CAS 741: SRS

Aqueous Speciation Diagram Generator

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Revision History

Table 1: Revision History

Date	Developer(s)	Change
10.5.2017	S. Palmer	First revision of document
12.18.2017	S. Palmer	Revision 1

Reference Material

This section records information for easy reference.

Notation

This section describes the notation conventions used in this document.

Chemical Notation

The following notation is used to describe chemical reactions:

$$\alpha_1 A_1 + \cdots + \alpha_n A_n \rightleftharpoons \beta_1 B_1 + \cdots + \beta_m B_m$$

where A_i are reactant species, α_i are the stoichiometric numbers of the reactant species, n is the number of reactant species, B_i are product species, β_i are the stoichiometric numbers of the product species, m is the number of product species.

Chemical species are denoted as follows:

$$E_{e1}^{1} \cdots E_{en(s)}^{n\ z}$$

where E^i are chemical elements, e_i are the number of each element E^i in the species, n is the number of distinct elements in the species, z is the charge, and s is the state. The state of a species ranges over the values aqueous (aq), solid (s), liquid (l), or gas (g).

Mathematical Notation

In addition to standard mathematical notation conventations, the Gries and Schneider notations Gries and Schneider (1993) for set building and the evaluation of operators applied over sets are use extensively in this document. Specifically, the expression $\{x : X \mid R \bullet P\}$ means the set of all values x that are members of X for which the range R is true and the predicate P is satisfied. A set preceded by Σ means the sum of all values in that set.

Spaces

All symbols that occur in this document have an associated space (a set which their values belong to). Standard mathematical spaces are used (e.g. $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{R}$, etc.) as well as some additional spaces defined in the following table.

symbol	description
Sp.	chemical species
Rx.	chemical reaction
Elt.	chemical element

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
mol	amount of substance	mole
l	volume	litre ($\mathrm{l} = 10^{-3} \cdot \mathrm{m}^3$)
Pa	pressure	pascal ($\mathrm{Pa} = \mathrm{kg\,m^{-1}\,s^{-2}}$)
bar	pressure	bar ($\mathrm{bar} = 10^5 \cdot \mathrm{Pa}$)

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 chemistry literature. The symbols are listed in alphabetical order.

symbol	space	unit	description
α	$\mathbb{N}$	–	stoichiometric coefficient of reactant species
β	$\mathbb{N}$	–	stoichiometric coefficient of product species
A	Sp.	–	reactant species in a chemical equation
B	Sp.	–	product species in a chemical equation
i	$\mathbb{N}$	–	index counter
j	$\mathbb{N}$	–	index counter
K	$\mathbb{R}$	–	equilibrium constant

K_{H_2O}	$\mathbb{R} \to \mathbb{R}$	–	equilibrium equation for the dissociation of water
$\overline{K}$	Set of $\mathbb{R}^n \to \mathbb{R}$	–	set of equilibria equations
k_+	$\mathbb{R}$	$\mathrm{mol\,s^{-1}}$	forward rate constant
k_-	$\mathbb{R}$	$\mathrm{mol\,s^{-1}}$	backward rate constant
$\overline{M}$	Set of $\mathbb{R}^n \to \mathbb{R}$	–	set of mass balance equations
m	$\mathbb{N}$	–	index counter
n	$\mathbb{N}$	–	index counter
P	$\mathbb{R}$	bar	pressure
R	Rx.	–	an arbitrary reversible reaction
$\overline{RK}_{in}$	Set of (Rx., $\mathbb{R}$)	–	the input set of all pairs of reactions and associated equilibrium constants
r_+	$\mathbb{R}$	$\mathrm{mol\,s^{-1}}$	forward reaction rate
r_-	$\mathbb{R}$	$\mathrm{mol\,s^{-1}}$	backward reaction rate
$\overline{S}$	Set of Sp.	–	a set of aqueous solute species in a chemical system
$\overline{S}_{in}$	Set of Sp.	–	the input set of all aqueous solute species in the chemical system
T	$\mathbb{R}$	°C	temperature
$\overline{T}_{in}$	Set of $\mathbb{R}$	–	the input set of total concentrations of chemical elements
X	Sp.	–	arbitrary chemical species
x	Elt.	–	arbitrary chemical element
x_{tot}	$\mathbb{R}$	mol/l	total concentration of an arbitrary chemical element x
$[X]$	$\mathbb{R}$	mol/l	concentration of the arbitrary chemical species X
$\{X\}$	$\mathbb{R}$	–	activity of the arbitrary chemical species X
z_X	$\mathbb{Z}$	–	charge number of an arbitrary aqueous solute X
$\#x\langle X\rangle$	$\mathbb{N}$	–	the number of occurrences of x in X

