CSCE 155N: Matlab

Final Project Proposal

Wednesday, April 25th, 2018

"*Balancing Equations Using Matlab*"

**Group Members -** Allen

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**Problem Description**

A chemical reaction occurs when some substances change chemically to other substances. Chemical reactions are represented by chemical equations. One important law that must be followed when writing a chemical reaction is the law of conservation of mass. This law says that matter cannot be created or destroyed. In every chemical reaction, the same mass of matter must end up in the products as started in the reactants. Balanced chemical equations show that mass is conserved in chemical reactions. The number of atoms before and after reaction does not change. Atoms cannot be lost.

Consider the following example in which water is broken into oxygen and hydrogen gas

Water → Oxygen Gas + Hydrogen Gas

H2O →           O2 +     H2

  The chemical formula for each of the molecule above is correct. However, it seems that we have gained an extra oxygen atom. This is not possible.

By balancing this equation, the law of conservation of mass will be satisfied.

Water → Oxygen Gas + Hydrogen Gas

**2**H2O →      O2 +    **2**H2

The purpose of this project is to take an unbalanced chemical reaction from the user, perform calculation, and return the balanced equation as an output.

**Solution Approach**

The determination of the stoichiometric coefficients in a chemical equation is mathematically equivalent to solving a system of linear algebraic equations. MATLAB is ideally suited to solve this problem. Below is a simple example of how this is the case:

x1CH4 + x2O2 → x3CO2 + x4H2O

Our program is tasked to determine the unknown coefficients x1 and x2. There are two species involved in this reaction: hydrogen (H) and oxygen (O). A balance equation can be written for each of these elements:

Carbon (C): 1⋅x1 + 0⋅x2 = 1⋅x3 + 0⋅x4

Hydrogen (H): 4⋅x1 + 0⋅x2 = 0⋅x3 + 2⋅x4

Oxygen (O): 0⋅x1 + 2⋅x2 = 2⋅x3 + 1⋅x4

We write these as homogeneous equations, each having zero on its right hand side:

x1 – x3 = 0

4x1 – 2x4 = 0

2x2 – 2x3 – x4 = 0

At this point, we have three equations in four unknowns. To complete the system, we define an auxiliary equation by arbitrarily choosing a value for one of the coefficients:

x4 = 1

The complete system of equations can be written in matrix form as Ax = b, where

A = [1 0 –1   0

       4 0 0 –2

       0 2 –2 –1

       0 0 0   1]

x = [x1

      x2

      x3

      x4]

b = [0

        0

        0

        1]

Solving for the x matrix will give us the coefficients we need.

Our program will consist of three main scripts:

1. countAtoms returns a structure array holding the numbers of atoms in each species of the chemical formulas. The input is a string or a cell array of string
   1. First, countAtoms will read input from a file provided by the user. This file should contain a chemical equation or a list of chemical equations needed to be balance
   2. An example of calling countAtoms
      1. N = countAtoms({‘CH4’, ‘02’, ‘CO2’, ‘H20’});
      2. N =
         1. Struct with fields
            1. C
            2. H
            3. O

such that

C 1 0 1 0

H 4 0 0 2

O 0 2 2 1

* 1. Elements, by convention, consist of one or two character abbreviations. The character is capitalized. If present, the second character is a lowercase letter. Therefore, error messages will be generated for invalid formulas input by the user

1. myMat computes the matrix for the given set of chemical species. The input is a structure array of the numbers of atoms each species have (the structure array obtained from countAtoms). In other word, the input of myMat is the output of countAtoms
   1. Example
      1. N = countAtoms({‘CH4’, ‘02’, ‘CO2’, ‘H20’});
      2. B = myMat(N);
      3. myMat =

1 0 1 0

4 0 0 2

1. 2 2 1
2. chemBalance computes a stoichiometry matrix for a chemical equation. The coefficient is negative for reactants and positive for products
   1. Example of calling this function:
      1. Out = chemBalance({‘CH4’, ‘02’, ‘CO2’, ‘H20’});
      2. Out =

-1

-2

1

2

* 1. A graph that shows the number of atoms at the beginning vs the number of atoms after being balanced will be displayed
  2. chemBalance will also write output to an output file

1. Our program will also calculate the molecular weight of the inputs if the user wish to attain this information.
   1. Another separate .m file will be created to implement this feature.
      1. We would need to input the atomic mass unit of all the elements. The input is a separate file with information of the atomic mass unit of all the elements on the periodic table. This file would then be the input data file when performing calculation.
      2. We will use the structure array attained in *countAtom* to perform molecular weight calculation

Our program will also consist of a GUI. The GUI will take input and provide the user with the proper output in a readable manner

**Task and Responsibilities Allocation**

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| **Last Name** | **First Name** | **CSE Username** | **Task** |
| **Giovanni** | Cruz Mojica | gcruzmojica | Responsible for creating the input file and the script that calculates the molecular weight of the inputs and displays the data |
| **Joshua** | Landers | jlanders | Responsible for creating the *myMat.m* file, the script that computes the matrix to be use, AND *chemBalance.m* file, the script that takes the resulting matrix from *myMat* and perform the balancing. Will also be responsible for creating the graph which shows the number of atoms before and after the balancing |
| **Xuan** | Le | ngochuongl | Responsible for creating the *countAtoms.m* file, the script that returns a structure array holding the numbers of atoms in species of the unbalanced equation |
| **Trevin** | Rezac | trezac | Responsible for creating the GUI of the program |

**Work cite:**

Andersen, and G.Bjedov. “ChemicalStoichiometry.” Mathgene.usc.es, mathgene.usc.es/matlab-profs-quimica/reacciones.