Composite Presentation/Project Profile

Project Scope:

My goal is to program a one-pager website on which chemical students can calculate required amounts of different solutions for them to mix their target solution together. This can serve as a calculator for anything from diluting a single solution to creating a complex mixture of several basic solutions (e.g., a DNA buffer). All a user needs to do is to enter the molarity of each solution they are using and the desired molarity of those solutions within the target mixture. The website will then calculate concentration and return a specific volume for each individual solution and the volume of the filler (e.g., distilled water). An example would be the creation of 1ml of G-quadruplexes with the components (and their molarity) potassium chloride (100mM), lithium cacodylate buffer (10mM), copper sulfate (4µM) and DNA (4µM). Available for use (with their respective molarities) are potassium chloride (1M), lithium cacodylate buffer (100mM), copper sulfate (1mM) and DNA (1mM). In this case the user would enter the values from above and click the "Calculate" button. For output they'd receive that they need 100µl of potassium chloride and lithium cacodylate buffer as well as 4µl of copper sulfate and DNA; the combination of those should be filled up with 792µl of distilled water.

Target Group:

As my brother is currently studying chemical biology and mentioned how that would be something nice to have, I thought this is a great project for my first web application. The target group of my project is of course not only my brother but everyone that needs to calculate solutions and concentrations frequently. This calculator should help speed up the process, especially when planning these things out in advance. While this is of course possible to calculate by hand, it takes time and a single human error in calculation can lead to hours of chemical processes and precious solutions being wasted. In my research online I've found several websites that offer similar calculators, but so far, I've not found one that would provide precisely this functionality. On the one hand I've found websites that are more specialized and come with preselected recipes, which makes them superior at calculating the creation of those specific recipes but unfortunately unable to provide functionality beyond their database of recipes. On the other hand, I've found simple concentration/molarity calculators that work the same way as my project, but only ever include a single solution; meaning calculating a solution of my test case would require 4 individual requests to the website and some additional manual calculation for the final solution. My goal with my project is to provide a simple to use, all in one solution to anyone in the filed of calculating molarity and mixing solutions.

Software development methodology:

