

Chemical Equation Processor

Project ID: 76

Authors:

**Aleksandar Obradovic, Andrew Zeng,
Donald Scott, Roger Liu, Kevin Baik**

Mentor:

Christopher Hayden

School:

Upper Dublin High School

Goals and Motivation

Motivation:

Reduce potential errors in manipulation of non-integral values from the periodic table of elements and the time spent executing tedious chemical operations. In doing so we will increase productivity in the field of chemistry and make chemistry more accessible to the masses.

Goals:

- Provide a tool for use in the balancing of chemical equations and stoichiometric analysis of reactions.
- Create a program that runs efficiently and is easily adaptable to many platforms.
- Equip the program to handle exceptions and impossibilities and inform the user of sources of error.

Processing Structure

User inputs reactants and products

Calculate balancing coefficients

User selects molecule

User enters
mass

User enters
volume

User enters quantity
(moles)

Run mass
algorithm

Run volume
algorithm

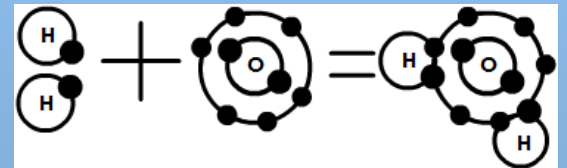
Run quantity
algorithm

Output mass/quantity/volume of other molecules

Background

•Balancing Equations

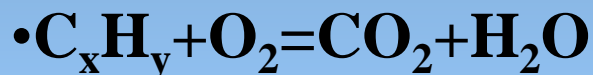
- A chemical equation consists of reactants and products which must obey the law of conservation of matter, retaining the same number of each element of either side of the reaction itself.
- Equations that represent known chemical reactions must be balanced to be practically applied, and the process is done by hand, via reactant-product tables, testing successive coefficient pairings for validity.



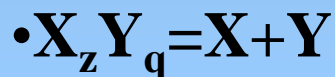
Background

•Types of Reactions

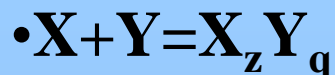
–Combustion



–Decomposition



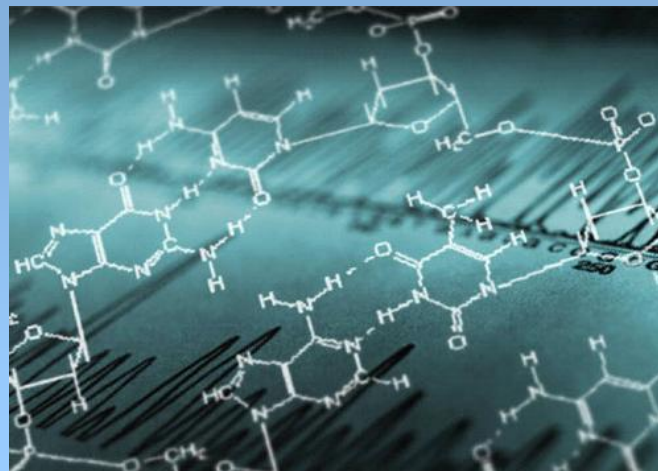
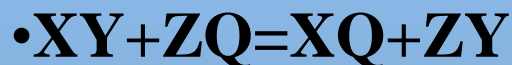
–Synthesis



–Single Replacement Reaction



–Double Replacement Reaction



Background

•Stoichiometry

- The portion of chemistry dealing with numerical relationships in chemical equations.
- Uses coefficients and molecular masses (from periodic table) to calculate quantities of substances involved in chemical equations.
- Given x mass (or quantity in moles) of product or reactant, find y mass (or quantity in moles) of different product or reactants.

•Avogadro's Law

- Extension of stoichiometry employing relations of volumes where standard temperature and pressure is assumed (1 atmosphere, 0 degrees Celsius). 1 mol of gas is contained in 22.414 liters.

Methods and Tools

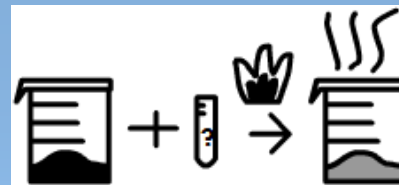
- **Programming Environment**
 - We programmed in Java, to provide compatibility with various systems.
 - We used Java swing to develop an elegant and efficient user interface that allows the user to enter an unbalanced chemical equation and navigate the stoichiometric functions of an automatically balanced and outputted equation.
 - We used Google SVN (subversion system) for a development workspace to allow all team members to edit the code and track changes.

Methods and Tools

• Algorithms

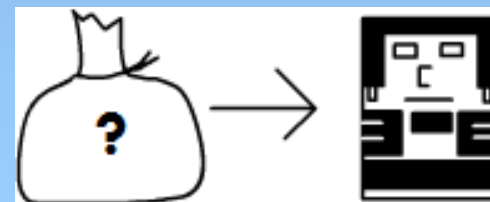
–Quantity conversions

- Specify molecule and quantity, divide the quantity by the coefficient of the specified molecule, multiply by the coefficient of the target molecule. Return that value.