Abbreviations and Acronyms

symbol	description
A	Assumption
DD	Data Definition
GD	General Definition
GS	Goal Statement
IM	Instance Model
LC	Likely Change
NF	Non-Functional Requirement
PS	Physical System Description
R	Requirement
SATP	Standard Ambient Temperature and Pressure
SRS	Software Requirements Specification
SpecGen	The Aqueous Speciation Diagram Generator program
T	Theoretical Model

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1 Introduction

1.1 Purpose of Document

The purpose of this document is to describe the requirements for the Aqueous Speciation Diagram Generator program (herein referred to as SpecGen), a software product that will produce a speciation diagram given a set of chemical reactions and element totals that define a chemical system as inputs. SpecGen is reimplementation of a MATLAB implementation by Smith (2007) (Wilfrid Laurier University) using a rational design process. The goals and theoretical models used in the SpecGen 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 all information necessary to understand and verify the transformation of inputs to outputs. The SRS is abstract: the contents describe the problem 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 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 (February 1986) point out, the most logical way to present the documentation is still to "fake" a rational design process.

1.2 Scope of Requirements

The scope of SpecGen is limited to the generation of speciation diagrams for aqueous chemical systems. Analysis of gas and solid phases will not be considered. The chemical systems under investigation are always assumed to be at Standard Ambient Temperature and Pressure (SATP). Diagrams generated by SpecGen will plot aqueous species concentrations over the pH range 0 to 14.

1.3 Characteristics of Intended Reader

Reviewers of this documentation should have an understanding of first year undergraduate physical chemistry.

1.4 Organization of Document

The organization of this document follows the template for an SRS for scientific computing software proposed by Smith and Lai (2005) and Koothoor (2013), with some aspects taken from Robertson and Robertson (1999). 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 data definitions in Sec:DataDefi and trace back to find any additional information they require.

The goal statements are refined to the theoretical models, and the theoretical models to the instance models. The data definitions are used to support the definitions of the different models.

2 General System Description

This section identifies the interfaces between the system and its environment, describes the user characteristics and lists the system constraints.

2.1 System Context

- User Responsibilities:
  - Ensure that the input data is correct.
  - Ensure that the input data is sufficient to specify a chemical system that has a unique speciation solution.
- SpecGen Responsibilities:
  - 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.
  - Solve the system of equations arising from the input data to generate the output data.
  - Generate a plot of the output data.

2.2 User Characteristics

The end user of SpecGen should have an understanding of first year undergraduate physical chemistry.

2.3 System Constraints

There are no system constraints.

3 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.

3.1 Problem Description

Chemical speciation refers to the stable (equilibrium) distribution of chemical species in a given chemical system. Speciation diagrams, which plot species concentrations against an independently varied parameter of the system, are useful tools for displaying speciation data in a concise and easy to use format. The production of speciation diagrams requires solving a set of non-linear equations which arise from the chemical reactions of the species present in a chemical system. As the number of reactions taking place in a system increases, producing speciation diagrams can quickly become a tedious undertaking when done manually.

SpecGen will produce a speciation diagram given a set of chemical reactions, equilibrium constants, and element totals that define a chemical system. SpecGen will be specific to speciation of ions in aqueous systems under varying pH, which is of particular importance in the fields of aqueous process engineering and hydrometallurgy. The diagram generated by SpecGen will plot speciation of all aqueous species (excluding H^+ and OH^-) across the pH range 0 to 14.