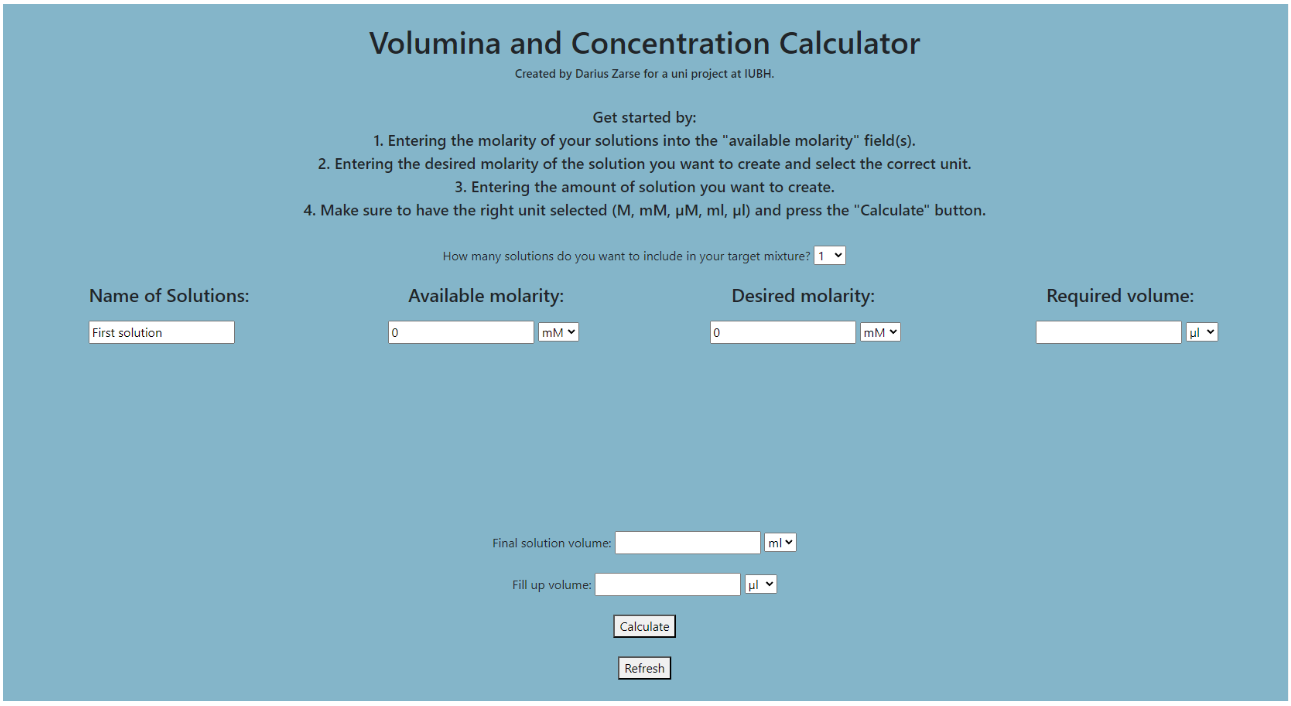
I plan on employing the big bang model I learned in my computer science class, as it is a simple and fast model and requires little planning or resources. The big bang model does not have a defined structure and order of processes. Following the big bang model means to focus all possible resources on coding and software development to get results as fast as possible. Requirements are implemented along the way whenever they arise. Its advantages include the extreme simplicity, the ease of management (as there are no hard structures to follow), the low amount of planning required, and the flexibility developers get. Additionally, it is considered a great tool for students or “newbies” to learn and practice their skills. The easy (almost nonexistent structure) also creates many disadvantages. For one, as there is no structure, there are no processes or milestones to discuss. This also means literature regarding this model is virtually nonexistent and it is only ever mentioned alongside other software development lifecycle models, but never discussed in detail as it lacks details to discuss. It carries very high risks and gets more and more unreliable the more complex the project gets. Especially for long projects that include many developers it is a bad fit as it can increase time and costs by a lot or even lead to a total abandonment of the project. But for small cases, such as this one-man project of an almost complete beginner, it seems like the perfect tool. As this is a one-person project with limited time and scope the risks regarding complexity and expensive failure cost are outweighed by the benefit of fast code delivery, learning along the way and massive flexibility. This means that I will write the code as fast as possible and solve issues I run into whenever I do. So, while I will lay out a clear idea in my composite presentation, this project has the potential to change along the way.

Tools:

I’m using visual studio code as my code editor. That’s the IDE/code editor I am most familiar and comfortable with, and I already used it for other university projects. As this is a web application and I will code the structure, style and functionality, I am using HTML, CSS and JavaScript. For my CSS framework I am using bootstrap (https://getbootstrap.com/) for their grid system and containers/rows/columns. That is the only CSS framework I’ve ever used so the choice was easy. I am currently trying to make a REST-API possible with node.js (https://nodejs.org/en) and express (https://expressjs.com/de/) as well as Insomnia (https://insomnia.rest/). As I am completely new to the topic of APIs and have no idea how to develop one, I just went with the most intuitive looking and popular tools I could find, so I’d have more tutorial material available.

User Interface:

For visualization purposes, here is a capture of my current website design:



Volumina and Concentration Calculator

Created by Darius Zarse for a uni project at IUBH.

Get started by:
1. Entering the molarity of your solutions into the "available molarity" field(s).
2. Entering the desired molarity of the solution you want to create and select the correct unit.
3. Entering the amount of solution you want to create.
4. Make sure to have the right unit selected (M, mM, µM, ml, µl) and press the "Calculate" button.

How many solutions do you want to include in your target mixture? 1

Name of Solutions:	Available molarity:	Desired molarity:	Required volume:
First solution	0 mM	0 mM	µl

Final solution volume: ml

Fill up volume: µl

Under the header of the page, I implemented a small introduction/guide on how to use the website. The first thing a user needs to decide is how many solutions they'd like to add together. They can select a number between 1-10 from the dropdown menu and that many rows of input fields will appear. The rows are divided into 4 columns. The outer left one is used to name the solution (this isn't necessary, but a quality of life feature my brother requested). On the central left column users can enter the molarity of their current solution into the input field and select the unit of concentration from a dropdown menu. The central right columns functions identically but is used to enter the desired molarity within the target solution. Finally, the outer right column is used for the output and includes read only fields of text that will be filled once the calculation is done. I also needed to include an option for users to input the amount of their target solution they want to create as that is essential for calculating the concentration of the individual solutions. This can be found under the input rows in the center. Under the target volume of the mixture is another read only text field that will show the fill up volume after the calculation. Lastly, I need a way to initiate the calculation which I plan on doing via the calculate button. Below the calculate button is a refresh button that will reset all input fields to their default values.

