

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

Samuel Crawford

February 3, 2023

Contents

1	Reference Material	iv
1.1	Table of Units	iv
1.2	Table of Symbols	iv
1.3	Abbreviations and Acronyms	v
1.4	Mathematical Notation	v
2	Introduction	2
2.1	Purpose of Document	2
2.2	Scope of Requirements	2
2.3	Characteristics of Intended Reader	2
2.4	Organization of Document	3
3	General System Description	3
3.1	System Context	3
3.2	User Characteristics	4
3.3	System Constraints	4
4	Specific System Description	5
4.1	Problem Description	5
4.1.1	Terminology and Definitions	5
4.1.2	Physical System Description	5
4.1.3	Goal Statements	6
4.2	Solution Characteristics Specification	6
4.2.1	Assumptions	7
4.2.2	Theoretical Models	8
4.2.3	General Definitions	9
4.2.4	Data Definitions	10
4.2.5	Data Types	11
4.2.6	Instance Models	12
4.2.7	Input Data Constraints	15
4.2.8	Properties of a Correct Solution	16
5	Requirements	16
5.1	Functional Requirements	16
5.2	Nonfunctional Requirements	17
6	Likely Changes	18
7	Unlikely Changes	18
8	Traceability Matrices and Graphs	18

9 Development Plan	21
10 Values of Auxiliary Constants	21

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 section
	0.2	Add IM for balancing a chemical reaction, along with relevant reference information
Jan. 23, 2023	0.2.1	Add IM for determining if a chemical reaction is feasible, along with relevant reference information
Jan. 25, 2023	0.2.2	Add references between sections for notation and definitions

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
m	length	metre
kg	mass	kilogram
s	time	second
°C	temperature	centigrade
J	energy	joule
W	power	watt ($W = J s^{-1}$)

[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 $Pa = N m^{-2}$ 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	m^2	coil surface area
A_{in}	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

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

[The introduction section is written to introduce the problem. It starts general and focuses on the problem domain. The general advice is to start with a paragraph or two that describes the problem, followed by a “roadmap” paragraph. A roadmap orients the reader by telling them what sub-sections to expect in the Introduction section. —TPLT]

2.1 Purpose of Document

[This section summarizes the purpose of the SRS document. It does not focus on the problem itself. The problem is described in the “Problem Description” section (Section 4.1). The purpose is for the document in the context of the project itself, not in the context of this course. Although the “purpose” of the document is to get a grade, you should not mention this. Instead, “fake it” as if this is a real project. The purpose section will be similar between projects. The purpose of the document is the purpose of the SRS, including communication, planning for the design stage, etc. —TPLT]

2.2 Scope of Requirements

[Modelling the real world requires simplification. The full complexity of the actual physics, chemistry, biology is too much for existing models, and for existing computational solution techniques. Rather than say what is in the scope, it is usually easier to say what is not. You can think of it as the scope is initially everything, and then it is constrained to create the actual scope. For instance, the problem can be restricted to 2 dimensions, or it can ignore the effect of temperature (or pressure) on the material properties, etc. —TPLT]

[The scope section is related to the assumptions section (Section 4.2.1). However, the scope and the assumptions are not at the same level of abstraction. The scope is at a high level. The focus is on the “big picture” assumptions. The assumptions section lists, and describes, all of the assumptions. —TPLT]

2.3 Characteristics of Intended Reader

[This section summarizes the skills and knowledge of the readers of the SRS. It does NOT have the same purpose as the “User Characteristics” section (Section 3.2). The intended readers are the people that will read, review and maintain the SRS. They are the people that will conceivably design the software that is intended to meet the requirements. The user, on the other hand, is the person that uses the software that is built. They may never

read this SRS document. Of course, the same person could be a “user” and an “intended reader.” —TPLT]

[The intended reader characteristics should be written as unambiguously and as specifically as possible. Rather than say, the user should have an understanding of physics, say what kind of physics and at what level. For instance, is high school physics adequate, or should the reader have had a graduate course on advanced quantum mechanics? —TPLT]

2.4 Organization of Document

This document is based on a template from [9], which is itself based on [5, 6].

