Problem Statement and Goals
ChemCode

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Table 1: Revision History

Date	Developer(s)	Change
Jan. 18, 2023	Sam	Create document and fill in Problem, Stakeholders, and Goals sections
Jan. 19, 2023	Sam	Format for Drasil upload and fill in Inputs and Outputs Section

1 Problem Statement

[You should check your problem statement with the problem statement checklist. —SS] [You can change the section headings, as long as you include the required information. —SS]

1.1 Problem

Chemistry is a broad field that studies matter and its interactions [1, pp. 8-9], primarily through chemical reactions. During a chemical reaction, bonds between some substances break and new ones are formed to create new substances; these reactions are often written as chemical equations [2]. Despite new chemicals being created, all atoms from the initial substances, or "reactants", must be present in the final substances, or "products" because of the Law of Conservation of Matter [2]. This means that for a chemical equation to be useful, it must be balanced by changing the coefficients of the substances involved in the reaction [2]. Additionally, since molecules only exist in whole numbers (since dividing a molecule changes its composition into new types of molecules), these coefficients must be whole numbers, and by convention should be as small as possible [2].

While these equations can be balanced by hand through the process of "balancing by inspection" [2], this can be time-consuming, prone to error, and inefficient, especially for more complicated chemical reactions. For each element

present in the reaction, an equality can be written for the number of elements in each substance, with the reactants on one side and the products on the other, using the coefficients of each substance as the variables [3]. These equalities then form a system of linear equations that can be solved through various methods to yield a relation between each coefficient, which can then be manipulated to find the require whole numbers [2, 3]. This method can also identify reactions that are "infeasible" and balance reactions involving fractional oxidation states [3], which "are used to describe the distribution of electrons in a molecule" [4].

1.2 Inputs and Outputs

[Characterize the problem in terms of "high level" inputs and outputs. Use abstraction so that you can avoid details. —SS]

Input:

- A representation of a chemical equation

Output:

- A representation of the inputted chemical equation in its balanced form with the smallest whole number coefficients possible

1.3 Stakeholders

The main stakeholder of this project is Dr. Spencer Smith, the instructor for the CAS 741 Development of Scientific Computing Software course for which this project is being completed. Dr. Smith and Dr. Jacques Carette are in charge of the Drasil project that ChemCode seeks to extend, so the implementation and process of getting there are of significance to them. Likewise, any future developers of Drasil, including myself [Can I use the first person? —SC], are potential stakeholders of this project, since they may use features added to Drasil, such as ideas about chemistry or systems of linear equations. Jason Balaci, another CAS 741 and Drasil contributor, is of particular mention, since there may be some overlap between our project, so we may be collaborating throughout this project.

More generally, anyone in the field of chemistry in at least a high-school level may be a stakeholder of this project, as they may use this tool in their work.

1.4 Environment

[Hardware and software —SS]

2 Goals

The goals of this project are to develop a program that:

- Can balance chemical equations using systems of linear equations.

3 Stretch Goals

References

[1] E. Gordon and Furman University, *CHM101: Chemistry and Global Awareness*. Greenville, SC, USA: LibreTexts, Jan. 2023.

[2] L. Lund and Anoka-Ramsey Community College, *Introduction to Chemistry*. Cambridge and Coon Rapids, MN, USA: LibreTexts, Jan. 2023.

[3] I. Hamid, "Balancing Chemical Equations by Systems of Linear Equations," *Applied Mathematics*, vol. 10, pp. 521–526, July 2019.

[4] Unacademy, "Fractional Oxidation States," 2023.