Functional requirements:

- As a user I should have the flexibility input any available solution with its respective molarity, so I can work with the solutions available to me.
- As a user I should be able to input the desired molarities of my solutions, so I am flexible to mix whatever target solution I want.
- As a user I want the website to calculate the volume of the specified available solutions and the fill up volume to save time and avoid potential human calculation errors.
- As a user I want to see the results in an ordered form, so I can quickly use them.
- As a user I want to decide when to initiate the calculation so I can start it whenever I am ready with my input.
- As the website provider I want to allow only the appropriate input into the input fields so that no errors fall back to me, and users are satisfied.
- As a user I want to be able to reset all input fields, so that I can start calculating the next target solution quickly.
- As the website provider I want the website to have a step-by-step guide on how to use its functionality, so that more people can benefit from it.
- As the user I want to choose the number of solutions I combine so I only see input fields that I must fill out.
- As the website provider I want to use responsive design, so that the website can be used on many different devices.

Nonfunctional requirements:

- I want the website to be usable for any high-school graduate within 5 minutes without any additional research.
- I want the website to give the user the opportunity to chose how many solutions they’d like to mix.
- The calculations and the result generation should be performed efficiently, providing a response within 2 seconds.
- The website should support keyboard navigation.
- The design should adapt to different screen sizes and resolutions.

Technical Details (for submission):

- I need to implement version control.
- I need to write tests to ensure functionality.
- I need to write an installation guide on how to run the web application.
- The website needs to be hosted on a cloud service (like AWS, google cloud)
- The website needs to be provided as docker-compose configuration.

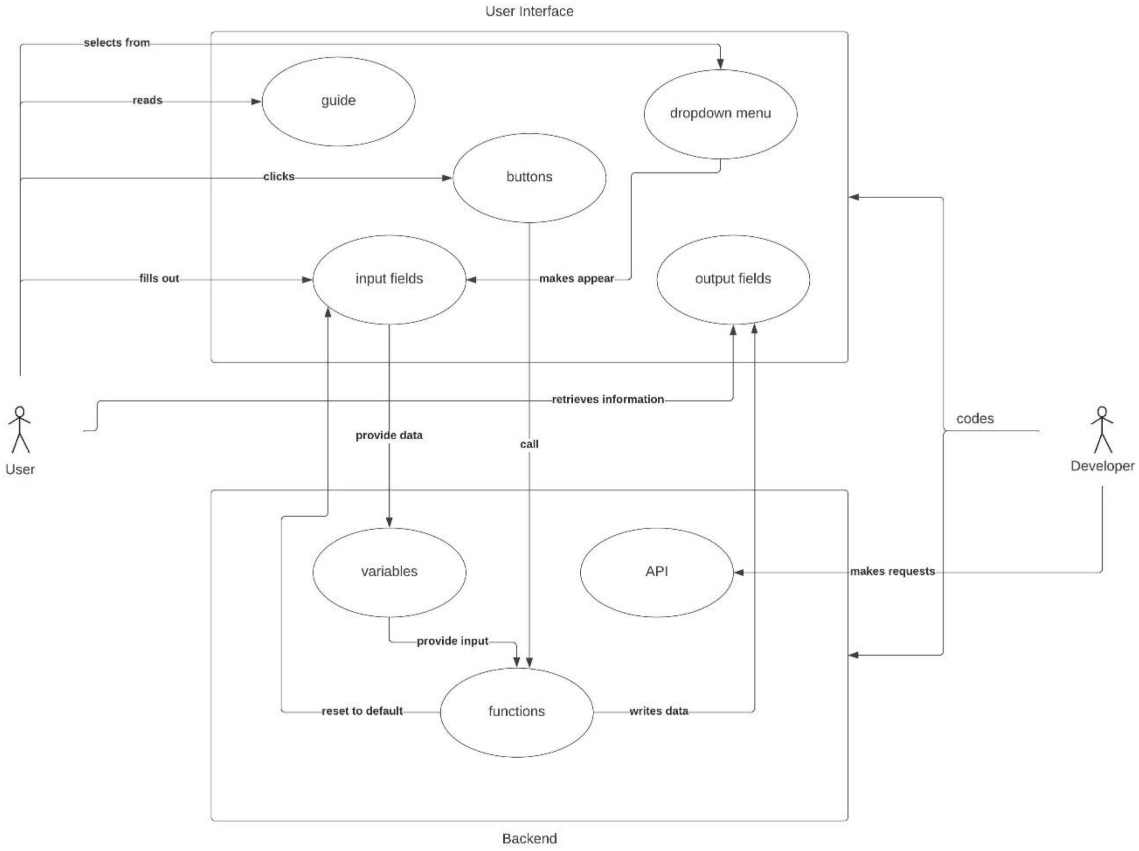
Glossary:

