Software Requirements Specification for Mass-Mass Stoichiometry Problem

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Contents

Revision History

Date	Version	Notes
07/10/2019	1.0	First version of document
28/10/2019	2.0	Second version of document
19/12/2019	3.0	Third version of document

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
g	mass	gram
g/mol	molecular weight	gram/mole
mol	mole ratio	mole

Table 1: Table of Units.

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 stoichiometry literature and with existing documentation for stoichiometry mass-mass program. The symbols are listed in alphabetical order.

symbol	**unit**	**description**
mass	g	mass.
mw	g/mol	molecular weight.

1.3 Abbreviations and Acronyms

symbol	description
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
SMMP	Stoichiometry Mass-Mass Program
T	Theoretical Model
B	Boolean result
R[0]	Reactant
R1	Reactant with known mass
R2	Reactant with unknown mass
R[1]	product

Table 2: Abbreviations and Acronyms

2 Introduction

2.1 Purpose of Document

The purpose of this document is to describe the requirements for Stoichiometry Mass-Mass Program. A software product that will produce a mass for unknown reactant in chemical reaction. The goal statements and theoretical models used in the SMMP code are provided, with an emphasis on explicitly identifying assumptions and unambiguous definitions. This document is intended to be used as a reference to provide ad hoc access to all information necessary to understand and verify the model. The SRS is abstract because the contents say what problem is being solved, but do not say 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 plan. The design document will show how the requirements are to be realized, including decisions on the numerical algorithms and programming environment. The verification and validation 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 [1], the most

logical way to present the documentation is still to "fake" a rational design process.

2.2 Scope of Requirements

The scope of SMMP is limited to get the mass of unknown reactant in chemical reaction.

2.3 Characteristics of Intended Reader

Reviewers of this documentation should have a background on Chemistry. Especially on chemical reactions and stoichiometry.

2.4 Organization of Document

The organization of this document follows the template for an SRS for scientific computing software proposed by [2] and [3]. 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 in Section: Instance Models and trace back to find any additional information they require.
The goal statements 4.1.3 are refined to the theoretical models and the theoretical models 4.2.3 to the instance models 4.2.6.

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.

3.1 System Context

Figure 1 shows the system context. A circle represents an external entity outside the software, the user in this case. A rectangle represents the software system itself (SMMP). Arrows are used to show the data flow between the system and its environment. SMMP is mostly self-contained. The only external interaction is through the user interface. The responsibilities of the user and the system are as follows:

- User Responsibilities:
  - Ensure the inputs are correct.
  - Ensure that all chemical reaction's elements entered are belong to chemical substances group.
  - Take care that consistent units are used for input variables.
- SMMP Responsibilities:

Figure 1: System Context

- Detect data type mismatch, such as a string of characters instead of a floating point number.
- Determine if the inputs satisfy the required physical and software constraints.
- Produce an error message in case input does not satisfy physical and software constraints.
- Do the necessary calculations to get the final result.
- Display the result to the end user.

3.2 User Characteristics

The end user of SMMP should have some basic knowledge on chemical stoichiometry.

3.3 System Constraints

There are no system constraints.

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.

4.1 Problem Description

SMMP is intended to solve Mass-Mass Stoichiometry problem in any chemical reaction.

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:

- Stoichiometry: Is the relationship between reactants and products in chemical reactions.
- Chemical reaction: Is a process that leads to the chemical transformation of one set of chemical substances to another.
- Reactant: A substance that takes part in and undergoes change during a reaction.
- Product: Is the substance formed from chemical reactions.
- Mole Ratio: Ratio of moles between any two compounds involved in chemical reaction.
- Coefficients: Is the number of molecules (or atoms) involved in the reaction.
- Molecular weight (Molar mass) : A measure of the sum of the atomic weight values of the atoms in a molecule.
- Molecule: A chemical reactant or product consist of chemical element with more than one atom.
- Compound: Molecule made up of two or more elements.

4.1.2 Physical System Description

The physical system of SMMP, as shown in Figure 2, includes the following elements:

PS1: Reactants mass.

PS2: Reactants mole ratio.

PS3: Reactants mole amount.

PS4: Reactants Molecular weight (molar mass).