3.1.1 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:

Activity: the "effective concentration" of a species in a chemical system

Equilibrium: the state of a chemical system in which species concentrations are stable

pH: Potential of Hydrogen: $\text{pH} = -\log\{H^+\}$

SATP: Standard Ambient Temperature and Pressure ($T = 25°\text{C},\ P = 1$ bar)

3.1.2 Physical System Description

The physical system of SpecGen includes the following elements:

PS1: An unspecified volume of liquid water containing dissolved chemical species under equilibrium conditions.

3.1.3 Goal Statements

Given a set of chemical species present in an aqueous chemical system, a set of reversible reactions and associated equilibrium constants that the species are subject to, and the total concentrations of all elements present in the species set (excluding O and H), the goal statements are:

GS1: Generate a plot of the equilibrium concentrations of all chemical species present in the system versus pH over the pH range 0 to 14.

3.2 Solution Characteristics Specification

The instance models that govern SpecGen are presented in § 3.2.5. The information to understand the meaning of the instance models and their derivation is also presented, so that the instance models can be verified.

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

A1: All generated speciation diagrams will cover the pH range 0 to 14. [IM1]

A2: All generated speciation diagrams are at SATP conditions. It follows that all user supplied equilibrium constants are assumed to be values measured under SATP conditions. [GD1, LC1]

A3: The chemical system is assumed be a single-solvent solution, where the solvent is liquid water at SATP. The chemical species in all of the user supplied equations are assumed to be aqueous solutes or water. [IM1, LC2]

A4: The activity of liquid water is assumed to be 1.0. [IM1, LC3]

A5: The activities of all aqueous solute species are assumed to be equal to their concentration. [IM1, LC3]

A6: All chemical equations supplied by the user are assumed to be reversible (finite equilibrium constant). [DD1]

3.2.2 Theoretical Models

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

Number	T1
Label	**Conservation of mass (concentration balance)**
Equation	$x_{tot} = \sum\{X : \overline{S} \mid x \in X \bullet \#x\langle X\rangle \cdot [X]\}$
Description	The total dissolved concentration of an element in an aqueous solution is equal to the sum of the concentrations of all species which contain that element. This is captured in the above equation, where: x is a chemical element x_{tot} is the total dissolved concentration of x in a solution X is an aqueous species in solution $\overline{S}$ is a set of all aqueous species in a solution $\#x\langle X\rangle$ is the number of occurrences of x in X $[X]$ is the concentration of X in solution
Source	–
Ref. By	DD2

Number	T2
Label	**Law of mass action (forward)**
Equation	$r_+ = k_+ \prod_{i=1}^{n} \{A_i\}^{\alpha_i}$
Description	The law of mass action describes the forward and backward reaction rates for a chemical reaction. For a given chemical reaction, the equation above expresses the law of mass action in the forward direction, where: r_+ is the forward reaction rate ($\mathrm{mol\,s^{-1}}$). k_+ is the forward rate constant ($\mathrm{mol\,s^{-1}}$). n is the number of reactants. A_i is the i^{th} reactant species. $\{A_i\}$ is the activity of A_i. α_i is the stoichiometric coefficient of the i^{th} reactant.
Source	Wikipedia (2017a)
Ref. By	T4

Number	T3
Label	**Law of mass action (backward)**
Equation	$r_- = k_- \prod_{j=1}^{m} \{B_j\}^{\beta_j}$
Description	The law of mass action describes the forward and backward reaction rates for a chemical reaction. For a given chemical reaction, the equation above expresses the law of mass action in the backward direction, where: r_- is the backward reaction rate ($\mathrm{mol\,s^{-1}}$). k_- is the backward rate constant ($\mathrm{mol\,s^{-1}}$). m is the number of products. B_j is the j^{th} product species. $\{B_j\}$ is the activity of B_j. β_j is the stoichiometric coefficient of the j^{th} product.
Source	Wikipedia (2017a)
Ref. By	T4