- Molarity (also molar concentration): a measure of concentration, in specific: the amount of substance per unit volume of a solution
- M, mM, µM: units for molarity. M (mole), mM (millimole), µM (micromole)
- Solution: a liquid mixture in which the solute (the minor component) is uniformly distributed within the solvent (the major component)
- potassium chloride, lithium cacodylate buffer, copper sulfate, DNA: chemical solutions that can be used together to produce G-quadruplexes.
- G-quadruplexes: secondary structures that can form in DNA/RNA by combination of four specific molecules combine and create a unique shape. They are the subject of much active research in the fields of molecular biology, biochemistry, and more.

System Design:

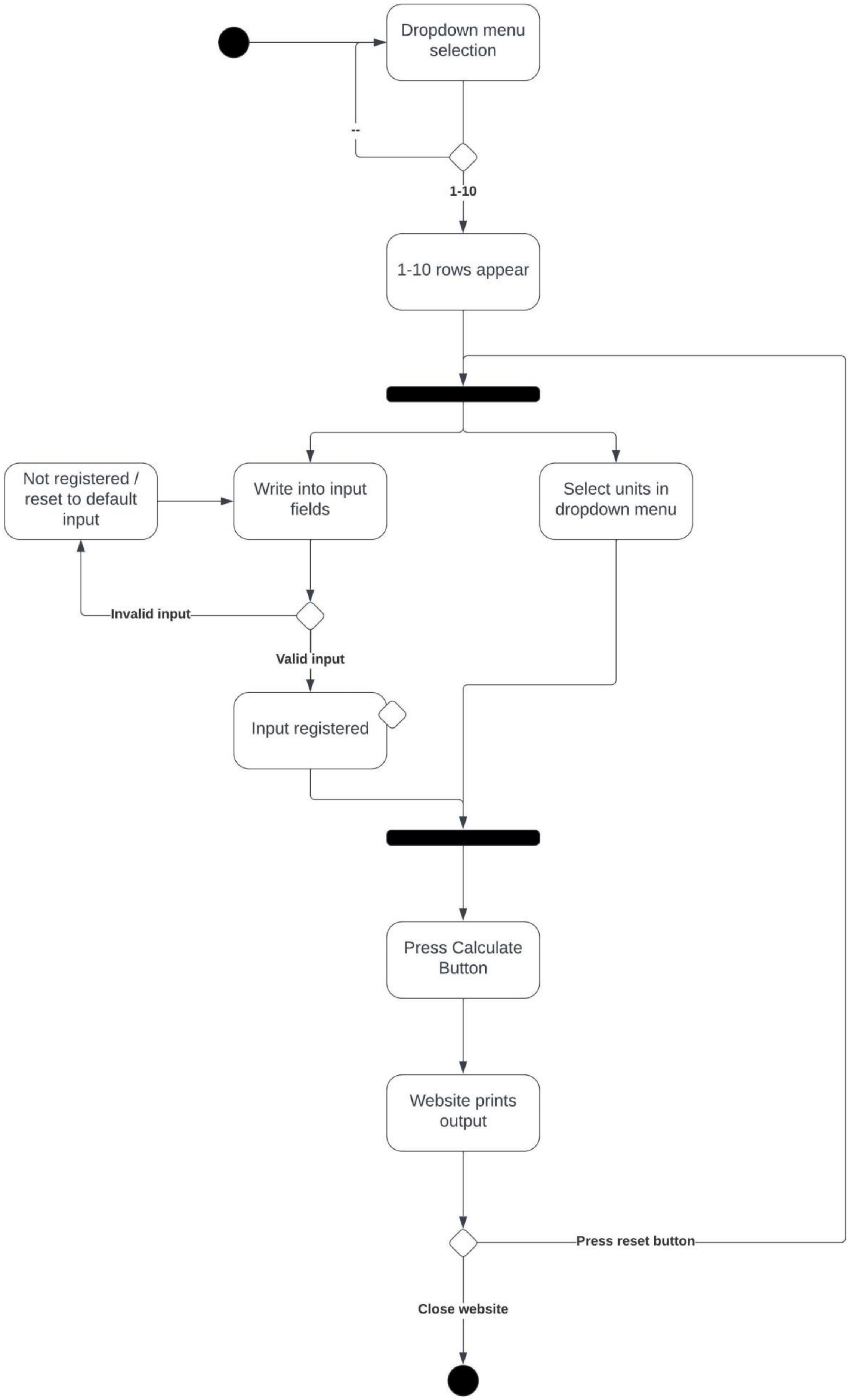
UML Use Case Diagram:

