Software Requirements Specification for ChemCode: A program for solving chemistry problems

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Revision History

Date	Version	Notes
Jan. 21, 2023	0.0	Start document, fill in title page, and add references
	0.1	Fill in Problem Description and Goal Statements sections, as well as all relevant definitions
Jan. 22, 2023	0.1.1	Replace the notion of "fractional oxidation state" with "non-stoichiometric compound"
	0.1.2	Fix capTemplate reference
	0.1.3	Update Abbreviations and Acronyms
	0.2	Add IM for balancing a chemical reaction (IM3), along with relevant reference information
Jan. 23, 2023	0.2.1	Add IM for determining if a chemical reaction is feasible (IM2), along with relevant reference information
Jan. 25, 2023	0.2.2	Add references between sections for notation and definitions
	0.2.3	Abstract IM2
	0.2.4	Add IM for converting chemical equation to a matrix (IM1), along with relevant reference information
	0.2.5	Rename and add input constraint to IM3
	0.2.6	Add note about IM3 returning the smallest solution
	0.2.7	Add TM for matrix equation (T1)
	0.2.8	Improve referencing, mainly for TMs, and add note about potential TM for Conservation of Mass
	0.2.9	Add check for Conservation of Mass in IM2
Jan. 26, 2023	0.3	Add Likely Changes from Problem Statement, add assumption about difference between number of elements and compounds (A1), and add mole to Table of Units
	0.3.1	Update T1 (and TM function) from feedback from presentation
	0.3.2	Fill in Scope of Requirements, fix A1 and change "infeasible" to "feasible"
Jan. 27, 2023	0.3.3	Improve section referencing in Revision History
	0.4	Fill in Functional Requirements
Jan. 28, 2023	0.4.1	Fill in main Nonfunctional Requirements, along with relevant reference information
	0.4.2	Add TM for the Law of Conservation of Mass (T2)
	0.4.3	Represent input to IM1 as two sequences of chemical formulas, add assumptions about user input, and remove infeasible likely change
Jan. 29, 2023	0.4.4	Add NFRs for understandability (NFR2) and verifiability (NFR6) and improve quality of other NFRs
	0.5	Fill in Introduction based on Drasil examples

1 Reference Material

This section records information for easy reference.

1.1 Table of Units

Throughout this document SI (Système International d'Unités) is employed as the unit system. In addition to the basic units, several derived units are used as described below. For each unit, the symbol is given followed by a description of the unit and the SI name.

symbol	unit	SI
mol	amount of substance	mole
m	length	metre
kg	mass	kilogram
s	time	second
°C	temperature	centigrade
J	energy	joule
W	power	watt ($\mathrm{W} = \mathrm{J\,s^{-1}}$)

[Only include the units that your SRS actually uses. —TPLT]

[Derived units, like newtons, pascal, etc, should show their derivation (the units they are derived from) if their constituent units are in the table of units (that is, if the units they are derived from are used in the document). For instance, the derivation of pascals as $\mathrm{Pa} = \mathrm{N\,m^{-2}}$ is shown if newtons and m are both in the table. The derivations of newtons would not be shown if kg and s are not both in the table. —TPLT]

[The symbol for units named after people use capital letters, but the name of the unit itself uses lower case. For instance, pascals use the symbol Pa, watts use the symbol W, teslas use the symbol T, newtons use the symbol N, etc. The one exception to this is degree Celsius. Details on writing metric units can be found on the NIST web-page. —TPLT]

1.2 Table of Symbols

The table that follows summarizes the symbols used in this document along with their units. The choice of symbols was made to be consistent with the heat transfer literature and with existing documentation for solar water heating systems. The symbols are listed in alphabetical order.

symbol	unit	description
A_C	$\mathrm{m^2}$	coil surface area
A_{in}	$\mathrm{m^2}$	surface area over which heat is transferred in

[Use your problems actual symbols. The si package is a good idea to use for units. —TPLT]

1.3 Abbreviations and Acronyms

symbol	description
1D	One-Dimensional
A	Assumption
DD	Data Definition
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
PS	Physical System Description
R	Requirement
SRS	Software Requirements Specification
T	Theoretical Model
VnV	Verification and Validation

1.4 Mathematical Notation

Matrices are written in bold uppercase letters (for example $\mathbf{A}$), while vectors (1D matrices) are written in bold lowercase letters, (for example $\mathbf{x}$) [1]. The zero matrix is a special type of matrix where each element is zero and is represented as $\mathbf{0}$ [2]. Individual entries in a matrix are written in lowercase letters with their row and column number, in that order, written as subscripts (for example a_{12}) [1]; these subscripts are sometimes separated by a comma for clarity (for example $a_{12,34}$) [3]. Two (or more) matrices with the same number of rows can be joined together to form an "augmented matrix", written as $(\mathbf{A}|\mathbf{B})$ [4].