Number	T4
Label	**Chemical equilibrium**
Equation	$k_+ \prod_{i=1}^{n} \{A_i\}^{\alpha_i} = k_- \prod_{j=1}^{m} \{B_j\}^{\beta_j}$
Description	When a chemical reaction is in equilibrium, the forward and reverse reaction rates are the same. Using T2 and T3, this idea is expressed in the equation above, where: k_+ is the forward rate constant ($\mathrm{mol\,s^{-1}}$). n is the number of reactants. A_i is the i^{th} reactant species. $\{A_i\}$ is the activity of A_i. α_i is the stoichiometric coefficient of the i^{th} reactant. k_- is the backward rate constant ($\mathrm{mol\,s^{-1}}$). m is the number of products. B_j is the j^{th} product species. $\{B_j\}$ is the activity of B_j. β_j is the stoichiometric coefficient of the j^{th} product.
Source	Wikipedia (2017a)
Ref. By	T5

Number	T5
Label	**Equilibrium equation**
Equation	$K = \frac{r_+}{r_-} = \frac{\prod_{j=1}^{m}\{B_j\}^{\beta_j}}{\prod_{i=1}^{n}\{A_i\}^{\alpha_i}}$
Description	The ratio of the forward and backward rate constants for a reaction forms a new constant called the equilibrium constant. Using T4, we can relate the equilibrium constant to the activities of the products and reactants. This is shown in the equation above, where: K is the equilibrium constant. r_+ is the forward reaction rate ($\mathrm{mol\,s^{-1}}$). k_+ is the forward rate constant ($\mathrm{mol\,s^{-1}}$). n is the number of reactants. A_i is the i^{th} reactant species. $\{A_i\}$ is the activity of A_i. α_i is the stoichiometric coefficient of the i^{th} reactant. r_- is the backward reaction rate ($\mathrm{mol\,s^{-1}}$). k_- is the backward rate constant ($\mathrm{mol\,s^{-1}}$). m is the number of products. B_j is the j^{th} product species. $\{B_j\}$ is the activity of B_j. β_j is the stoichiometric coefficient of the j^{th} product.
Sources	Wikipedia (2017a)
Ref. By	GD1, DD1

3.2.3 General Definitions

This section collects the laws and equations that will be used in deriving the data definitions, which in turn are used to build the instance models.

Number	GD1
Label	**Water dissociation equilibrium**
SI Units	–
Equation	$K_{H_2O}: \ 10^{-14} = \{H^+\} \cdot \{OH^-\}$
Description	This is the equilibrium equation for the dissociation of water. The equation arises from T5 using the value of 10^{-14} for the equilibrium constant at SATP, where: $\{H^+\}$ is the activity of H^+ $\{OH^-\}$ is the activity of OH^-
Source	Wikipedia (2017b)
Ref. By	DD1

3.2.4 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	**Set of equilibria**
Symbol	$\overline{K}$
SI Units	–
Equation	$\overline{K} = \left\{ (R, K_R) : \overline{RK}_{in} \ \bullet \ K_R = \frac{\prod_{j=1}^{m} \{B_j\}^{\beta_j}}{\prod_{i=1}^{n} \{A_i\}^{\alpha_i}} \text{ with reaction } R \right\} \cup K_{H_2O}$
Description	By A6, all of the input reactions are reversible with finite equilibrium constants. Thus, we can express the input reactions as a set of equilibria via T5. The equilibrium equation for the dissociation of water (GD1) is added to this set since it is not supplied by the user.
Sources	–
Ref. By	IM1

Number	DD2
Label	**Set of mass balance equations**
Symbol	$\overline{M}$
SI Units	–
Equation	$\overline{M} = \{x_{tot} : \overline{T}_{in} \bullet \sum\{X : \overline{S}_{in} \mid x \in X \bullet \#x\langle X\rangle \cdot [X]\} = x_{tot}\}$
Description	Instantiation of T1 using the input sets $\overline{T}_{in}$ and $\overline{S}_{in}$ yields a set of mass (concentration) balance equations.
Sources	–
Ref. By	IM1

3.2.5 Instance Models

This section transforms the problem defined in § 3.1 into one which is expressed in mathematical terms. It uses concrete symbols defined in § 3.2.4 to replace the abstract symbols in the models identified in § 3.2.2 and § 3.2.3.

The goal GS1 is accomplished by plotting the results of IM1.