[This section provides a roadmap of the SRS document. It will help the reader orient themselves. It will provide direction that will help them select which sections they want to read, and in what order. This section will be similar between project. —TPLT]

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 \rightarrow Calculations \rightarrow 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]

[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

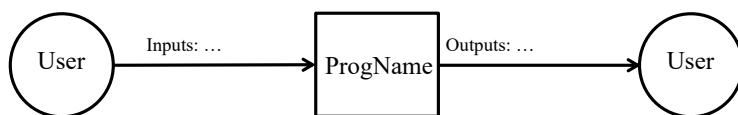


Figure 1: System Context

user will need to assume that responsibility. The list of responsibilities 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

[This section summarizes the knowledge/skills expected of the user. Measuring usability, which is often a required non-function requirement, requires knowledge of a typical user. As mentioned above, the user is a different role from the “intended reader,” as given in Section 2.3. As in Section 2.3, the user characteristics should be specific and unambiguous. For instance, “The end user of ChemCode should have an understanding of undergraduate Level 1 Calculus and Physics.” —TPLT]

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 [10]. 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 [10].

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:

- **Infeasible:** (Referring to a chemical equation) not able to be balanced [11].
- **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” [12].
- **Product:** A substance created by a chemical reaction [10].
- **Reactant:** A substance present at the beginning of, and involved in, a chemical reaction [10].
- **Reduced Row Echelon Form:** A form of a matrix where every row with only zeros is at the bottom and every column but the rightmost one has all zeroes except for one one (which has only zeroes to its left) [13].
- [Should I include “matrix”, “vector”, and/or “augmented matrix”? —SC]

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 infeasible (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]

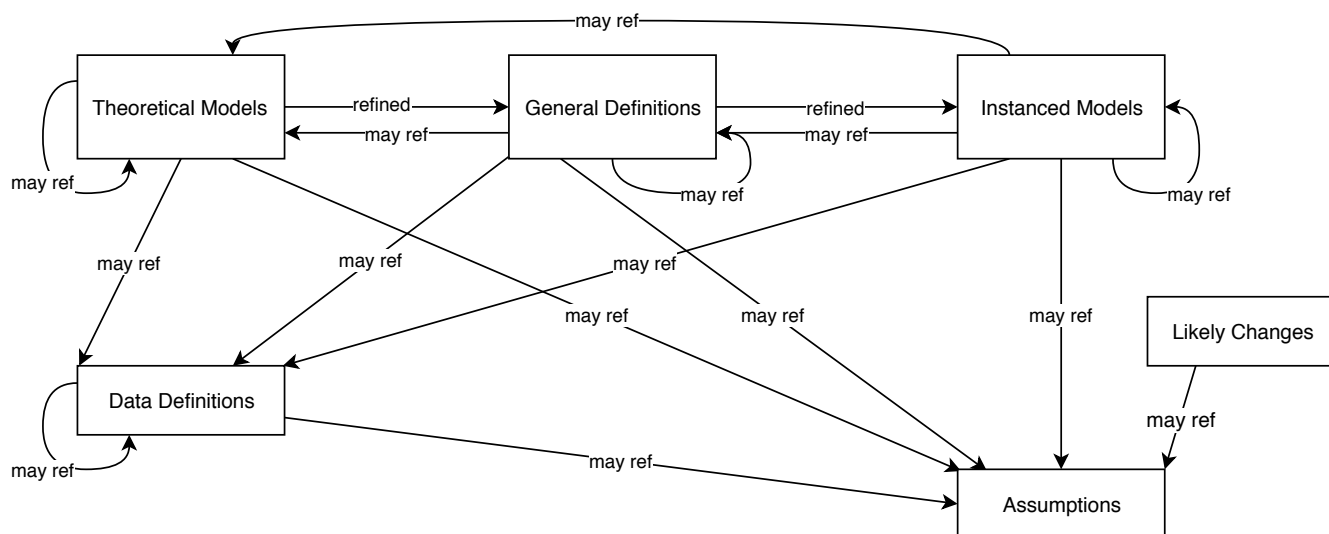
[This section presents the solution characteristics by successively refining models. It starts with the abstract/general Theoretical Models (TMs) and refines them to the concrete/specific Instance Models (IMs). If necessary there are intermediate refinements to General Definitions (GDs). All of these 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: [Short description of each assumption. Each assumption should have a meaningful label. Use cross-references to identify the appropriate traceability to T, GD, DD etc., using commands like dref, ddref etc. Each assumption should be atomic - that is, there should not be an explicit (or implicit) “and” in the text of an assumption. —TPLT]

