to see how the molecules react with each other. There is an information box that states the temperature of the reaction, actual velocity of molecules and velocity scale. Unless the molecules have the right orientation and they collide with the proper amount of energy, the reaction would be unsuccessful. Some characteristics that the user can adjust in the reaction are temperature, which would consequently affect the velocity of the molecules since they the kinetic energy they posses would change and therefore, the rate of reaction would vary. A quiz at the end will test whether the user understood the learning outcome or not.



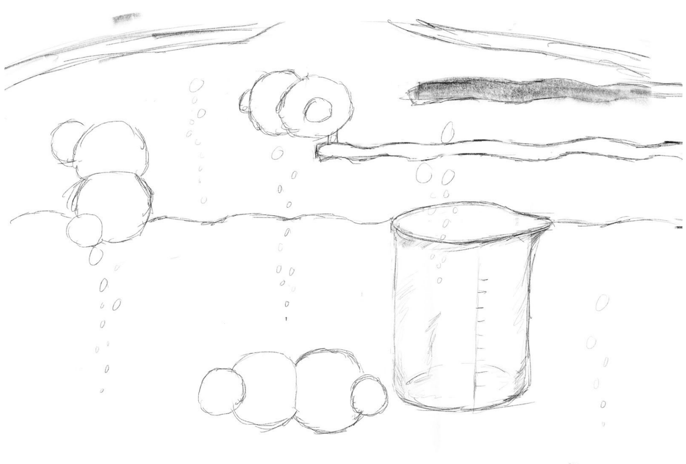
1.2 Scale map

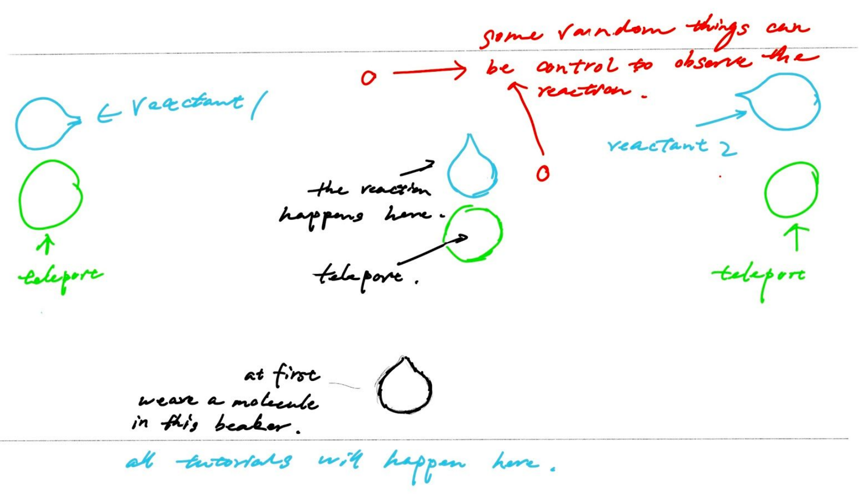
In this scenario, the VR home page starts with a map that contains different levels of a reaction which must be explored in order. The first place on the map will be an instructions page. The user will be using the map (guides and voice suggestions) and start exploring the reaction from macro level to micro level. The mission will be separated into three main parts, each section will have a quiz at the end, if the user correctly answers the quiz (by using the bow and arrow to shoot at the right answer), the user will be able to move up to the next level. In the micro level the user will be able to move the molecule in different positions and collide it with another molecule (with the right position and right power, the reaction will occur). After the user correctly finishes all the challenges, the user will be rewarded. Levels are unblocked once the user finishes the mission on the map, which allows the user to go back to any of them and review the reaction.



1.3 Swimming and leaping

In the third possibility, the user will be exploring the connection between molecular and macroscopic levels by leaping between equipment and molecules to get different visuals of the reaction. In this scenario, the user will see each level of the reaction and will be in the environment as the reactants particles. This version of the virtual reality is entailed to be very animated for the user to physically cause change to the reaction. and At the start of the game, the reaction is happening inside a beaker, the user will find themselves inside of this reaction as the solution at the macroscopic level. At this point the user will be at the first level and will be “swimming” inside of the beaker with the solution or will be added as a solution into another beaker to start the reaction. At the next point of the reaction, the user will be surrounded by the molecules of the reaction at the microscopic level. At this point the user will be able to interact with the molecules around them. The focus of this level is to allow the user to grab the molecules around them and make them interact, as well as observing their nature movement in the reaction. We want the users interactions with the molecules in the microscopic level to be very dramatic. The user will have to take a quiz at the end to see if they reached the learning outcome.