[If symbols are used to show mathematical operations, these should be summarized here. In some cases the easiest way to summarize the notation is to point to a text or other source that explains the notation. —TPLT]

[This SRS template is based on [5, 6]. It will get you started. You should not modify the section headings, without first discussing the change with the course instructor. Modification means you are not following the template, which loses some of the advantage of a template, especially standardization. Although the bits shown below do not include type information, you may need to add this information for your problem. If you are unsure, please can ask the instructor. —TPLT]

[Feel free to change the appearance of the report by modifying the LaTeX commands. —TPLT]

[This template document assumes that a single program is being documented. If you are documenting a family of models, you should start with a commonality analysis. A separate template is provided for this. For program families you should look at [7, 8]. Single family member programs are often programs based on a single physical model. General purpose tools are usually documented as a family. Families of physical models also come up. —TPLT]

[The SRS is not generally written, or read, sequentially. The SRS is a reference document. It is generally read in an ad hoc order, as the need arises. For writing an SRS, and for reading one for the first time, the suggested order of sections is:

- Goal Statement
- Instance Models
- Requirements
- Introduction
- Specific System Description

—TPLT]

[Guiding principles for the SRS document:

- Do not repeat the same information at the same abstraction level. If information is repeated, the repetition should be at a different abstraction level. For instance, there will be overlap between the scope section and the assumptions, but the scope section will not go into as much detail as the assumptions section.

—TPLT]

[The template description comments should be disabled before submitting this document for grading. —TPLT]

[You can borrow any wording from the text given in the template. It is part of the template, and not considered an instance of academic integrity. Of course, you need to cite the source of the template. —TPLT]

[When the documentation is done, it should be possible to trace back to the source of every piece of information. Some information will come from external sources, like terminology. Other information will be derived, like General Definitions. —TPLT]

[An SRS document should have the following qualities: unambiguous, consistent, complete, validatable, abstract and traceable. —TPLT]

[The overall goal of the SRS is that someone that meets the Characteristics of the Intended Reader (Section 2.3) can learn, understand and verify the captured domain knowledge. They should not have to trust the authors of the SRS on any statements. They should be able to independently verify/derive every statement made. —TPLT]

2 Introduction

Chemical equations are common ways of representing chemical reactions (as described in Physical System Description), but must be balanced for use in other calculations [9]. Therefore, it is useful to have a tool to automatically balance these chemical reactions for efficiency and accuracy.

The following section provides an overview of the Software Requirements Specification (SRS) for ChemCode. This section explains the purpose of this document, the scope of the requirements, the characteristics of the intended reader, and the organization of the document.

2.1 Purpose of Document

The primary purpose of this document is to record the requirements of the program for solving chemistry problems [Is this a good description? —SC]. Goals, assumptions, theoretical models, definitions, and other model derivation information are specified, allowing the reader to fully understand and verify the purpose and scientific basis of ChemCode. With the exception of system constraints, this SRS will remain abstract, describing what problem is being solved, but not how to solve it.

This document will be used as a starting point for subsequent development phases, including writing the design specification and the software Verification and Validation (VnV) Plan. The design document will show how the requirements are to be realized, including decisions on the numerical algorithms and programming environment. The VnV Plan will show the steps that will be used to increase confidence in the software documentation and the implementation. Although the SRS fits in a series of documents that follow the so-called "waterfall model", the actual development process is not constrained in any way. Even when the waterfall model is not followed, as Parnas and Clements point out in [10], the most logical way to present the documentation is still to "fake" a rational design process.

2.2 Scope of Requirements

The scope of the requirements includes determining if a given chemical equation is feasible (see Terminology and Definitions) and, if it is, balancing it using the smallest whole number coefficients possible, regardless of whether or not the chemical formulas in the equation are correct or if the reaction would take place in a real-world setting.

2.3 Characteristics of Intended Reader

Reviewers of this documentation should have an understanding of high-school level chemistry, namely stoichiometry (see Terminology and Definitions), and undergraduate Level 1 linear algebra, namely solving systems of linear equations. The end user of ChemCode, as described in User Characteristics, does not require knowledge of linear algebra, since relevant concepts will be implemented by the code and hidden from the user.

2.4 Organization of Document

The organization of this document is based a template from, [11], which is based on the template for an SRS for scientific computing software proposed by [5], [6], and [12]. The presentation follows the standard pattern of presenting goals, theories, definitions, and assumptions. For readers that would like a more bottom-up approach, they can start reading the Instance Models and trace back to find any additional information they require.

The Goal Statements are refined to the Theoretical Models, which are refined to the Instance Models.

