Module Interface Specification for Stoichiometry Mass-Mass Program

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1 Revision History

Date	**Version**	**Notes**
Date 1	1.0	First version of document

2 Symbols, Abbreviations and Acronyms

See SRS Documentation here

Contents

3 Introduction

The following document details the Module Interface Specifications for Stoichiometry Mass-Mass Program

Complementary documents include the System Requirement Specifications and Module Guide. The full documentation and implementation can be found here

4 Notation

The structure of the MIS for modules comes from **?**, with the addition that template modules have been adapted from **?**. The mathematical notation comes from Chapter 3 of **?**. For instance, the symbol := is used for a multiple assignment statement and conditional rules follow the form $(c_1 \Rightarrow r_1 | c_2 \Rightarrow r_2 | ... | c_n \Rightarrow r_n)$.

The following table summarizes the primitive data types used by SMMP.

Data Type	**Notation**	**Description**
character	char	a single symbol or digit
integer	$\mathbb{Z}$	a number without a fractional component in (-∞, ∞)
natural number	$\mathbb{N}$	a number without a fractional component in [1, ∞)
real	$\mathbb{R}$	any number in (-∞, ∞)

The specification of SMMP uses some derived data types: sequences, strings, and tuples. Sequences are lists filled with elements of the same data type. Strings are sequences of characters. Tuples contain a list of values, potentially of different types. In addition, SMMP uses functions, which are defined by the data types of their inputs and outputs. Local functions are described by giving their type signature followed by their specification.
Since chemical reaction is central to SMMP, the following notation is introduced in an attempt to simplify the presentation of the MIS.

Chemical reaction:

$$c_1 R[0]_1 + c_2 R[0]_2 = cc_1 R[1]_1 + cc_2 R[1]_2$$

where $R[0]_1$ is reactant with known mass, c_1 is the coefficient number associated to this reactant , $R[0]_2$ is reactant with unknown mass, c_2 is the coefficient number associated to this reactant , $R[1]_i$ is a product and cc_i is he coefficient number associated to this product.

5 Module Decomposition

The following table is taken directly from the Module Guide document for this project.

Level 1	**Level 2**
Hardware-Hiding	
Behaviour-Hiding	Input Module Atomic Mass Module Chemical Reaction Balancing Module Mass Calculation Module
Software Decision	GUI Module

Table 1: Module Hierarchy

6 MIS of Input Module

6.1 Module

Input

6.2 Uses

Not Applicable.

6.3 Syntax

6.3.1 Exported Constants

None.

6.3.2 Exported Types

ReactionT = ?

6.3.3 Exported Access Programs

Name	**In**	**Out**	**Exceptions**
$input_1$	chemical reaction: ReactionT	-	-
$input_2$	Mass: $\mathbb{R}$	-	-

6.4 Semantics

Not Applicable.

7 MIS of Atomic Mass Module

7.1 Module

Atomic Mass

7.2 Uses

Balancing (Section 8)

7.3 Syntax

7.3.1 Exported Constants

None.

7.3.2 Exported Types

ElementT = ?

7.3.3 Exported Access Programs

Name	**In**	**Out**	**Exceptions**
Atomic-Mass	element: ElementT	Atomic-Mass: $\mathbb{R}$	element $\notin$ ElementT

7.4 Semantics

7.4.1 State Variables

1. e: ElementT
2. Atomic-Mass: $\mathbb{R}$

7.4.2 Environment Variables

Atomic Mass library file.

7.4.3 Assumptions

None.

7.4.4 Access Routine Semantics

(Atomic Mass):

- transition: None.
- output: AtomicMass $:=$ $\mathbb{R}$
- exception: if (e $\notin$ ElementT) $\rightarrow$ no-Atomic-Mass

7.4.5 Local Functions

AtomicMass: ElementT $\rightarrow$ $\mathbb{R}$
AtomicMass(e) $\equiv$ (e= H $\rightarrow$ 1.0079 | e= He $\rightarrow$ 4.002 |...)

8 MIS of Chemical Reaction Balancing Module

8.1 Template Module

Balancing

8.2 Uses

Input (Section 6)

8.3 Syntax

8.3.1 Exported Constants

None.