1.4 Advantages and disadvantages of the environment setup options

The following table has the ranking scale 1(worst)-5(best):

	#1 (jumping in)	#2 (scale map)	#3 (swimming)
# of levels of scale	2	3	2
Interactivity	3	5	4
uniqueness	5	5	5
Engagement with user	4	4	5
Best Learning environment	4	5	4
Method of testing user's acquired knowledge	3	5	3
Ease of use	3	5	3
TOTAL	24	32	26

2. Reaction Options

2.1 The traffic light reaction
Summary:
Involves indigo carmine being converted to different forms based on the pH, and also getting oxidized and reduced.
Possible user interaction: The user could shake it on the macro level, or change pH on the micro level.
Pros: common reaction used by science demonstrators (the user may already be familiar with it)
Cons: Very complicated: a lot of research is needed, and the reactants have complicated structure (on top of indigo carmine (http://molview.org/?cid=2723854), it also involves starch (http://molview.org/?cid=439341)). Also, it seems like it isn’t fully known how this reaction works.
More info: https://youtu.be/1ueSa6-UqYo

2.2 Silver mirror
Summary:
Tollen's reagent is added to a solution that includes aldehydes (or a couple other things). The diamminesilver (H3N-Ag-NH3) is reduced by the aldehyde to form ammonia and elemental silver, then some of the silver sticks to the sides of the glass vessel forming a mirror.
Possible user interaction: The user could change the concentration of aldehydes (or switch between aldehydes and ketones), temperature, pH, etc.
Pros: Tollen's reagent is often used in a teaching lab to distinguish between glucose and fructose, and the reaction is done industrially using glucose to make high quality mirrors.
Cons: Fairly complicated reaction, so it's probably harder than we want
More info: https://en.wikipedia.org/wiki/Tollens%27_reagent#Qualitative_organic_analysis

2.3 Acid-base reaction
Summary:
An indicator (probably phenolphthalein) is in solution, and an acid is reacting with a base (one of them could be organic - vinegar or ammonia). The user observes the indicator changing colour on the macro level and sees it change shape on the micro level.
Possible user interaction: Could change type of acid --> Ka, concentration of acid --> pH, temperature --> rate
Pros: Fairly simple (in comparison to the others), the user would have seen this in titrations in labs already
Cons: Modelling of phenolphthalein is complicated.
More info: https://en.wikipedia.org/wiki/Phenolphthalein#pH_indicator

2.4 Advantages and disadvantages of the reaction options

The reactions are ranked on each criterion, then coloured to reflect how good they are compared to each other. Red will be given a value of 1, yellow 2, and green 3. The value for each option will then be multiplied by their weights and summed to get an idea of how they compare. This will not make our final decision, but it may help us decide.

	wt.	#1 (stop light)	#2 (silver mirror)	#3 (acid-base)
Complexity/confusingness	4	3	2	1
# of controllable variables	3	2	3	3
Interestingness	4	3	3	2
Future usefulness	4	1	2	3
Most familiar to students	5	1	2	3
Client Preference	5	1	1	3
Weighted sum		36	52	71

3. Discussion

For our final design, we have decided to show the acid-base reaction using the scale map format. On top of the fact that the client stated that she preferred it, we chose the acid base reaction for our VR environment because we decided that the users familiarity with the reaction would enhance the overall learning experience of the VR. Ultimately the purpose of this environment is to effectively display to the user the connection between molecular and macroscopic views of molecular chemistry. Although the other reactions were very fun and engaging, we want the user to be most focused on the dynamics properties of molecules during a reaction. Using a reaction that the user has already seen in the past will put less attention on learning new organic chemistry reaction, but will enhance the users understanding of the microscopic properties of molecules, structures, dynamics. Furthermore, understanding the underlying chemistry behind the way that indicators work will help students' conceptual understanding whenever they do an acid-base titration or something similar in a future lab. We chose the scale map format because we found that it scored the highest in benchmarking. This environment excelled in all categories, and our team preferred it over our other two options. We found that the scale map is also easier to manipulate between the macroscopic and microscopic levels of chemistry.

4. Conclusion

In conclusion, after careful consideration to each of the possible solutions our team chose a final solution for the project. Since students in organic chemistry have trouble visualizing the dynamic nature of molecules, our VR environment will help demonstrate the connection between molecular and macroscopic views of molecular chemistry. For our final design, we have decided to show the acid-base reaction in the scale map VR environment designed throughout this deliverable.