MEng Group Project Specification & Design

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Project Summary

- Objective: Develop software capable of calculating, storing and predicting chemical compound formulas based on user input, and displaying results in a meaningful way

- Primary deliverables:
  - Web server: For providing a front end interface for remote user interaction and formulae calculation
  - Database: For storing information related to user accounts, chemical information and commonly used formulae

- Additional programming: Stoichiometry and precursor calculators

Functionality

- Users with account can log in with username and password
- Presented with a periodic table from which they can select elements
- Selection presents a list of available precursors that may be selected. User may also choose maximum size of desired output compounds
- Data points representing possible precursor mixtures displayed and explorable using the WebGL interface

Web Server

- Provides remote access and web-based UI for users, as well as a base for calculations and processing

- Utilizes several packages, including:
  - Node.js for handling server-side scripts outside the context of the web browser
  - Express framework for handling server traffic
  - PUG for HTML templates and allowing for easier customization of data and presentation
  - ExpressSession for handling user sessions to keep track of user favourites and preferences
  - Python Script/C++ through Node.js for computation
  - bCrypt2 for password encryption

Database

- Utilizes MongoDB for independent scalability of both database and software

- Consists of three main relations:
  - UserInfo: Holds usernames and encrypted passwords for login purposes
  - ElementData: Holds information regarding available element configurations (name, charge, etc.)
  - CalcedPoints: Holds information on previously calculated results
    - Makes repeat calculation unnecessary and lightens computational load

Stoichiometry Calculator

- Takes a set of elements defined by the user and an atomic limit, outputs a selection of charge-balanced compounds that can be generated from these elements
- Computation handled by transforming elements into matrix form and utilizing LU decomposition to solve linear equations

If the user selected Al and O with a limit of 5 atoms in the result:

$$\mathbf{A} = \begin{matrix} \text{Al} & \text{O} \\ \end{matrix} \begin{bmatrix} 1 & 1 \\ 3 & -2 \end{bmatrix} \begin{matrix} \text{Initial Quantity} \\ \text{Charge Imbalance} \end{matrix}$$

$$\mathbf{B} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \begin{matrix} \text{Resulting Proportion} \\ \text{Desired Charge Imbalance} \end{matrix}$$

$$\begin{bmatrix} 1 & 1 \\ 3 & -2 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Via LU decomposition:

$$\begin{bmatrix} 1 & 1 \\ 3 & -2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 1 \\ 0 & -5 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} \times \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -3 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 \\ 0 & -5 \end{bmatrix} \times \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -3 \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0.4 \\ 0.6 \end{bmatrix}$$

Precursor Calculator

- Takes a target compound and a set of other compounds as input, outputs combinations of compounds that would produce the desired result

- Works with matrices as well, but takes more complicated approach to arrive at solution

Precursor Calculator

If the user selected Li_2S, Al_2S_3, Al_2O_3, $LiAlO_2$, Li_2O as precursors, and a desired end ratio of $Li_1 : Al_1 : S_1 : O_1$ we construct:

$$\mathbf{A} = \begin{array}{c} \begin{matrix} Li_2S & Al_2S_3 & Al_2O_3 & LiAlO_2 & Li_2O \end{matrix} \\ \begin{bmatrix} 2 & 0 & 0 & 1 & 2 \\ 0 & 2 & 2 & 1 & 0 \\ 1 & 3 & 0 & 0 & 0 \\ 0 & 0 & 3 & 2 & 1 \end{bmatrix} \end{array} \begin{matrix} Li \text{ in compound} \\ Al \text{ '} \\ S \text{ '} \\ O \text{ '} \end{matrix}$$

$$\mathbf{B} = \begin{array}{c} \text{Ratio in output} \\ \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \end{array} \begin{matrix} \text{Li} \\ \text{Al} \\ \text{S} \\ \text{O} \end{matrix}$$

Precursor Calculator

We then find the null space of $\mathbf{A}$, firstly we apply Gauss-Jordan elimination to put it into reduced row echelon form:

$$\text{rref}(\mathbf{A}) = \begin{bmatrix} 1 & 0 & 0 & \frac{1}{2} & 1 \\ 0 & 1 & 0 & -\frac{1}{6} & -\frac{1}{3} \\ 0 & 0 & 1 & \frac{2}{3} & \frac{1}{3} \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

Taking the 'free' section of the $\text{rref}(\mathbf{A})$ and multiplying by -1:

$$\begin{bmatrix} -\frac{1}{2} & -1 \\ \frac{1}{6} & \frac{1}{3} \\ -\frac{2}{3} & -\frac{1}{3} \end{bmatrix}$$

Then adding identity to these rows so the height of our new matrix is the same as the width of the initial matrix $\mathbf{A}$:

$$\begin{bmatrix} -\frac{1}{2} & -1 \\ \frac{1}{6} & \frac{1}{3} \\ -\frac{2}{3} & -\frac{1}{3} \\ 1 & 0 \\ 0 & 1 \end{bmatrix}$$

Precursor Calculator

The null space is then defined by scalar multiples of the columns of this matrix:

$$x \cdot \begin{bmatrix} -\frac{1}{2} \\ \frac{1}{6} \\ -\frac{2}{3} \\ 1 \\ 0 \end{bmatrix} + y \cdot \begin{bmatrix} -1 \\ \frac{1}{3} \\ -\frac{1}{3} \\ 0 \\ 1 \end{bmatrix}$$

Where x and y are any real numbers.

Finally, via the same method demonstrated in the Stoichiometry calculator, we find a solution S to our initial equations:

$$\begin{bmatrix} 2 & 0 & 0 & 1 & 2 \\ 0 & 2 & 2 & 1 & 0 \\ 1 & 3 & 0 & 0 & 0 \\ 0 & 0 & 3 & 2 & 1 \end{bmatrix} \times \mathbf{S} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \qquad \mathbf{S} = \begin{bmatrix} \frac{1}{2} \\ \frac{1}{6} \\ \frac{1}{3} \\ 0 \\ 0 \end{bmatrix}$$

Using this solution and the null space we can then find the space of all possible solutions to the system of equations:

$$\mathbf{S} + x \cdot \begin{bmatrix} -\frac{1}{2} \\ \frac{1}{6} \\ -\frac{2}{3} \\ 1 \\ 0 \end{bmatrix} + y \cdot \begin{bmatrix} -1 \\ \frac{1}{3} \\ -\frac{1}{3} \\ 0 \\ 1 \end{bmatrix}$$

Each solution we return is cached in the database as a possible point and can be presented to the user graphically via the web server.