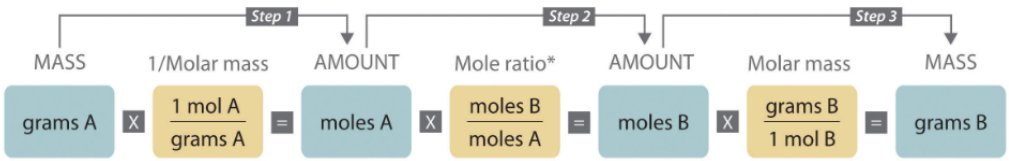

Figure 2: Physical representation of SMMP.

4.1.3 Goal Statements

Given unbalanced chemical reaction with sets of reactants and products , the goal statement are:

GS1: Balance the chemical reaction.

GS2: Get the mass of one of unknown reactant.

4.2 Solution Characteristics Specification

The instance models that govern SMMP 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

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 type definition[TD], theoretical model [T], general definition [GD], data definition [DD], instance model [IM], or likely change [LC], in which the respective assumption is used.

A1: Chemical reaction with two chemical reactants. [T1, DD9, DD10, DD11, R1, R3, NF4, ULC2].

A2: Chemical reactant could be single element, molecule or Compound with two elements. [DD1, DD3, DD4, DD5, DD6, DD7, DD9, DD10, DD12, IM1, R1, R3, NF1, NF4]

A3: Chemical product could be single element, molecule or compound with two elements. [DD3, DD4, DD5, DD6, DD7, DD9, DD10, IM1, R1, R2, R3, NF1, NF4, LC2]

A4: Known mass of one chemical reactant. [IM2, IM4, R1, R2, R3, R4, NF1, NF2]

A5: Known mass entered in g unit. [IM2, R1, R2, R3, R4, NF1, NF2, NF4, ULC1]

4.2.2 Type Definition

This section focuses on the general variable's types that SMMP is based on.

TD1: ElementT = $\forall$ e $\in$ set of chemical element = { H,He,Li,Be,B,C,N,O,F,Ne,Na,Mg,Al,Si,P,S,Cl,Ar,K, Ca,Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu,Zn,Ga,Ge,As,Se,Br,Kr,Rb,Sr,Y,Zr,Nb,Mo,Tc,Ru,Rh,Pd,Ag,Cd,In, Sn,Sb,Te,I,Xe,Cs,Ba,La,Ce,Pr,Nd,Pm,Sm,Eu,Gd,Tb,Dy,Ho,Er,Tm,Yb,Lu,Hf,Ta,W,Re,Os,Ir,Pt, Au,Hg,Tl,Pb,Bi,Po,At,Rn,Fr,Ra,Ac,Th,Pa,U,Np,Pu,Am,Cm,Bk,Cf,Es,Fm,Md,No,Lr,Rf,Db,Sg, Bh,Hs,Mt,Ds,Rg,Cn,Nh,Fl,Mc,Lv,Ts,Og }

TD2: MoleculeT = tuple of (number : $\mathbb{N}$, element : ElementT).

TD3: CompoundT = set of MoleculeT.

TD4: StoichiometricT = tuple of (coefficient : $\mathbb{N}$, Compound : CompoundT)

TD5: ChemicalEqT = set of StoichiometricT

TD6: ReactionT = sequence [2] of ChemicalEq.

4.2.3 Theoretical Models

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

Number	T1
Label	**Law of Conservation of Mass**
Equation	$\sum$ mass for $R = \sum$ mass for P.
Description	The above equation states that there is no change in total mass occurs in a chemical reaction. The total number of products mass is equal to the total number of reactants mass.
Source	[4]
Ref. By	IM1

4.2.4 General Definitions

N.A

4.2.5 Data Definitions

This section collects and defines all the data needed to build the instance models. The dimension of each quantity is also given.

