**DSCI6001 – Final Project**

**Applications of Linear Algebra to Chemistry**

In this project we discuss two applications of linear algebra to chemistry:

* To balance chemical equations.
* To calculate the right mix of volumes of chemical substances to produce a chemical solution.

**Balance of Chemical Equations**

We start by describing step by step how to balance an example of a chemical equation.

In this application, we will always have a parametrized solution as we will have more independent variables than equations, been the system homogeneous.

After that, we introduce the case of the combustion of saturated hydrocarbons, creating a general solution to balance any saturated hydrocarbon.

We also have a function that will balance the above scenario. This function relies on a helper one to validate the user entry, which I have tried to use regex (using the python re library): since I was not getting satisfactory results, I abandoned it, although I would have prefer the use of regex as it is very flexible and scalable.

**Mixing of Chemical Substances to Create a Chemical Solution**

This type of application requires a full rank linear system in order to work.

For example, if we have three chemical compounds to be mixed, we will require a system of three linear equations in order to find the proper mix of volumes of chemical compounds.

We show an example of how to solve a system like the one described above.

Following that, we develop a general solution to find the right mix of volumes for two components producing a chemical solution. We describe all the conditions that need to be met in order for the linear system to be able to produce a solution.

Another function is presented that will help on finding the proper volumes of two chemical substances to be mixed.

References:

* http://www.slideshare.net/rasen58/linear-algebra-application-to-chemistry
* http://ndu2009algebra.blogspot.com/2011/04/as-we-struggle-to-increase-number-of.html
* https://regexone.com/references/python