ChemBox Project Documentation

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1 Analysis

1.1 Introduction

Technology gives us the benefits of saving time and doing work more efficiently. The use of software and technology in chemistry does not only help increase accuracy and decrease human error, but also reduces the time spent performing repetitive tasks by hand. ChemBox is a software project with the aim of creating an interactive, user-friendly and intuitive toolbox for automating and simplifying complex and repetitive tasks that come up on a daily basis for students, educators and professionals in the field of chemistry. The application features a range of different tools that should help chemists work more efficiently and also carry out their work more accurately. ChemBox is split into three distinct modules with different functionalities.

The first module is the "ChemCalculator". The aim of this part of the program is to help the user carry out calculations by filling in equations and formulae. Although substituting numbers into predefined equations is a rather trivial task, it leaves a lot of room for human error when it comes to things like converting between units or applying mathematical laws correctly. This module should help the user with the most important and at the same time most trivial tasks in chemistry.

The second module, "ChemBalancer", is for balancing chemical equations, as the name already suggests. Chemical equations come up in every lab experiment, calculation or research problem. While balancing short equations made up of very few different elements is arguably a rather easy task, it can get quite tricky when you have to work with a large number of different elements, complex ions or just very long equations. Making just a tiny mistake when balancing an important equation can cause a big set back as it can take long to find small errors like mixing up a 2 with a 3.

The third and last module is the "ChemEditor". Visualising molecular structures can play a vital role in understanding a substances chemical properties or understanding interactions with other substances. Drawing molecules out by hand is pretty straight forward. It is knowing when a bond is valid and which atoms bond together and which don't that is the tricky part. Having a tool that can help you make sure the chemical molecule you want to draw can even exist, can be a great help not only for beginner level chemists but also for more experienced chemists.

1.2 Prospective Users

Chembox will provide valuable tools to a diverse user base, spanning from students to professional chemists. The intuitive and straight forward design will allow users with varying backgrounds and degrees to use ChemBox for their own specific needs.
In the early stage, the main users of this system will be pupils and staff attending Ellesmere College, but it could be a goal to make the software available open source to anyone online.
Engaging with pupils at the college during the early stages allows for a valuable user feedback loop. This direct interaction with the user group will provide insights into the software's usability, identify potential improvements, and address any specific requirements that may arise within the college context.

1.3 Specific Objectives

Through being an A-Level Chemistry student myself, I have learned a lot about using chemical equations and performing calculations as well as balancing chemical equations and visualising chemical substances and molecules. I was able to identify a number calculations that processes that come up on a regular basis and divide them into non-negotiable and nice-to-have objectives.

1.3.1 Chemical Equations and Calculations - ChemCalculator

The first module of the program is for performing calculations which are based on chemical formulae. Where appropriate the program should allow the user to choose from a range of different units for each calculation, so the user doesn't have to calculate the conversions like the one from cm^3 to dm^3 for example.

Required functionalities:

1. Standard moles calculation:
$$moles = \frac{mass}{molar\ mass}$$
2. Calculation to find the concentration:
$$concentration = \frac{moles}{volume}$$

3. Avogadro's number calculations. The user should be able to give a number of different inputs, including mass, moles, molecular weight and the number of atoms. After giving two independent inputs, the program should be able to calculate the rest of the values using Avogadro's number.
   The equation the calculator will be based on is:

$$number\ of\ atoms = Avogadro's\ number \times moles$$

   This should be paired with a mole calculator for the possibility use the following formula:

$$number\ of\ atoms = Avogadro's\ number \times \frac{mass}{molar\ mass}$$

4. Atom Economy calculation:

$$Atom\ Economy = \frac{Mr\ of\ desired\ product}{Sum\ of\ Mr\ of\ all\ reactants} \times 100$$

5. Percentage Yield calculation:

$$\%Yield = \frac{Actual\ yield}{Theoretical\ yield} \times 100$$

6. Calculation for the Specific Heat Capacity and Enthalpy changes:

$$q = mc\Delta T$$

   (q = energy change) (m = mass) (c = specific heat capacity) (ΔT = temperature change)

7. Equilibrium Constant calculation for a reversible reaction:

$$a[A] + b[B] \rightleftharpoons c[C] + d[D]$$

$$K_C = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

   (K_C = Equilibrium Constant) (Upper case letter = Concentration) (Lower case letter = Moles in Equation)

8. Rate Equation and Rate constant calculation:

$$Rate = k[A]^m[B]^n$$

Non-essential objectives:

1. Gibbs Free Energy calculation:

$$\Delta G = \Delta H - T\Delta S$$

(ΔG = Gibbs Free Energy) (ΔH = enthalpy)
(T = temperature) (ΔS = entropy)

2. Acid calculations - pH and $[H^+]$

$$pH = -log[H^+]$$

$$[H^+] = 10^{-pH}$$

3. Acid dissociation constants K_a and pK_a

$$K_a = \frac{[H^+][A^-]}{[HA]}$$

$$pK_a = -logK_a$$

$$K_a = 10^{-pK_a}$$

1.3.2 Chemical Equation Balancer - ChemBalancer

A substantial part of the project will be the ChemBalancer which will be the module that balances chemical equations. This system must be able to take complex unbalanced equations and convert them into a balanced version. It must be able to handle subscript numbers, brackets and complex ions.

1.3.3 Visualisation of Chemical Molecules - ChemEditor

The third part of the program will be the ChemEditor module, which can be used for visualising the structures of chemical molecules. This module will require a user-friendly and easy to use interface, with the main focus on the canvas. The user should have the option to choose from a range of different elements what he wants to add to the canvas. In a tool bar, the user should also be able to choose the bond order (single, double, triple) and the charge on each atom. When clicking on an atom, there should be an option to add a bond to another atom or delete the atom.
When the user constructs their molecules, ChemEditor will have to conduct real-time checks to ensure that atoms do not exceed their valence electrons and that it is chemically possible to have a molecule with the given structure. The required objectives for this module are:

1. Tool bar:
   In the tool bar on the top end of the application, there has to be a list of buttons for choosing the element, which must include the most common elements (Carbon, Hydrogen, Sulphur, Chlorine, etc.). There also has to be the option to choose the bond order (single, double or triple bond) as well as choosing the option to form a dative bond. Another essential option in form of buttons should be removing atoms and bonds as well as being able to safe the drawn structures as a document. A possible non-essential enhancement would be getting extra information about atoms upon highlighting as well as getting information like the molar mass and the empirical formula of a molecule after highlighting.

2. Canvas:
   The canvas is the area in which the user can draw their molecules. There are a number of essential features that must be included here.

   (a) The user must be able to draw atoms by clicking on the canvas.

(b) Upon selecting an existing atom on the canvas, depending on the chosen action type, the user should have different options:

i. When the chosen action type is "Draw", a number of greyed out atoms and bonds to those atoms should be drawn, out of which the user can choose where he wants to place his next atom.

ii. When the chosen action type is "Bond", the program should draw a bond from the selected atom to every existing atom on the canvas, with which a bond would be possible. The colour of those bonds needs to be different to the colour of the actual existing bonds, to avoid confusion.

1.4 Current and Proposed Systems

The current standard is to work out chemical equations or draw molecules on paper. This might make sense for simple equations or small molecules, but it gets less efficient and more difficult as complexity increases. Although there are some software solutions for very specific tasks, there isn't one intuitive and easy to use application that combines the different tasks in one place.

Naturally, drawing molecules with pen and paper feels best and is the preferred choice by most people. This project is not here to replace that, it should merely pose as a help for chemists when working certain things out.

2 Documented Design

3 Testing

4 Evaluation