Problem Statement and Goals
ChemCode

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January 20, 2023

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, fill in Inputs and Outputs and Environment sections, update Stakeholders section, and move Environment 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], 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 Environment

[Hardware and software —SS]

ChemCode will be developed using Drasil [5], "a framework for generating high-quality documentation and code for Scientific Computing Software" [6, p. iii] by encapsulating scientific knowledge as "chunks" to be reused among projects [6]. The implementation in Drasil places some constraints on this project.

Since Drasil is built on the idea of reusability, external libraries will be used to solve these systems of linear equations. This was previously done with ordinary differential equation (ODE) solvers, since "creating a complete ODE solver in Drasil would take considerable time, and there are already many reliable external libraries have been tested by long use" [7, p. 24].

Additionally, Drasil can currently generate code in Python, C++, C#, Java, and Swift [7], so these will be the languages that will be focused on for the ChemCode project. While using external ODE solvers in Drasil, the developers "did not find a suitable library for Swift" [7, p.24], so a similar problem may arise when using external system of linear equations solvers; this means that ChemCode may not be generated in all five languages.

1.4 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 development process 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, a fellow CAS 741 student and Drasil contributor, is of particular mention, since there may be some overlap between our projects so we may be collaborating throughout this project. I am also a stakeholder of ChemCode as the developer.

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.

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.

[5] J. Carette, D. Szymczak, B. MacLachlan, M. Niazi, S. Crawford, D. Scime, AKM11, S. Palmer, S. Smith, O. Owojaiye, A. Elwazani, Mornix, Muhammadaliog3, D. P. R. Guttapati, N. Hu, J. Wu, L. Mawarid, J. Seger, Aida, N. G. Muralidharan, Azer-X, D. Genkin, and R. Jain, "JacquesCarette/Drasil," Feb. 2021.

[6] B. MacLachlan, *A Design Language for Scientific Computing Software in Drasil*. PhD thesis, McMaster University, Hamilton, ON, Canada, June 2020.

[7] D. Chen, *Solving Higher-Order ODEs in Drasil*. PhD thesis, McMaster University, Hamilton, ON, Canada, Sept. 2022.