8.3.2 Exported Types

ElementT = ∀ e ∈ 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 }

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

CompoundT = set of MoleculeT.

StoichiometricT = tuple of (coefficient : N , Compound : CompoundT)

ChemicalEqT = set of StoichiometricT

ReactionT = sequence [2] of ChemicalEq.

8.3.3 Exported Access Programs

Name	In	Out	Exceptions
Molecule's atoms	Molecule: MoleculeT	Number-of-Atoms: $\mathbb{N}$	-
compound's atoms	Compound: CompoundT	Number-of-Atoms: $\mathbb{N}$	-
Elements of a compound	Compound: CompoundT	set of Element: ElementT	-
number of atoms in ChemicalEq	Compound: CompoundT coefficient : $\mathbb{N}$	Number-of-Atoms: $\mathbb{N}$	-
Elements of a ChemicalEq	ChemicalEq: ChemicalEqT	set of Element: ElementT	-
Balanced reaction for an element	Reaction: ReactionT Element: ElementT	B: Boolean	number of atoms in each side for one element is not equal
Balanced reaction	Reaction: ReactionT	B: Boolean	number of atoms in each side for all element is not equal
balanced chemical reaction	Reaction: ReactionT	Reaction*: ReactionT	number of atoms in each side for all element is not equal

8.4 Semantics

8.4.1 State Variables

e: ElementT
m : MoleculeT
C: CompoundT
S: StoichiometricT

Ce: ChemicalEq
R: ReactionT

8.4.2 Environment Variables

None.

8.4.3 Assumptions

None.

8.4.4 Access Routine Semantics

(Number-of-Atoms-in-Molecule):

- transition: None.
- output: Number-of-Atoms-in-Molecule $:= \mathbb{N}$
- exception: None

(Number-of-Atoms-in-Compound):

- transition: None.
- output: Number-of-Atoms-in-Compound $:= \mathbb{N}$
- exception: None

(Number-of-Atoms-in-Stoichiometric):

- transition: None.
- output: Number-of-Atoms-in-Stoichiometric $:= \mathbb{N}$
- exception: None

(Number-of-Atoms-in-ChemicalEq):

- transition: None.
- output: Number-of-Atoms-in-ChemicalEq $:= \mathbb{N}$
- exception: None

(ElementsInCompoundT):

- transition: None.
- output: set of ElementT

- exception: None

(Elements of a ChemicalEq):

- transition: None.
- output: set of ElementT
- exception: None

(Balanced reaction for an element):

- transition: None
- output: if (Number-of-Atoms-in-ChemicalEq(R[0],e) = Number-of-Atoms-in-ChemicalEq (R[1] ,e)) then True
  if (Number-of-Atoms-in-ChemicalEq(R[0],e) $\neq$ Number-of-Atoms-in-ChemicalEq (R[1] ,e)) then False
- exception: None

(Balanced reaction):

- transition: None.
- output: if $\forall$(Number-of-Atoms-in-ChemicalEq(R[0],e) = Number-of-Atoms-in-ChemicalEq (R[1] ,e)) then True
  if $\exists$(Number-of-Atoms-in-ChemicalEq(R[0],e) $\neq$ Number-of-Atoms-in-ChemicalEq (R[1] ,e)) then False
- exception: None

8.4.5 Local Functions

1. Number-of-Atoms-in-Molecule: MoleculeT X ElementT $\rightarrow \mathbb{N}$
Number-of-Atoms-in-Molecule(m,e) $\equiv$ (m.element = e $\rightarrow$ m.number | m.element $\neq$ e $\rightarrow$ 0)

2. Number-of-Atoms-in-Compound: CompoundT X ElementT $\rightarrow \mathbb{N}$
Number-of-Atoms-in-Compound(C,e) $\equiv$ + (m : MoleculeT| m $\in$ C $\cdot$ Number-of-Atoms-in-Molecule(m,e))

3. Number-of-Atoms-in-Stoichiometric: StoichiometricT $\times$ ElementT $\rightarrow \mathbb{N}$
Number-of-Atoms-in-Stoichiometric(S,e) $\equiv$ (S.coefficient $\cdot$ Number-of-Atoms-in-Compound (S.Compound,e))