3 General System Description

This section provides general information about the system. It identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints. [This text can likely be borrowed verbatim. —TPLT]

[The purpose of this section is to provide general information about the system so the specific requirements in the next section will be easier to understand. The general system description section is designed to be changeable independent of changes to the functional requirements documented in the specific system description. The general system description provides a context for a family of related models. The general description can stay the same, while specific details are changed between family members. —TPLT]

3.1 System Context

[Your system context will include a figure that shows the abstract view of the software. Often in a scientific context, the program can be viewed abstractly following the design pattern of Inputs → Calculations → Outputs. The system context will therefore often follow this pattern. The user provides inputs, the system does the calculations, and then provides the outputs to the user. The figure should not show all of the inputs, just an abstract view of the main categories of inputs (like material properties, geometry, etc.). Likewise, the outputs should be presented from an abstract point of view. In some cases the diagram will show other external entities, besides the user. For instance, when the software product is a library, the user will be another software program, not an actual end user. If there are system constraints that the software must work with external libraries, these libraries can

also be shown on the System Context diagram. They should only be named with a specific library name if this is required by the system constraint. —TPLT]

Figure 1: System Context

[For each of the entities in the system context diagram its responsibilities should be listed. Whenever possible the system should check for data quality, but for some cases the user will need to assume that responsibility. The list of responsibilites should be about the inputs and outputs only, and they should be abstract. Details should not be presented here. However, the information should not be so abstract as to just say "inputs" and "outputs". A summarizing phrase can be used to characterize the inputs. For instance, saying "material properties" provides some information, but it stays away from the detail of listing every required properties. —TPLT]

- User Responsibilities:
  -
- ChemCode Responsibilities:
  - Detect data type mismatch, such as a string of characters instead of a floating point number
  -

3.2 User Characteristics

The end user of ChemCode should have an understanding of high-school level chemistry, namely stoichiometry (see Terminology and Definitions).

3.3 System Constraints

[System constraints differ from other type of requirements because they limit the developers' options in the system design and they identify how the eventual system must fit into the world. This is the only place in the SRS where design decisions can be specified. That is, the quality requirement for abstraction is relaxed here. However, system constraints should only be included if they are truly required. —TPLT]

4 Specific System Description

This section first presents the problem description, which gives a high-level view of the problem to be solved. This is followed by the solution characteristics specification, which presents the assumptions, theories, definitions and finally the instance models. [Add any project specific details that are relevant for the section overview. —TPLT]

4.1 Problem Description

ChemCode is intended to balance chemical equations (including ones with nonstoichiometric compounds; see Terminology and Definitions) so they can be useful for other computations [9]. Additionally, since molecules only exist in whole numbers (since dividing a molecule changes its composition into new types of molecules), the coefficients used to balance the equation must be whole numbers, and by convention should be as small as possible [9].

4.1.1 Terminology and Definitions

This subsection provides a list of terms that are used in the subsequent sections and their meaning, with the purpose of reducing ambiguity and making it easier to correctly understand the requirements:

- **Feasible**: (Referring to a chemical equation) able to be balanced [13].
- **Hydrate**: "A compound formed by the chemical combination of water and some other substance in a definite molecular ratio" [14].
- **Nonstoichiometric Compound**: "Any solid chemical compound in which the numbers of atoms of the elements present cannot be expressed as a ratio of small whole numbers" [15].
- **Product**: A substance created by a chemical reaction [9].
- **Reactant**: A substance present at the beginning of, and involved in, a chemical reaction [9].
- **Stoichiometry**: "The calculation of the quantities of reactants or products in a chemical reaction using the relationships found in a balanced chemical equation" [9, p. 337].

4.1.2 Physical System Description

[The purpose of this section is to clearly and unambiguously state the physical system that is to be modelled. Effective problem solving requires a logical and organized approach. The statements on the physical system to be studied should cover enough information to solve the problem. The physical description involves element identification, where elements are defined as independent and separable items of the physical system. Some example elements

include acceleration due to gravity, the mass of an object, and the size and shape of an object. Each element should be identified and labelled, with their interesting properties specified clearly. The physical description can also include interactions of the elements, such as the following: i) the interactions between the elements and their physical environment; ii) the interactions between elements; and, iii) the initial or boundary conditions. —TPLT]

The physical system of ChemCode, as shown in Figure ?, includes the following elements:

PS1:

PS2: ...

[A figure here makes sense for most SRS documents —TPLT]

4.1.3 Goal Statements

Given a representation of a chemical equation, the goal statements of ChemCode are:

GS1: Determine if a given chemical reaction is feasible (see Terminology and Definitions).

GS2: Balance the inputted chemical equation with the smallest whole number coefficients possible.