4.2.2 Theoretical Models

[Theoretical models are sets of abstract mathematical equations or axioms for solving the problem described in Section “Physical System Description” (Section 4.1.2). 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. [Modify the examples below for your problem, and add additional models as appropriate. —TPLT]

RefName: T:COE

Label: Conservation of thermal energy

Equation: $-\nabla \cdot \mathbf{q} + g = \rho C \frac{\partial T}{\partial t}$

Description: The above equation gives the conservation of energy for transient heat transfer in a material of specific heat capacity C ($\text{J kg}^{-1} \text{°C}^{-1}$) and density ρ (kg m^{-3}), where \mathbf{q} is the thermal flux vector (W m^{-2}), g is the volumetric heat generation (W m^{-3}), T is the temperature (°C), t is time (s), and ∇ is the gradient operator. For this equation to apply, other forms of energy, such as mechanical energy, are assumed to be negligible in the system (A??). In general, the material properties (ρ and C) depend on temperature.

Notes: None.

Source: http://www.efunda.com/formulae/heat_transfer/conduction/overview_cond.cfm

Ref. By: GD??

Preconditions for T:COE: None

Derivation for T:COE: Not Applicable

[“Ref. By” is used repeatedly with the different types of information. This stands for Referenced By. It means that the models, definitions and assumptions listed reference the current model, definition or assumption. This information is given for traceability. Ref. By provides a pointer in the opposite direction to what we commonly do. You still need to have a reference in the other direction pointing to the current model, definition or assumption. As an example, if T1 is referenced by G2, that means that G2 will explicitly include a reference to T1. —TPLT]

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	W m^{-2}
Equation	$q(t) = h\Delta T(t)$
Description	<p>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.</p> <p>$q(t)$ is the thermal flux (W m^{-2}).</p> <p>h is the heat transfer coefficient, assumed independent of T (A??) ($\text{W m}^{-2} \text{ } ^\circ\text{C}^{-1}$).</p> <p>$\Delta T(t) = T(t) - T_{\text{env}}(t)$ is the time-dependent thermal gradient between the environment and the object ($^\circ\text{C}$).</p>
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	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 ($^{\circ}\text{C}$). T_W is the temperature of the water ($^{\circ}\text{C}$). The heat flux out of the coil, q_C (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 (m^2) and heat transfer coefficient h_C ($\text{W m}^{-2} ^{\circ}\text{C}^{-1}$). 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	IM1

4.2.5 Data Types

[This section is optional. In many scientific computing programs it isn’t necessary, since the inputs and output 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 [14]. —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” (Section 4.1.2) 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 Section 4.1 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 [reference your goals —TPLT] are solved by [reference your instance models —TPLT]. [other details, with cross-references where appropriate. —TPLT] [Modify the examples below for your problem, and add additional models as appropriate. —TPLT]

Number	IM1
Label	Energy balance on water to find T_W
Input	$m_W, C_W, h_C, A_C, h_P, A_P, t_{\text{final}}, T_C, T_{\text{init}}, T_P(t)$ from IM?? The input is constrained so that $T_{\text{init}} \leq T_C$ (A??)
Output	$T_W(t)$, $0 \leq t \leq t_{\text{final}}$, such that $\frac{dT_W}{dt} = \frac{1}{\tau_W}[(T_C - T_W(t)) + \eta(T_P(t) - T_W(t))]$, $T_W(0) = T_P(0) = T_{\text{init}}$ (A??) and $T_P(t)$ from IM??
Description	T_W is the water temperature ($^{\circ}\text{C}$). T_P is the PCM temperature ($^{\circ}\text{C}$). T_C is the coil temperature ($^{\circ}\text{C}$). $\tau_W = \frac{m_W C_W}{h_C A_C}$ is a constant (s). $\eta = \frac{h_P A_P}{h_C A_C}$ is a constant (dimensionless). The above equation applies as long as the water is in liquid form, $0 < T_W < 100^{\circ}\text{C}$, where 0°C and 100°C are the melting and boiling points of water, respectively (A??, A??).
Sources	Citation here
Ref. By	IM??