Number	DD1
Label	**Atomic Mass.**
Symbol	-
SI Units	-
Equation	AtomicMass: ElementT $\rightarrow \mathbb{R}$
Description	AtomicMass(e) $\equiv$ ($e = \text{H} \rightarrow 1.0079 \mid e = \text{He} \rightarrow 4.002 \mid ...$) Where e is an element $\in$ ElementT The function will take the element(e) and return the number of atomic mass of that element.
Sources	[5]
Ref. By	DD12

Number	DD2
Label	**Count number of atoms in Molecule**
Symbol	-
SI Units	-
Equation	Number-of-Atoms-in-Molecule: MoleculeT $\times$ ElementT $\rightarrow \mathbb{N}$
Description	Number-of-Atoms-in-Molecule(m,e) $\equiv$ (m.element $= e \rightarrow m$.number $\mid$ m.element $\neq e \rightarrow 0$) Where e is an element $\in$ ElementT m is a molecule $\in$ MoleculeT The function will compare the molecule(m) with element(e) if they are equal it returns the number of atoms in that element else it will return 0
Sources	[6]
Ref. By	DD3

Number	DD3
Label	**Count number of atoms in compound**
Symbol	-
SI Units	-
Equation	Number-of-Atoms-in-Compound: CompoundT $\times$ ElementT $\rightarrow \mathbb{N}$
Description	Number-of-Atoms-in-Compound $(C,e) \equiv +$ $(m :$ MoleculeT $\mid m \in C \cdot$ Number-of-Atoms-in-Molecule(m,e) $)$ Where e is an element $\in$ ElementT m is a molecule $\in C$ C is the compound. The function will take all set of molecules$(m) \in$ compound(C) and apply Number-of-Atoms-in-Molecule(m,e) function on them then add them together.
Sources	[6]
Ref. By	DD4

Number	DD4
Label	**Count number of atoms in Stoichiometric**
Symbol	-
SI Units	-
Equation	Number-of-Atoms-in-Stoichiometric: StoichiometricT $\times$ ElementT $\rightarrow \mathbb{N}$
Description	Number-of-Atoms-in-Stoichiometric$(S,e) \equiv$ $(S.$coefficient $\cdot$ Number-of-Atoms-in-Compound$(S.$Compound$,e)$ $)$ Where $S \in$ StoichiometricT *coefficient* $\in$ StoichiometricT C is the compound $\in$ StoichiometricT The function will take the compound(C) and get Number-of-Atoms-in-Compound(C) then multiply it with compound coefficient.
Sources	[6]
Ref. By	DD5

Number	DD5
Label	**Count number of atoms in one side of chemical reaction**
Symbol	-
SI Units	-
Equation	Number-of-Atoms-in-ChemicalEq: ChemicalEqT $\times$ ElementT $\rightarrow \mathbb{N}$
Description	Number-of-Atoms-in-ChemicalEq $(Ce, e) \equiv +$ $(S :$ StoichiometricT $\mid S \in Ce \cdot$ Number-of-Atoms-in-Stoichiometric$(S, e))$ Where $S \in$ StoichiometricT $S \in Ce$ Ce is one side of chemical equation. The function will take each Stoichiometric$(S) \in$ ChemicalEq(Ce) and apply number-of-Atoms-in-Stoichiometric(S, e) function on it then add them together.
Sources	[7]
Ref. By	DD8

Number	DD6
Label	**Elements of a compoundT**
Symbol	-
SI Units	-
Equation	ElementsInCompoundT : CompoundT $\rightarrow$ set of ElementT.
Description	ElementsInCompound$(C) \equiv \cup \{ m :$ MoleculeT $\mid m \in C \cdot m$.element$\}$ where C is the compound. m is Molecule $\in C$. The function will take each Molecule in Compound(C) and return its element then apply union to all molecules $\in C$.
Sources	[6]
Ref. By	DD7

Number	DD7
Label	**Elements of a ChemicalEq**
Symbol	-
SI Units	-
Equation	ElementsInChemicalEq : ChemicalEqT $\rightarrow$ set of ElementT.
Description	ElementsInChemicalEq(Ce) $\equiv \cup \{ C : \text{CompoundT} \mid C \in Ce \cdot \text{ElementsInCompound}(C)\}$ where C is the compound $\in Ce$. ChemicalEq(Ce) is one side of chemical equation The function will take each compound in ChemicalEq(Ce) and return its elements then apply union to all compound $\in Ce$.
Sources	[7]
Ref. By	DD9