4.2 Solution Characteristics Specification

[This section specifies the information in the solution domain of the system to be developed. This section is intended to express what is required in such a way that analysts and stakeholders get a clear picture, and the latter will accept it. The purpose of this section is to reduce the problem into one expressed in mathematical terms. Mathematical expertise is used to extract the essentials from the underlying physical description of the problem, and to collect and substantiate all physical data pertinent to the problem. —TPLT]

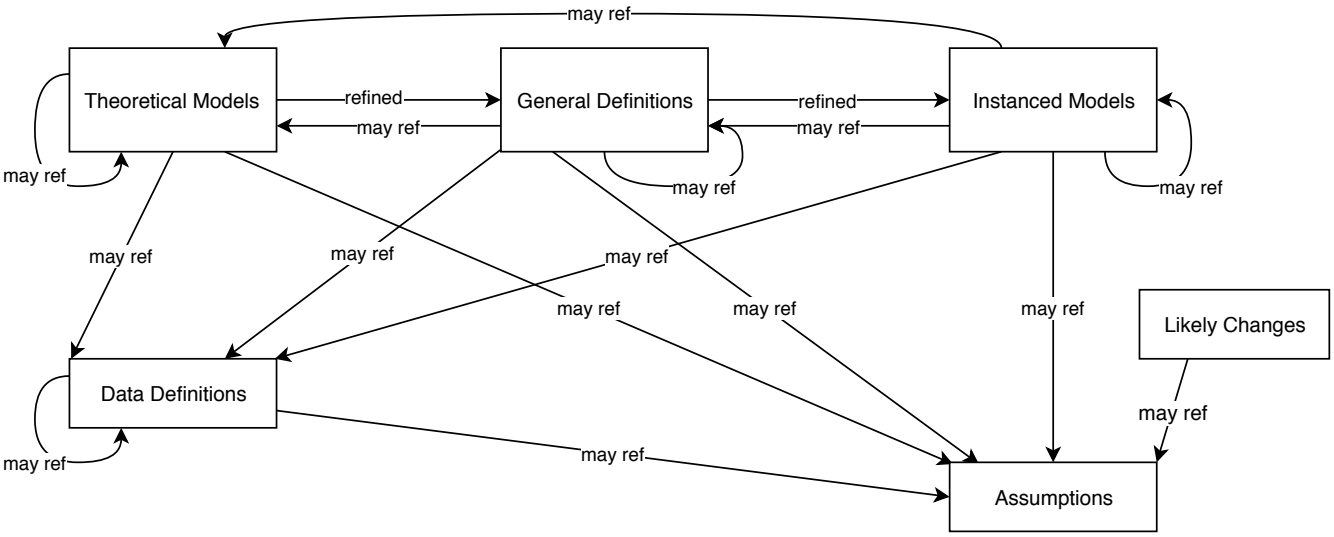
[This section presents the solution characteristics by successively refining models. It starts with the abstract/general Theoretical Models (TMs) and refines them to the concrete/specific Instance Models (IMs). If necessary there are intermediate refinements to General Definitions (GDs). All of these refinements can potentially use Assumptions (A) and Data Definitions (DD). TMs are refined to create new models, that are called GMs or IMs. DDs are not refined; they are just used. GDs and IMs are derived, or refined, from other models. DDs are not derived; they are just given. TMs are also just given, but they are refined, not used. If a potential DD includes a derivation, then that means it is refining other models, which would make it a GD or an IM. —TPLT]

[The above makes a distinction between "refined" and "used." A model is refined to another model if it is changed by the refinement. When we change a general 3D equation to a 2D equation, we are making a refinement, by applying the assumption that the third dimension does not matter. If we use a definition, like the definition of density, we aren't refining, or changing that definition, we are just using it. —TPLT]

[The same information can be a TM in one problem and a DD in another. It is about how the information is used. In one problem the definition of acceleration can be a TM, in another it would be a DD. —TPLT]

[There is repetition between the information given in the different chunks (TM, GDs etc) with other information in the document. For instance, the meaning of the symbols, the units etc are repeated. This is so that the chunks can stand on their own when being read by a reviewer/user. It also facilitates reuse of the models in a different context. —TPLT]

[The relationships between the parts of the document are show in the following figure. In this diagram "may ref" has the same role as "uses" above. The figure adds "Likely Changes," which are able to reference (use) Assumptions. —TPLT]



The instance models that govern ChemCode are presented in Subsection 4.2.6. The information to understand the meaning of the instance models and their derivation is also presented, so that the instance models can be verified.

4.2.1 Assumptions

[The assumptions are a refinement of the scope. The scope is general, where the assumptions are specific. All assumptions should be listed, even those that domain experts know so well that they are rarely (if ever) written down. —TPLT] [The document should not take for granted that the reader knows which assumptions have been made. In the case of unusual assumptions, it is recommended that the documentation either include, or point to, an explanation and justification for the assumption. —TPLT]

This section simplifies the original problem and helps in developing the theoretical model by filling in the missing information for the physical system. The numbers given in the square brackets refer to the theoretical model [T], general definition [GD], data definition [DD], instance model [IM], or likely change [LC], in which the respective assumption is used.