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 IM??
Output	$r_{m,n-1} = 0 \wedge r_{m,n} \neq 0$
Description	<p>A is a matrix of coefficients so 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 (see Terminology and Definitions), negative entries indicate the compound is a product, and zeroes indicate the corresponding element is not present in the corresponding compound.</p> <p>R is the $m \times n$ matrix (A 0) as close to reduced row echelon form (see Terminology and Definitions) as possible from IM??. [Is the relationship between R and $r_{m,n-1}$ clear? —SC] [Where should R be defined? —SC]</p> <p>0 is the zero matrix (see Mathematical Notation). [Recursive descriptions? —SC]</p>
Sources	[11] , [15]
Ref. By	IM??

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	Calculation of compound coefficients
Input	A from IM??
Output	x , such that $\mathbf{Ax} = \mathbf{0}$ from IM?? [Is this sufficient? Does matrix multiplication need to be explained? —SC]
Description	A is a matrix of coefficients so 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 (see Terminology and Definitions), negative entries indicate the compound is a product, and zeroes indicate the corresponding element is not present in the corresponding compound. [This description should go with wherever A is defined. —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	[11]
Ref. By	IM??

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	$L > 0$	$L_{\min} \leq L \leq L_{\max}$	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

[The requirements refine the goal statement. They will make heavy use of references to the instance models. —TPLT]

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: [Requirements for the inputs that are supplied by the user. This information has to be explicit. —TPLT]

- R2: [It isn't always required, but often echoing the inputs as part of the output is a good idea. —TPLT]
- R3: [Calculation related requirements. —TPLT]
- R4: [Verification related requirements. —TPLT]
- R5: [Output related requirements. —TPLT]

[Every IM should map to at least one requirement, but not every requirement has to map to a corresponding IM. —TPLT]

5.2 Nonfunctional Requirements

[List your nonfunctional requirements. You may consider using a fit criterion to make them verifiable. —TPLT] [The goal is for the nonfunctional requirements to be unambiguous, abstract and verifiable. This isn't easy to show succinctly, so a good strategy may be to give a "high level" view of the requirement, but allow for the details to be covered in the Verification and Validation document. —TPLT] [An absolute requirement on a quality of the system is rarely needed. For instance, an accuracy of 0.0101 % is likely fine, even if the requirement is for 0.01 % accuracy. Therefore, the emphasis will often be more on describing how well the quality is achieved, through experimentation, and possibly theory, rather than meeting some bar that was defined a priori. —TPLT] [You do not need an entry for correctness in your NFRs. The purpose of the SRS is to record the requirements that need to be satisfied for correctness. Any statement of correctness would just be redundant. Rather than discuss correctness, you can characterize how far away from the correct (true) solution you are allowed to be. This is discussed under accuracy. —TPLT]

- NFR1: **Accuracy** [Characterize the accuracy by giving the context/use for the software. Maybe something like, "The accuracy of the computed solutions should meet the level needed for <engineering or scientific application>. The level of accuracy achieved by ChemCode shall be described following the procedure given in Section X of the Verification and Validation Plan." A link to the VnV plan would be a nice extra. —TPLT]
- NFR2: **Usability** [Characterize the usability by giving the context/use for the software. You should likely reference the user characteristics section. The level of usability achieved by the software shall be described following the procedure given in Section X of the Verification and Validation Plan. A link to the VnV plan would be a nice extra. —TPLT]
- NFR3: **Maintainability** [The effort required to make any of the likely changes listed for ChemCode should be less than FRACTION of the original development time. FRACTION is then a symbolic constant that can be defined at the end of the report. —TPLT]

NFR4: **Portability** [This NFR is easier to write than the others. The systems that ChemCode should run on should be listed here. When possible the specific versions of the potential operating environments should be given. To make the NFR verifiable a statement could be made that the tests from a given section of the VnV plan can be successfully run on all of the possible operating environments. —TPLT]

- Other NFRs that might be discussed include verifiability, understandability and reusability.