Number	DD8
Label	**Balanced reaction for an element**
Symbol	-
SI Units	-
Equation	IsBalancedReactionForElement : ReactionT $\times$ ElementT $\rightarrow$ B
Description	IsBalancedReactionForElement (R, e) $\equiv$ Number-of-Atoms-in-ChemicalEq($R[0]$,e) = Number-of-Atoms-in-ChemicalEq ($R[1]$,e) Where $R[0]$ is the reactant on the left side of chemical reaction. $R[1]$ is reactant on the right side of chemical reaction called "products" R is a reaction The function will take one reactant $\in$ chemical reaction and check if it balanced or not.
Sources	[8].
Ref. By	DD9

Number	DD9
Label	**Balanced reaction**
Symbol	-
SI Units	-
Equation	IsBalancedReaction : ReactionT $\rightarrow$ B
Description	IsBalancedReaction(R) $\equiv$ $\forall$ (e : ElementT $\mid$ $e \in$ ElementsInChemicalEq($R[0]$) $\cdot$ IsBalancedReactionForElement(R, e)) Where $R[0]$ is the reactant $\in$ R. R is reaction The function will take each reactant in Reaction and return if its balanced or not. if all reactants $\in$ R is balanced then R is balanced.
Sources	[8].
Ref. By	IM1

Number	DD10
Label	**Coefficient**
Symbol	-
SI Units	-
Equation	AreAllCoefficientOnes : ChemicalEqT $\rightarrow$ B
Description	AreAllCoefficientOnes(Ce) $\equiv$ $\forall$ (C : CompoundT | $C \in Ce$ · $Ce.coefficient$=1) The function will take every coefficient in compound $\in$ ChemicalEqReaction and return if its equal to 1 or not. where ChemicalEq(Ce) is one side of chemical equation
Sources	[9]
Ref. By	IM1

Number	DD11
Label	**Mole ratio**
Symbol	–
SI Units	mol
Equation	Mole ratio: CompoundT $\rightarrow \mathbb{N}$
Description	Mole ratio $\equiv \div($ C : CompoundT | $C \in Ce \cdot Ce$.coefficient) The above function will take the coefficient for each compound in the ChemicalEq and divide them together. where ChemicalEq(Ce) is one side of chemical reaction.
Sources	[10].
Ref. By	IM3.

Number	DD12
Label	**molecular weight**
Symbol	mw
SI Units	g/mol
Equation	mw : CompoundT $\rightarrow \mathbb{R}$
Description	$mw(C)$: + (m : MoleculeT | $m \in C \cdot$ Number-of-Atoms-in-Molecule(m,e) $\times$ AtomicMass(m,e) where mw is the molecular weight of reactant . It is computed by multiplying the AtomicMass for the molecule with the Number-of-Atoms-in-Molecule. If the reactant is compound it will take the add all its Molecule's molecular weight.
Sources	[11]
Ref. By	IM2 , IM4

4.2.6 Instance Models

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 4.2.5 to replace the abstract symbols in the models identified in Sections 4.2.3 and 4.2.4.

The goals 1 and 2 are solved by 4.2.6.

Number	IM1
Label	**balanced chemical reaction**
Input	Reaction
Output	Reaction*
Description	Reaction is ReactionT such that AreAllCoefficientOnes(R[0]) $\wedge$ AreAllCoefficientOnes(R[1]) Reaction* is same as Reaction, but with coefficients changed such that IsBalancedReaction(R*).
Sources	[8]
Ref. By	GS1

Number	IM2
Label	**Converting mass to mole**
Input	$mass$, mw
Output	$mole = \frac{mass}{mw}$
Description	$mass$ is the substance mass. mw is the substance molecular weight. The above equation gives the amount of mole for particular substance by dividing the mass amount with molecular weight.
Sources	[12]
Ref. By	IM3

Number	IM3
Label	**Converting mole ratio to mole.**
Input	*mole-of-R1* , *mole-ratio*.
Output	*mole amount of R2* $= \frac{\textit{mole-of-R1}}{\textit{mole-ratio}}$
Description	*mole-of-R1* is the mole amount for known reactant. *mole-ratio* is the mole ratio between *R1* and *R2*. The above equation gives the amount of mole for R2 substance by dividing the mole amount of *R1* with the *mole-ratio*.
Sources	[13]
Ref. By	IM4

Number	IM4
Label	**Converting mole to mass**
Input	mole amount , *mw*
Output	$mass = mole \times mw$
Description	*mole* is the mole amount for the substance. *mw* is the substance molecular weight. The above equation gives the mass for substance by multiplying the mole amount with the molecular weight .
Sources	[13]
Ref. By	GS2

4.2.7 Input Data Constraints

Table 3 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.