A1: For all inputted chemical equations, there is at most one more compound than element. (Through empirical analysis, chemical equations without this constraint lead to unexpected results that require a deeper analysis.)

A2: All inputted chemical formulas describe real chemical formulas. [IM1]

A3: All inputted chemical formulas are formatted following some set of agreed-upon conventions. [IM1, LC6]

A4: All inputted chemical formulas are simple; i.e., only consist of atomic symbols and subscripts. [IM1, LC1]

4.2.2 Theoretical Models

[Theoretical models are sets of abstract mathematical equations or axioms for solving the problem described in Physical System Description. Examples of theoretical models are physical laws, constitutive equations, relevant conversion factors, etc. —TPLT]

This section focuses on the general equations and laws that ChemCode is based on.

Number: T1

Label: Matrix equation

Equation: $\mathbf{Ax} = \mathbf{b}$

Description: The above equation gives the general form of the matrix equation where $\mathbf{A}$ is an $m \times n$ matrix, $\mathbf{b}$ is a vector in $\mathbb{R}^m$, and $\mathbf{x}$ is a vector in $\mathbb{R}^n$ with unknown values to be solved for [16].

Notes: For any $\mathbf{A}$ and $\mathbf{b}$, there is either zero, one, or infinite values for $\mathbf{x}$ [17].

Source: https://textbooks.math.gatech.edu/ila/matrix-equations.html [Is this a good enough source? —SC]

Ref. By: IM3

Derivation for T1: Not Applicable

Number: T2

Label: Law of Conservation of Mass

Equation: Not Applicable

Description: This law states that "matter can neither be created nor destroyed in a chemical reaction . . . but it may change forms to other substances" [9, p. 112].

Notes: None

Source: https://chem.libretexts.org/Courses/Anoka-Ramsey_Community_College/Introduction_to_Chemistry/03%3A_Matter_and_Energy/3.06%3A_Conservation_of_Mass

Ref. By: IM2

Derivation for T2: Not Applicable

4.2.3 General Definitions

[General Definitions (GDs) are a refinement of one or more TMs, and/or of other GDs. The GDs are less abstract than the TMs. Generally the reduction in abstraction is possible through invoking (using/referencing) Assumptions. For instance, the TM could be Newton's Law of Cooling stated abstracting. The GD could take the general law and apply it to get a 1D equation. —TPLT]

This section collects the laws and equations that will be used in building the instance models.

[Some projects may not have any content for this section, but the section heading should be kept. —TPLT] [Modify the examples below for your problem, and add additional definitions as appropriate. —TPLT]

Number	GD1
Label	**Newton's law of cooling**
SI Units	$\mathrm{W\,m^{-2}}$
Equation	$q(t) = h\Delta T(t)$
Description	Newton's law of cooling describes convective cooling from a surface. The law is stated as: the rate of heat loss from a body is proportional to the difference in temperatures between the body and its surroundings. $q(t)$ is the thermal flux ($\mathrm{W\,m^{-2}}$). h is the heat transfer coefficient, assumed independent of T (A**??**) ($\mathrm{W\,m^{-2}\,{}^{\circ}C^{-1}}$). $\Delta T(t) = T(t) - T_{\mathrm{env}}(t)$ is the time-dependent thermal gradient between the environment and the object (°C).
Source	Citation here
Ref. By	DD1, DD**??**

Detailed derivation of simplified rate of change of temperature

[This may be necessary when the necessary information does not fit in the description field. —TPLT] [Derivations are important for justifying a given GD. You want it to be clear where the equation came from. —TPLT]

4.2.4 Data Definitions

[The Data Definitions are definitions of symbols and equations that are given for the problem. They are not derived; they are simply used by other models. For instance, if a problem depends on density, there may be a data definition for the equation defining density. The DDs are given information that you can use in your other modules. —TPLT]

[All Data Definitions should be used (referenced) by at least one other model. —TPLT]

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given. [Modify the examples below for your problem, and add additional definitions as appropriate. —TPLT]

Number	DD1
Label	**Heat flux out of coil**
Symbol	q_C
SI Units	$\mathrm{W\,m^{-2}}$
Equation	$q_C(t) = h_C(T_C - T_W(t))$, over area A_C
Description	T_C is the temperature of the coil (°C). T_W is the temperature of the water (°C). The heat flux out of the coil, q_C ($\mathrm{W\,m^{-2}}$), is found by assuming that Newton's Law of Cooling applies (A**??**). This law (GD1) is used on the surface of the coil, which has area A_C ($\mathrm{m^2}$) and heat transfer coefficient h_C ($\mathrm{W\,m^{-2}\,°C^{-1}}$). This equation assumes that the temperature of the coil is constant over time (A**??**) and that it does not vary along the length of the coil (A**??**).
Sources	Citation here
Ref. By	IM**??**