I've decided to go for a UML use case diagram in order to visualize the system. It looks like this:



UML Activity Diagram:

In order to portrait the processes on the website I've created an activity diagram as follows:


Dropdown menu selection
--
1-10
1-10 rows appear
Not registered / reset to default input
Write into input fields
Select units in dropdown menu
Invalid input
Valid input
Input registered
Press Calculate Button
Website prints output
Press reset button
Close website

Implementation:

Explanation of your design and implementation procedure in written form (approx. 1/2 page)
I have a html file that encompasses most of my website structure. Ever since I implemented bootstrap my CSS code shrunk a lot as I could save myself lots of work by using bootstraps row, column and container-fluid objects. I have a header area in which I wrote my short introduction and guide, below that my rows that can be toggled on or off, each with 4 columns. The 3 columns starting on the left all include input fields (1 text, 2 number) that all have their individual id (from 1 to 10). Each input field has a default value that allows me to calculate the volumes even if rows are left empty. The number fields are restricted to only enter numbers as I want to avoid undetected errors in calculation. The right most column is read only as it only will present the output calculated. Below the bootstrap grid I added 2 more centered input fields, one to take the target volume, the other (read only) to output the fill up volume. Lastly, I implemented a calculate and a refresh button below.

Regarding functionality, I have two functions that get called on load of the website via an event listener. One toggles the rows so that on website load the rows initially are not visible, the other stores the default values assigned to the individual input fields in an array so that they can be restored via the refresh button. The toggle rows function also allows for the user to select the number of rows made visible (the amount a user wants to use). To make the use of the input fields easier I implemented an event listener that clear the default values when an input field is focused. If the field already has some user input, it won’t get cleared though so users have the option to correct their input without having to type it again.

The base functionality of getting the input data, doing the volume calculation and providing output works as follows. When the calculate button get clicked the functions create an array, convert the value of the input fields to micromole (for calculations), and save the converted values in the array. The volume then gets calculated by dividing the total volume of the target solution by the quotient out of the available molarity and the desired molarity. The fill up volume simply is the difference between the previously calculated individual volumes and the total volume. Once calculated, these values then are output in the required volume column of the grid, and the fill up volume in its own text field.

Next steps:

I still need to work on the API. I’d like to make my calculator functionality available through a GET API request. In my research online and communication with my brother I’ve learned that there is thousand over thousands of different potential recipes, so a databank for that wouldn’t be very helpful, especially as different situations oftentimes require the same ingredients but with different molarities. Therefore, I thought making an API and using it to make the calculator available for other applications to use might be a better solution.