Table 3: Input Variables

Var	Physical Constraints	Software Constraints	Typical Value	Uncertainty
mass	$mass > 0$	-	-	-

4.2.8 Properties of a Correct Solution

Table 4 shows the data constraints on the output variables. The column for physical constraints gives the physical limitations on the range of values that can be taken by the variable.

Table 4: Output Variables

Var	Physical Constraints
mass	$mass > 0$
atoms	$\sum$ atoms for *R[0]*= $\sum$ atoms for *R[1]*.

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: The system will use the following inputs:
1- Unbalanced chemical reaction.
2- Mass of R1.

R2: The system will produce the followings:
1- Balanced chemical reaction.
2- Mass for R2.

R3: The system needs to calculate the followings:
1- number of atoms used in each reactant and product.
2- Coefficients needed for balance chemical reaction.
3- molecular weight for R1, R2.
4- Mole amount for R1.
5- Mole ratio between R1 and R2.
6- Mole amount for R2.

R4: The system will verify the followings:
1- Output is correct.
2- Inputs satisfy the required physical constraints.
3- Mass Conservation Low applied in the chemical reaction.
4- No integer overflow.
5- Outputs satisfy the required output constraints.

5.2 Nonfunctional Requirements

This section provides the non-functional requirements, the qualities that the software is expected to exhibit.

NF1: The ability to provide a correct Solution.

NF2: The ability to test and verify the system.

NF3: The system is understandable for novel users without any ambiguities.

NF4: The system could be used for different applications and modified easily.

6 Likely Changes

LC1: The system may ask the the user enter the molecular weight of the reactants.

LC2: The system may ask the user to enter balance chemical reaction.

7 Unlikely Changes

ULC1: The units used in the system will not likely to be change.

ULC2: The system will not change the number of entered reactants.

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 5 shows the dependencies of theoretical models, general definitions, data definitions, instance models, and likely changes on the assumptions. Table 6 shows the dependencies of theoretical models, general definitions, data definitions, and instance models with each other. Table 7 shows the dependencies of instance models, requirements, and data constraints on each other.

	A1	A2	A3	A4	A5
T1	X				
DD1		X			
DD2					
DD3		X	X		
DD4		X	X		
DD5		X	X		
DD6		X	X		
DD7		X	X		
DD8					
DD9	X	X	X		
DD10	X	X	X		
DD11	X				
DD12		X			
IM1		X	X		
IM2				X	X
IM3					
IM4				X	
R1	X	X	X	X	X
R2			X	X	X
R3	X	X	X	X	X
R4				X	X
NF1		X	X	X	X
NF2				X	X
NF3					
NF4	X	X	X		X
LC1					
LC2			X		
ULC1					X
ULC2	X				

Table 5: Traceability Matrix Showing the Connections Between Assumptions and Other Items

	T1	DD1	DD2	DD3	DD4	DD5	DD6	DD7	DD8	DD9	DD10	DD11	DD12	IM1	IM2	IM3	IM4
T1														X			
DD1			X	X			X										
DD2		X		X			X										
DD3		X	X		X												
DD4				X		X											
DD5					X			X									
DD6		X	X	X				X									
DD7						X	X		X								
DD8							X		X								
DD9									X		X			X			
DD10										X		X		X			
DD11											X					X	
DD12		X	X	X											X		X
IM1	X								X	X							
IM2													X				
IM3													X		X		
IM4													X			X	

Table 6: Traceability Matrix Showing the Connections Between Items of Different Sections

	IM1	IM2	IM3	IM4	4.2.7	R1	R2	R3	R4
IM1			X		X	X	X		X
IM2			X		X	X		X	X
IM3	X	X		X				X	
IM4			X					X	
R1	X	X			X		X	X	X
R2	X			X	X	X		X	X
R3	X	X	X	X		X		X	
R4	X			X	X	X	X	X	

Table 7: Traceability Matrix Showing the Connections Between Requirements and Instance Models

9 Values of Auxiliary Constants

NA

References

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