4.2.5 Data Types

[This section is optional. In many scientific computing programs it isn't necessary, since the inputs and outpus are straightforward types, like reals, integers, and sequences of reals and integers. However, for some problems it is very helpful to capture the type information. —TPLT]

[The data types are not derived; they are simply stated and used by other models. —TPLT]

[All data types must be used by at least one of the models. —TPLT]

[For the mathematical notation for expressing types, the recommendation is to use the notation of [18]. —TPLT]

This section collects and defines all the data types needed to document the models. [Modify the examples below for your problem, and add additional definitions as appropriate. —TPLT]

Type Name	Name for Type
Type Def	mathematical definition of the type
Description	description here
Sources	Citation here, if the type is borrowed from another source

4.2.6 Instance Models

[The motivation for this section is to reduce the problem defined in Physical System Description to one expressed in mathematical terms. The IMs are built by refining the TMs and/or GDs. This section should remain abstract. The SRS should specify the requirements without considering the implementation. —TPLT]

This section transforms the problem defined in Problem Description into one which is expressed in mathematical terms. It uses concrete symbols defined in Section 4.2.4 to replace the abstract symbols in the models identified in Sections 4.2.2 and 4.2.3.

The goals GS1 and GS2 are solved by IM2 and IM3, respectively.

Number	IM1
Label	**Matrix representation of elements present in reaction**
Input	Two sequences of representations of chemical formulas; one for the reactants and one for the products (see Terminology and Definitions).
Output	A matrix such that each entry indicates the amount of a given element in a given compound; each row corresponds to a different element and each column corresponds to a different compound. Positive entries indicate the compound is a reactant, negative entries indicate the compound is a product, and zeroes indicate the corresponding element is not present in the corresponding compound.
Description	Each chemical formula present in the inputted sequences are assumed to be valid (A2), be formatted correctly (A3), and only consist of atomic symbols and subscripts (A4).
Sources	[13]
Ref. By	IM2, IM3

Derivation of ...

[The derivation shows how the IM is derived from the TMs/GDs. In cases where the derivation cannot be described under the Description field, it will be necessary to include this subsection. —TPLT]

Number	IM2
Label	**Determination of feasibility**
Input	**A** from IM1
Output	F if a row of **A** does not have a positive and a negative entry or if (**A**|**0**) has no solutions and T otherwise
Description	**A** is a matrix representing the amount of each element in each compound in a reaction from IM1. [Is this necessary? —SC] If a row of **A** only has either a positive or negative entry, then there is an element that is either a reactant or a product (see Terminology and Definitions) but not both, which breaks the Law of Conservation of Mass (T2). [Is this a good place for this? —SC] **0** is the zero matrix (see Mathematical Notation).
Sources	[13]
Ref. By	IM3

Derivation of ...

[The derivation shows how the IM is derived from the TMs/GDs. In cases where the derivation cannot be described under the Description field, it will be necessary to include this subsection. —TPLT]

Number	IM3
Label	**Vector of compound coefficients in balanced equation**
Input	**A** from IM1 The input is constrained so that **A** is feasible (IM2). [Is this correct? —SC]
Output	**x**, such that it is the smallest solution to $\mathbf{Ax} = \mathbf{0}$ from T1 [Is this sufficient? —SC]
Description	**A** is a matrix representing the amount of each element in each compound in a reaction from IM1. [Is this necessary? —SC] **x** is a vector of coefficients for each compound in the reaction (in the order inputted) so that the equation is balanced. **0** is the zero matrix (see Mathematical Notation).
Sources	[13]
Ref. By	N/A

Derivation of ...

[The derivation shows how the IM is derived from the TMs/GDs. In cases where the derivation cannot be described under the Description field, it will be necessary to include this subsection. —TPLT]

4.2.7 Input Data Constraints

Table 1 shows the data constraints on the input output variables. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable. The column for software constraints restricts the range of inputs to reasonable values. The software constraints will be helpful in the design stage for picking suitable algorithms. The constraints are conservative, to give the user of the model the flexibility to experiment with unusual situations. The column of typical values is intended to provide a feel for a common scenario. The uncertainty column provides an estimate of the confidence with which the physical quantities can be measured. This information would be part of the input if one were performing an uncertainty quantification exercise.

The specification parameters in Table 1 are listed in Table 2.

