Concept Presentation

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. For creating the API I used node.js (<https://nodejs.org/en>) and express (<https://expressjs.com/de/>) as well as Insomnia (<https://insomnia.rest/>). For CSS styles I am using the bootstraps framework.

Composite Presentation/Project Profile

User Interface:

The webpage should have a small introduction and explanation on how to use it, then I will have several text fields structured like a table. The user should be able to select how many solutions they’d like to mix. Implementing several rows will allow users to calculate target solutions including several components. On the 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 second columns functions identically but is used to enter the desired molarity within the target solution. It also includes a dropdown menu. The 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 need 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. Lastly, I need a way to initiate the calculation which I plan on doing via a button.

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

Ein Bild, das Text, Screenshot, Schrift, Design enthält.

Automatisch generierte Beschreibung

Functional requirements:

* The website needs a way for user input regarding their available solutions and their molarity.
* The website needs a way for user input regarding the desired molarity of their target solution.
* The website needs to calculate the volume of the specified available solutions to mix the target solution, as well as the fill up volume.
* The website needs a way to display the calculated volumes.
* The website needs a way to initiate the calculation once user input is finished.
* The website needs to allow only the appropriate input into the input fields.
* The website should include the opportunity for users to input the name of the solutions they’d like to mix.
* The website should have a way to reset all input fields to their default value.

Nonfunctional requirements:

* The website needs to have a “guide” on how to use it.
* The web application needs to be provided as docker-compose configuration.
* The web application needs to be provided as cloud-hosted application (preferably with unrestricted access).
* I need to write an installation guide on how to run the web application.
* I need to write tests to ensure functionality.
* I need to implement version control.

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 (molar), mM (millimolar), µM (micromolar)
* 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: several solutions that can be used together to produce G-quadruplexes.
* G-quadruplexes: secondary structures that can form in DNA/RNA by four

System Design:

Ein Bild, das Text, Screenshot, Schrift, Diagramm enthält.

Automatisch generierte BeschreibungAs I’ve employed the big bang model, I’ve already started coding the website. So far, I’ve run with the design outlined in my project profile. I am working on this kind of functionality:

I will split my code into 3 files (1 HTML, 1 CSS, 1 JavaScript).

For now, I am still considering potential additions to user functionality. First, a way to alert users to potential “wrong” input, in case they are entering letters or invalid characters instead of valid molarity. And additionally, a way for the user to select the number of different solutions their target solution should include (in contrast to just a set number of 5, which according to my research is covering most of the field already). This would work in form of a dropdown menu that selects a number out of a list which in turn would make that number of rows appear. As I am completely new to HTML, CSS and JavaScript I will evaluate along the way for how much additional functionality I can include, and which steps should take priority.