Number	IM1
Label	**System of non-linear equations to find equilibrium concentrations**
Input	$\overline{K}$, $\overline{M}$
Output	$\{X : \overline{S}_{in} \mid X \neq OH^- \wedge X \neq H^+ \bullet \{[X] \text{ for } 0 \leq pH \leq 14\}\}$, when the system of non-linear equations $\overline{K} \cup \overline{M}$ is satisfied
Description	The union of $\overline{K}$ (DD1) and $\overline{M}$ (DD2) makes up the system of non-linear equations that must be solved. By A3, all activities in the system of equations $\overline{K} \cup \overline{M}$ are either that of water or that of an aqueous solute species. By A4, all instances of $\{H_2O\}$ can be replaced with 1.0. By A5, all activities of aqueous solute species can be replaced by their concentrations. This results in a non-linear system of equations where the set of unknowns is the set $\overline{S}_{in}$. By A1, the system is solved on the pH range 0 to 14.
Sources	–
Ref. By	–

3.2.6 Data Constraints

Tables 2 and 4 show the data constraints on the input and output variables, respectively. 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 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 2 are listed in Table 3.

Table 2: Input Variables

Input	Physical Constraints	Software Constraints	Typical Value	Uncertainty
x_{tot}	–	$x_{tot_{\min}} \leq x_{tot}$	0.1 mol/l	1%
R	–	–	–	–
K	–	–	10^{-4}	2.5%

* The user will supply a set of each input variable.

** There must be an accompanying equilibrium constant for every equation supplied by the user.

*** The set of pairs (R, K) is $\overline{RK}_{in}$.

**** The set of x_{tot} is $\overline{T}_{in}$.

Table 3: Specification Parameter Values

Var	Value
$x_{tot_{\min}}$	0 mol$\,$l^{-1}

Table 4: Output Variables

Output	Physical Constraints
$\{X : \overline{S}_{in} \mid X \neq OH^- \wedge X \neq H^+ \bullet \{[X] \text{ for } 0 \leq pH \leq 14\}\}$	$[X] \geq 0$

3.2.7 Properties of a Correct Solution

A correct solution must satisfy the system of non-linear equations described by IM1.

4 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.

The goal GS1 is solved by R5.

4.1 Functional Requirements

R1: SpecGen will take the following inputs:

1. $\overline{RK}_{in}$: the set of all pairs of reactions and associated equilibrium constants
2. $\overline{T}_{in}$: the set of total concentrations of chemical elements

R2: SpecGen will derive $\overline{S}_{in}$ (the set of all aqueous solute species in the chemical system) from the set of reactions in R1.

R3: SpecGen will ensure that the inputs do not violate the constraints specified in § 3.2.6.

R4: SpecGen will calculate equilibrium concentrations for all species in $\overline{S}_{in}$ (excluding H^+ and OH^-) via IM1.

R5: SpecGen will generate a speciation diagram of all species in $\overline{S}_{in}$ (excluding H^+ and OH^-) in the pH range 0 to 14 using the results of the calculation in R4.

4.2 Nonfunctional Requirements

SpecGen is small in size and relatively simple, so performance is not a priority. Any reasonable implementation will be very quick and use minimal storage. Rather than performance, the non-functional requirement priorities are correctness, understandability, reusability, maintainability, and portability.

NF1: SpecGen will generate diagrams with readable titles, axis labels, legends, and plot lines.

5 Likely Changes

LC1: Generation of diagrams under non-SATP conditions [A2]

LC2: Consideration of gas and solid equilibria [A3]

LC3: Calculation using true activity, with user supplied activity coefficients for more accurate speciation [A4, A5]

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

	T1	T2	T3	T4	T5	GD1	DD1	DD2	IM1
T1									
T2									
T3									
T4		X	X						
T5				X					
GD1					X				
DD1					X	X			
DD2	X								
IM1							X	X	

Table 5: Traceability Matrix Showing the Connections Between TM, GD, DD, IM

	IM1	§ 3.2.6
R1		
R2		
R3		X
R4	X	
R5		

Table 6: Traceability Matrix Showing the Connections Between Requirements and Instance Models

	A1	A2	A3	A4	A5	A6
T1						
T2						
T3						
T4						
T5						
GD1		X				
DD1						X
DD2						
IM1	X		X	X	X	
LC1		X				
LC2			X			
LC3				X	X	

Table 7: Traceability Matrix Showing the Connections Between Assumptions and Other Items

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