PD-C Design Criteria

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 team developed the design criteria for the project.The team outlined the functional and non-functional requirements as well as any constraints that could affect the design on the VR system. In this deliverable we also completed product benchmarking. From looking at other VR projects we compared them to our own design criteria to further outline our software.

- Functional requirements
    - Show macroscopic/microscopic levels
    - Show dynamic and random nature of molecules
    - Test user on the comprehension of the learning outcome
    - Show changes in the reaction and the impact
    - Facilitate students understanding of molecules' behaviour
    - Simple to use
- Non-functional requirements
    - Aesthetics
    - Specific molecules/reaction shown - organic molecules
    - Additional features (audio, pedagogical agent)
    - Molecule colour scheme
- Constraints
    - Using a specific version of Unity
    - Time to make the code
    - Knowledge of using software
    - Follow the laws of physics (ex. gravity)
    - Creative Commons designation

The following table organizes the needs of the client and our elementary design solution to implement each need into the project.

Needs	Design Criteria
Immersive Environment	-change between macroscopic and microscopic levels -reflecting changes in both levels -random movements -constantly moving -user perspective (feedback) -accurate scale for molecules -different modes in code -users' feeling of Immersion (subj) -sufficient animation -magnitude of molecules -differentiate atoms and molecules (colour/size) -show successful/unsuccessful collisions -visualize full reaction (include solvent) -include different states and effect of changing temperatures

The environment has audio	-introduction -sound effects when things collide -optional audio
State the learning outcome	-minimize text -agenda
Test the user whether they achieved the learning outcome or not	-test scores can indicate usefulness of app -agreement of our testing method and traditional tests
Help organic chemistry students	-visuals -follows their curriculum
Provide a tutorial on how to use the environment	-Users' comprehension (test scores) -interactive (game type)
Be simple enough for beginner VR users to comprehend	-Include a tutorial -Have a help button -Users' ratings -also have a seperate advanced mode
Have a Pedagogical agent	-teaching assistants -Users' comprehension (test scores)
Show the relationship between 2D and 3D diagrams	-specified graphics curated on solidworks
Use organic molecules in demonstrations	-Complexity of molecules (length of chain or ring)
Content is scientifically accurate	-Expert's opinion
Molecules follow the colour scheme conventions	-Boolean
Molecules are shown using one of the typical representations	-Similarity between representations used and traditional ones

*User ratings will be determined throughout the prototyping stages. We will have random users come and test the VR.

To ensure that the project is completed to its fullest potential, our team will take the required steps to acquire a skill set that will allow our project to succeed. Skills that our team identifies important for each team member to have for the functionality of the project are:

- Know how to use Unity.
- Programming in C#.
- Know how to use Solidworks.

- Know the first year organic chemistry reactions and having passed the principles of chemistry course.

Design Benchmarking

		ODYSSEY (WAVEFUN)	Molview	**Our Project**
Description		A VR app produced by an education company which shows molecules and reactions	A website where the user can draw a molecule and see it displayed in 3d	An app for at least one VR system which shows a specific reaction on micro and macro scales and has options for the user to change certain parameters (possibilities: pH, temperature, etc.)

Features		- VR
		- Shows reactions and motion
		- Lots of options
		  - Gas sim
		  - Reactions
			- Open source
			- User draws molecules
			- Respects colour standards
			- Can go from name to drawing or vice versa
				- Open source
				- Respects colour
				- Shows reactions and motion
				- shows both successful and unsuccessful collision
				-

Drawbacks		- Really expensive	- No VR - Few representations	- user has little control over reaction (other than specific parameters) - only one reaction
Price	5	$750 (instructor) $7500 (20 students) (university edition)	Free (GNU GPL)	Free (CC)
Representations	3	4?	2	1-2
Shows collisions	5	Y	N	Y
Shows dynamic molecules	5	Y	N	Y

Connection between micro and macro	5	N	N	Y
Easy to use	4	?	Y	Y
Audio	2	N	N	Ideally Y, marginally N
Relationship between 2d & 3d	2	?	Y	Ideally Y, marginally N
Organic molecules	4	Y	Y	Y

Target range of design specifications:

- Number of representations: 1
- Price (to use): free ($0)
- Reaction shown: 1
- Number of levels shown: 2+
- Successful collisions: 10+
- Unsuccessful collisions: 10+
- Speed of collisions: x1 (normal), x2 (double), x0.5 (half), x0.25 (quarter)
- Temperature: -100ºC to 100ºC (variable depending on reaction)