6 Likely Changes

LC1: [Give the likely changes, with a reference to the related assumption (aref), as appropriate. —TPLT]

7 Unlikely Changes

LC2: [Give the unlikely changes. The design can assume that the changes listed will not occur. —TPLT]

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 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

	T??	T??	T??	GD1	GD??	DD1	DD??	DD??	DD??	IM1	IM??	IM??	IM??
T??													
T??			X										
T??													
GD1													
GD??	X												
DD1				X									
DD??				X									
DD??													
DD??								X					
IM1					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

	IM1	IM??	IM??	IM??	4.2.7	R??	R??
IM1		X				X	X
IM??	X			X		X	X
IM??						X	X
IM??		X				X	X
R??							
R??						X	
R??					X		
R2	X	X				X	X
R??	X						
R??		X					
R??			X				
R??				X			
R4			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??																			
IM1											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

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

- [1] D. O’Sullivan and D. J. Unwin, “Appendix A: Notation, Matrices, and Matrix Mathematics,” in *Geographic Information Analysis*, pp. 373–394, Hoboken, NJ, USA: Wiley, 2 ed., Mar. 2010.
- [2] E. W. Weisstein, “Zero Matrix,” 2023. Publisher: Wolfram Research, Inc.
- [3] L. J. Latecki, “Matrices,” 2018.
- [4] M. Taboga, “Augmented matrix,” 2021.
- [5] W. S. Smith and L. Lai, “A new requirements template for scientific computing,” in *Proceedings of the First International Workshop on Situational Requirements Engineering Processes – Methods, Techniques and Tools to Support Situation-Specific Requirements Engineering Processes, SREP’05* (J. Ralyté, P. Ågerfalk, and N. Kraiem, eds.), (Paris, France), pp. 107–121, In conjunction with 13th IEEE International Requirements Engineering Conference, 2005.
- [6] W. S. Smith, L. Lai, and R. Khedri, “Requirements analysis for engineering computation: A systematic approach for improving software reliability,” *Reliable Computing, Special Issue on Reliable Engineering Computation*, vol. 13, pp. 83–107, February 2007.
- [7] W. S. Smith, “Systematic development of requirements documentation for general purpose scientific computing software,” in *Proceedings of the 14th IEEE International Requirements Engineering Conference, RE 2006*, (Minneapolis / St. Paul, Minnesota), pp. 209–218, 2006.
- [8] W. S. Smith, J. McCutchan, and J. Carette, “Commonality analysis for a family of material models,” Technical Report CAS-17-01-SS, McMaster University, Department of Computing and Software, 2017.
- [9] W. S. Smith, “capTemplate,” Sept. 2022.
- [10] L. Lund and Anoka-Ramsey Community College, *Introduction to Chemistry*. Cambridge and Coon Rapids, MN, USA: LibreTexts, Jan. 2023.
- [11] I. Hamid, “Balancing Chemical Equations by Systems of Linear Equations,” *Applied Mathematics*, vol. 10, pp. 521–526, July 2019.
- [12] The Editors of Encyclopaedia Britannica, “nonstoichiometric compound,” Oct. 2010.
- [13] M. Taboga, “Reduced row echelon form,” 2021.
- [14] D. M. Hoffman and P. A. Strooper, *Software Design, Automated Testing, and Maintenance: A Practical Approach*. New York, NY, USA: International Thomson Computer Press, 1995.

- [15] R. Pramoditha, “How do you use NumPy, SciPy and SymPy to solve Systems of Linear Equations?,” Sept. 2021.

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

[Grammar, flow and L^AT_EX advice:

- For Mac users *.DS_Store should be in .gitignore
- L^AT_EX 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?