Table 1: Input Variables

Var	Physical Constraints	Software Constraints	Typical Value	Uncertainty
L	$L > 0$	$L_{\text{min}} \leq L \leq L_{\text{max}}$	1.5 m	10%

(*) [you might need to add some notes or clarifications —TPLT]

Table 2: Specification Parameter Values

Var	Value
L_{min}	0.1 m

4.2.8 Properties of a Correct Solution

A correct solution must exhibit [fill in the details —TPLT]. [These properties are in addition to the stated requirements. There is no need to repeat the requirements here. These additional properties may not exist for every problem. Examples include conservation laws (like conservation of energy or mass) and known constraints on outputs, which are usually summarized in tabular form. A sample table is shown in Table 3 —TPLT]

Table 3: Output Variables

Var	Physical Constraints
T_W	$T_{\text{init}} \leq T_W \leq T_C$ (by A??)

[This section is not for test cases or techniques for verification and validation. Those topics will be addressed in the Verification and Validation plan. —TPLT]

5 Requirements

This section provides the functional requirements, the business tasks that the software is expected to complete, and the nonfunctional requirements, the qualities that the software is expected to exhibit.

5.1 Functional Requirements

R1: Input a representation of a chemical equation.

R2: Convert the inputted equation to matrix form (from IM1).

R3: Determine if the inputted equation is feasible (see Terminology and Definitions; from IM2).

R4: If the inputted equation is feasible, balance the chemical equation with the smallest whole number coefficients possible (from IM3).

R5: If the inputted equation is infeasible, output a descriptive message. [Should this go before R4? —SC]

R6: If the inputted equation is feasible, output a balanced form of the equation in the same format as the input, using the coefficients from IM3.

5.2 Nonfunctional Requirements

NFR1: **Accuracy:** Computed solutions should have a relative error no greater than 0.1%, since the most finely-calibrated chemistry equipment has a relative error of 0.1-0.2% [19, 20]. This means that computed integers should be exact.

NFR2: **Understandability:** A new intended user (as described by User Characteristics) should be able to learn how to use ChemCode in an acceptable amount of time, as measured by the procedure in Section X of the Verification and Validation (VnV) Plan.

NFR3: **Usability:** An intended user (as described by User Characteristics) should find ChemCode easy to use, as measured by the procedure in Section X of the VnV Plan.

NFR4: **Maintainability:** The traceability between requirements, assumptions, theoretical models, general definitions, data definitions, instance models, likely changes, and unlikely changes is completely recorded in traceability matrices in the SRS.

NFR5: **Portability:** ChemCode should be able to run on systems with the corresponding programming language installed, including systems running on Windows or macOS. The tests from the VnV Plan should pass in these environments.

NFR6: **Verifiability:** ChemCode is tested following the VnV Plan.

6 Likely Changes

LC1: The user will be able to input complex chemical formulas, such as hydrates (see Terminology and Definitions) or those with polymers or isotopes (A4).

LC2: Given the amount of one substance in a reaction (in moles), ChemCode will be able to calculate the amount of every other substance in the reaction (also in moles).[1]

LC3: Given the amount of each reactant (in moles) in a reaction, ChemCode will be able to determine the limiting reactant(s).[1]

LC4: Given the amount of each [Is "each" a requirement? —SC] reactant (in moles) in a reaction, ChemCode will be able to calculate the theoretical yield of each product (also in moles).[1] This is dependent on LC3.

LC5: Given the amount of each [Is "each" a requirement? —SC] reactant (in moles) in a reaction, ChemCode will be able to calculate the amount of excess reactant(s) (also in moles).[1] This is dependent on LC3.

[1] These examples of problems related to chemical equations were taken from [9].

LC6: ChemCode will be able to parse valid but incorrectly-formatted chemical formulas inputted by the user and format them correctly when outputting them (A3).

LC7: For ease of use, the user will be able to enter the amounts required by LC2, LC3, LC4, and LC5 in terms of mass.[1]

LC8: ChemCode will be able to classify a chemical reaction as "combination (or synthesis), decomposition, combustion, single replacement, ... double replacement" [9, p. 301] or some combination of these.[1]

LC9: ChemCode will allow the user to input phase labels.[1]

LC10: ChemCode will be able to identify the phase labels for compounds, which will involve determining solubility.[1] This is dependent on LC9.

LC11: ChemCode will be able to identify when a reaction will not take place.[1] This is dependent on LC10.

7 Unlikely Changes

LC12: [Give the unlikely changes. The design can assume that the changes listed will not occur. —TPLT] [Is this supposed to be "LC" or "UC"? —SC]

8 Traceability Matrices and Graphs

The purpose of the traceability matrices is to provide easy references on what has to be additionally modified if a certain component is changed. Every time a component is changed, the items in the column of that component that are marked with an "X" may have to be modified as well. Table 4 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 5 shows the dependencies of instance models, requirements, and data constraints on each other. Table 6 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions.