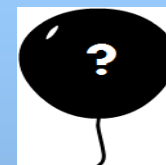
–Mass Conversions

- Specify molecule and mass, divide mass by the molecular mass of the specified molecule, follow the quantity conversion, and multiply by molecular mass of target molecule. Return that value.



–Volume Conversions

- Specify molecule and volume, divide the volume by 22.414 (the STP volume), then follow the quantity conversion, and multiply by 22.414. Return that value.



Methods and Tools

• Algorithms

–Balancing Equations

- Read elements and parenthesized ions as variables and create a system of equations. Solve with matrices.

Example:



$$\bullet \text{Fe: } 1a + 0b - 3c = 0d$$

$$\text{Cl: } 2a + 0b + 0c = 1d$$

$$\text{Na: } 0a + 3b + 0c = 1d$$

$$\text{(PO}_4\text{): } 0a + 1b - 2c = 0d$$

$$\begin{bmatrix} x_1^3 & x_1^2 & x_1 & 1 \\ x_2^3 & x_2^2 & x_2 & 1 \\ x_3^3 & x_3^2 & x_3 & 1 \\ x_4^3 & x_4^2 & x_4 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ b \\ c \\ d \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

Results

- **Software demo (my computer) example of each type of reaction**
- **Some screenshots**
- **Talk about memory load time and calc time, catches nonexistent elements and unbalanceable equations (element on one side is not repeated on the other side)**

Results

The screenshot shows the 'FOC Equation Solver' application window. It features a menu bar with 'File' and 'About'. The main interface is divided into three sections: 'Equation', 'Balanced Equation', and 'Stoichiometric Data'. The 'Equation' section has two input fields separated by an equals sign and a greater-than sign, with a 'Balance' button below them. The 'Balanced Equation' section currently displays 'Waiting for Input'. The 'Stoichiometric Data' section includes a table for inputting data, with columns for 'molecule', 'value', 'prefix', and 'unit type'. The first row contains 'Item 1', a blank value field, 'giga', and '(g)mass'. There are 'Add' and 'Remove' buttons to the right of the table. Below the table, it indicates 'Limiting Reactant: none'.

molecule	value	prefix	unit type
Item 1		giga	(g)mass

The initial state of the program upon running. Blank fields are for input of reactants and products of the equation. Information will be outputted and further input will be accepted in currently blank space. Balance button continues the algorithm.

Results

The screenshot shows the 'FOC Equation Solver' application window. The interface is divided into several sections:

- Equation:** A text input field contains the unbalanced equation $\text{C}_2\text{H}_4 + \text{O}_2 \Rightarrow \text{CO}_2 + \text{H}_2\text{O}$. Below it is a 'Balance' button.
- Balanced Equation:** A text area displays the balanced equation: $\text{C}_2\text{H}_4 + 3 \text{O}_2 \rightarrow 2 \text{CO}_2 + 2 \text{H}_2\text{O}$.
- Stoichiometric Data:** A section titled 'Input data relating to your scenario.' contains a table with columns for 'molecule', 'value', 'prefix', and 'unit type'.

molecule	value	prefix	unit type
C2H4		BASE	(g)mass

Below the table are 'Add' and 'Remove' buttons. To the right, it indicates 'Limiting Reactant: none'.

The program outputs the balanced equation, or returns an error if user entered a non-existent element or an unbalanceable equation, then asks for molecule, value, unit type, and decimal prefix of unit.

Results

The screenshot shows the 'FOC Equation Solver' application window. The interface is divided into several sections:

- Equation:** A text input field contains the unbalanced equation C2H4 + O2 => CO2 + H2O. Below it is a 'Balance' button.
- Balanced Equation:** The balanced equation is displayed as $\text{C}_2\text{H}_4 + 3 \text{O}_2 \rightarrow 2 \text{CO}_2 + 2 \text{H}_2\text{O}$.
- Stoichiometric Data:** A section for inputting data. It includes a table with columns for 'molecule', 'value', 'prefix', and 'unit type'. One entry is shown: 'O2' with a value of '23.1', a prefix of 'BASE', and a unit type of '(g)mass'. There are 'Add' and 'Remove' buttons. Below the table, it says '23.1 grams of C2H4'. A 'Limiting Reactant:' field shows 'None'.
- Stoichiometric Calculations:** A scrollable list of results for each molecule:
 - C2H4:** Quantity 0.8234 mol, Mass 23.1 g, Volume 18.4446 L.
 - O2:** Quantity 2.4703 mol, Mass 79.0453 g, Volume 55.3338 L.
 - CO2:** Quantity 1.6468 mol, Mass 72.477 g, Volume 36.8892 L. A ball-and-stick model of a CO2 molecule is shown.
 - H2O:** Quantity 1.6468 mol, Mass 29.6683 g, Volume 36.8892 L. A ball-and-stick model of a H2O molecule is shown.

The final state of the program. Final results of stoichiometric analysis are outputted in the box on the right and user can restart the process with new equations

Future Work

- **Predict products dynamically given only one side of the equation.**
- **Extend to handle Gas Laws at temperature and pressure variance (not assuming STP).**
- **Illustrate chemical structures of reactants and products (electron structures).**
- **Enable equation ion charge handling capabilities.**
- **Specify physical states of reactants and products (use of solubility rules to determine states).**