4. Number-of-Atoms-in-ChemicalEq: ChemicalEqT X ElementT $\rightarrow \mathbb{N}$

Number-of-Atoms-in-ChemicalEq (Ce,e) ≡ + (S : StoichiometricT | S ∈ Ce · Number-of-Atoms-in-Stoichiometric(S,e))

5. ElementsInCompoundT : CompoundT → set of ElementT.
ElementsInCompound(C) ≡ ∪ { m : MoleculeT | m ∈ C · m.element}

6. ElementsInChemicalEq : ChemicalEqT → set of ElementT.
ElementsInChemicalEq(Ce) ≡ ∪ { C : CompoundT | C ∈ Ce · ElementsInCompound(C)}

7. IsBalancedReactionForElement : ReactionT x ElementT → B
IsBalancedReactionForElement (R, e) ≡ Number-of-Atoms-in-ChemicalEq(R[0],e) = Number-of-Atoms-in-ChemicalEq (R[1] ,e)

8. IsBalancedReaction : ReactionT → B
IsBalancedReaction(R) ≡ ∀ (e : ElementT | e ∈ ElementsInChemicalEq(R[0]) · IsBalancedReactionForElement(R, e))

9 MIS of Mass Calculation Module

9.1 Module

Mass

9.2 Uses

Balancing (Section 8) , Atomic Mass (Section 7)

9.3 Syntax

9.3.1 Exported Constants

None.

9.3.2 Exported Access Programs

Name	In	Out	Exceptions
Molecular weight	Atomic-Mass: $\mathbb{R}$ Number-of-Atoms-in-Compound: $\mathbb{N}$	Molecular-weight:$\mathbb{R}$	-
mole-ratio	coefficient1 : $\mathbb{N}$ coefficient2 : $\mathbb{N}$	mole-ratio: $\mathbb{N}$	-
$mole_1$	mass : $\mathbb{R}$ Molecular-weight: $\mathbb{R}$	mole: $\mathbb{R}$	-
$mole_2$	mole1: $\mathbb{R}$ mole-ratio: $\mathbb{R}$	mole2: $\mathbb{R}$	-
mass	mole2: $\mathbb{R}$ Molecular-weight: $\mathbb{R}$	mass:$\mathbb{R}$	-

9.4 Semantics

9.4.1 State Variables

None

9.4.2 Environment Variables

None

9.4.3 Assumptions

None

9.4.4 Access Routine Semantics

(Molecular-weight):

- transition: None
- output: Molecular-weight := $\mathbb{R}$
- exception: None

(Mass-to-Mole):

- transition: None
- output: Mole := $\mathbb{R}$
- exception: None

(mole ratio):

- transition: None
- output: mole-ratio := $\mathbb{N}$
- exception: None

(Mole-ratio-to-Mole):

- transition: None
- output: Mole2 := $\mathbb{R}$
- exception: None

(Mole-to-Mass):

- transition: None
- output: Mass := $\mathbb{R}$
- exception: None

9.4.5 Local Functions

1. Molecular-weight : CompoundT → $\mathbb{R}$
Molecular-weight := Atomic-Mass × Number-of-Atoms-in-Compound

2. Mole := $\frac{Mass}{Molecular_weight}$

3. Mole-ratio: CompoundT → $\mathbb{N}$
Mole-ratio := $\frac{coefficient2}{coefficient1}$

4. Mole2 := $\frac{Mole1}{mole-ratio}$

5. Mass := $\frac{Mole}{Molecular-weight}$

10 MIS of GUI Module

10.1 Module

GUI

10.2 Uses

Balancing (Section 8) , Mass (Section 9)

10.3 Syntax

10.3.1 Exported Constants

None.

10.3.2 Exported Types

ReactionT = ?

10.3.3 Exported Access Programs

Name	In	Out	Exceptions
GUI	-	Mass: $\mathbb{R}$ balanced-reaction: ReactionT	-

10.4 Semantics

10.4.1 State Variables

None

10.4.2 Environment Variables

screen interface

10.4.3 Assumptions

None

10.4.4 Access Routine Semantics

(display):

- transition: None
- output: Mass: $\mathbb{R}$, balanced reaction: ReactionT
- exception: None

10.4.5 Local Functions

None