[You will have to modify these tables for your problem. —TPLT]

[The traceability matrix is not generally symmetric. If GD1 uses A1, that means that GD1's derivation or presentation requires invocation of A1. A1 does not use GD1. A1 is "used by" GD1. —TPLT]

[The traceability matrix is challenging to maintain manually. Please do your best. In the future tools (like Drasil) will make this much easier. —TPLT]

The purpose of the traceability graphs is also to provide easy references on what has to be additionally modified if a certain component is changed. The arrows in the graphs represent dependencies. The component at the tail of an arrow is depended on by the component at

	T??	T??	T??	GD1	GD??	DD1	DD??	DD??	DD??	IM??	IM??	IM??	IM??
T??													
T??			X										
T??													
GD1													
GD??	X												
DD1				X									
DD??				X									
DD??													
DD??								X					
IM??					X	X	X				X		
IM??					X		X		X	X			X
IM??		X											
IM??		X	X				X	X	X		X		

Table 4: Traceability Matrix Showing the Connections Between Items of Different Sections

	IM??	IM??	IM??	IM??	4.2.7	R??	R??
IM??		X				X	X
IM??	X			X		X	X
IM??						X	X
IM??		X				X	X
R??							
R??						X	
R??					X		
R??	X	X				X	X
R??	X						
R??		X					
R??			X				
R??				X			
R??			X	X			
R??		X					
R??		X					

Table 5: Traceability Matrix Showing the Connections Between Requirements and Instance Models

	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??	A??
T??	X																		
T??																			
T??																			
GD1		X																	
GD??			X	X	X	X													
DD1							X	X	X										
DD??			X	X						X									
DD??																			
DD??																			
IM??											X	X		X	X	X			X
IM??												X	X			X	X	X	
IM??														X					X
IM??													X					X	
LC??				X															
LC??								X											
LC??									X										
LC??											X								
LC??												X							
LC??															X				

Table 6: Traceability Matrix Showing the Connections Between Assumptions and Other Items

the head of that arrow. Therefore, if a component is changed, the components that it points to should also be changed. Figure **??** shows the dependencies of theoretical models, general definitions, data definitions, instance models, likely changes, and assumptions on each other. Figure **??** shows the dependencies of instance models, requirements, and data constraints on each other.

9 Development Plan

[This section is optional. It is used to explain the plan for developing the software. In particular, this section gives a list of the order in which the requirements will be implemented. In the context of a course this is where you can indicate which requirements will be implemented as part of the course, and which will be "faked" as future work. This section can be organized as a prioritized list of requirements, or it could should the requirements that will be implemented for "phase 1", "phase 2", etc. —TPLT]

10 Values of Auxiliary Constants

[Show the values of the symbolic parameters introduced in the report. —TPLT]

[The definition of the requirements will likely call for SYMBOLIC_CONSTANTS. Their values are defined in this section for easy maintenance. —TPLT]

[The value of FRACTION, for the Maintainability NFR would be given here. —TPLT]

References

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[The following is not part of the template, just some things to consider when filing in the template. —TPLT]
[Grammar, flow and LaTeXadvice:

- For Mac users `*.DS_Store` should be in `.gitignore`
- LaTeX and formatting rules
  - Variables are italic, everything else not, includes subscripts (link to document)
    - Conventions
    - Watch out for implied multiplication
  - Use BibTeX
  - Use cross-referencing
- Grammar and writing rules
  - Acronyms expanded on first usage (not just in table of acronyms)
  - "In order to" should be "to"

—TPLT]
[Advice on using the template:

- Difference between physical and software constraints
- Properties of a correct solution means *additional* properties, not a restating of the requirements (may be "not applicable" for your problem). If you have a table of output constraints, then these are properties of a correct solution.
- Assumptions have to be invoked somewhere
- "Referenced by" implies that there is an explicit reference
- Think of traceability matrix, list of assumption invocations and list of reference by fields as automatically generatable
- If you say the format of the output (plot, table etc), then your requirement could be more abstract

—TPLT]

Appendix — Reflection

The information in this section will be used to evaluate the team members on the graduate attribute of Lifelong Learning. Please answer the following questions:

1. What knowledge and skills will the team collectively need to acquire to successfully complete this capstone project? Examples of possible knowledge to acquire include domain specific knowledge from the domain of your application, or software engineering knowledge, mechatronics knowledge or computer science knowledge. Skills may be related to technology, or writing, or presentation, or team management, etc. You should look to identify at least one item for each team member.

2. For each of the knowledge areas and skills identified in the previous question, what are at least two approaches to acquiring the knowledge or mastering the skill? Of the identified approaches, which will each team member pursue, and why did they make this choice?