M4SF-17LL010301071: Thermodynamic Database Development

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Thermodynamic Database Development

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Contents

1. Introduction

This progress report (Level 4 Milestone Number M4SF-17LL010301071) summarizes research conducted at Lawrence Livermore National Laboratory (LLNL) within the Argillite Disposal R&D Work Package Number M4SF-17LL01030107. The DR Argillite Disposal R&D control account is focused on the evaluation of important processes in the analysis of disposal design concepts and related materials for nuclear fuel disposal in clay-bearing repository media. The objectives of this work package are to develop model tools for evaluating impacts of THMC process on long-term disposal of spent fuel in argillite rocks, and to establish the scientific basis for high thermal limits. This work is contributing to the GDSA model activities to identify gaps, develop process models, provide parameter feeds and support requirements providing the capability for a robust repository performance assessment model by 2020.

In FY17, LLNL continued efforts in the development of thermodynamic databases in support of the Spent Fuel and Waste and Science Technology (SFWST) program. Thermodynamic models provide the basis for understanding the stability of solid phases and speciation of aqueous species and modeling the evolution of repository conditions. LLNL's efforts included

- Illustrating the concepts developed by Wolery and Jove-Colon in FY15 and FY16 and applying them to mineralogic components of greatest interest to SFWST research, starting with a re-analysis of the mineral data model of Helgeson et al. (1978).
- Testing the PhreeqC-PEST fitting routine using various surface complexation models (non-electrostatic, diffuse double layer, etc.) and applying the method to larger sets of sorption data (all U(VI)-quartz data available in the literature) in a comprehensive manner. This effort is intended to build the principles of database development for use in GDSA models.
- Continued engagement with the NEA TDB project through the support of Dr. Atkins-Duffin as the SFWST representative for international thermodynamic database development effort. This effort ensures that US GDSA model efforts are aligned with internationally accepted practices for repository performance assessment calculations. This effort is supported by the Crystalline International work package.

In this report, we focus our summary on thermodynamic database development efforts. Our engagement with the NEA TDB project is summarized in a separate Level 4 Milestone associated with the Crystalline and Crystalline International work packages.

In addition to re-analyzing the mineral data of Helgeson et al., (1978), LLNL has been updating the thermochemical data for aqueous species and making comparisons with the mineral data of Holland and Powell (2011). We have been creating a modified SUPCRT92 data file, and producing a modified version of SUPCRT92 that contains key reference data based on the CODATA (Cox et al., 1989) values or updated values. We are merging these improvements with others made in SUPCRTBL (Zimmer et al., 2016). This is providing a core for additional database development. As much as possible, LLNL is leveraging the efforts of the NEA TDB effort and other investigators.

2. Update to FY16 Thermodynamic Database Delevopment Efforts

The paper "Chemical Thermodynamic Data. I. The Concept of Links to the Chemical Elements and the Historical Development of Key Thermodynamic Data" by Thomas J. Wolery (LLNL) and Carlos F. Jové-Colón (SNL) was accepted by Geochimica et Cosmochimica Acta on September

26, 2016. This paper was published in 2017. The full reference to the article is the following: Thomas J. Wolery and Carlos F. Jove-Colon. 2017. Chemical thermodynamic data. 1. The concept of links to the chemical elements and the historical development of key thermodynamic data, Geochimica et Cosmochimica Acta, 213: 635–676.

A second paper, "Chemical Thermodynamic Data. II. Water in SUPCRT92 and Similar Codes: Thermochemical Properties in Relation to Equations of State," by Wolery and Jové-Colón, was submitted to Computers & Geosciences on Sept. 13, 2016. This was returned by the editors without review. This journal has recently adopted a new focus on "modern computer science paradigms," and this paper does not fit the focus of this journal. The document is available in draft form from the authors.

In FY16, we began making modifications to the SUPCRT92 program (Johnson et al., 1992). This code is still widely used and is featured in two geochemistry textbooks (Anderson, 2005; Walther, 2009). In FY16, we eliminated the obsolete direct-access data file, converted the code to operate in Joule (as opposed to calorie) units, and created a code to convert database files in calorie units to Joule units. The plan was to subsequently combine the modified version with another modified SUPCRT92, the SUPCRTBL of Zimmer et al., 2016, which can use the mineral thermodynamic model of Holland and Powell (2011). While we do not necessarily believe that the Holland and Powell mineral database should be directly included in a future database owing to consistency issues with aqueous species data, the forms used to represent mineral heat capacities and mineral transitions are superior to those in the old SUPCRT92.

3. FY17 Thermodynamic Database Development Efforts

We are evaluating how to disseminate the information contained in the second manuscript prepared in FY16. We now expect that this will evolve into a somewhat lengthy institutional report including all the relevant details and a shorter paper with only key results, to be submitted to a suitable journal. Although the original Part II paper discussed both SUPCRT92 and the IAPWS-95 equation of state for water (Wagner and Pruss, 2002), we did not produce a version of SUPCRT92 that actually contained the IAPWS-95 model. SUPCRT92 contains the earlier water equation of state model of Haar et al., (1984), which the International Association for the Properties of Water and Steam (IAPWS) recognized as an earlier standard (IAPS-84). This model is not valid near the critical point (647.096K and 22.064 MPa). SUPCRT92 uses the Levelt-Sengers et al. (1983) equation of state model in a close region around the critical point. IAPWS-95 in contrast covers the whole region from the triple point temperature (273.16K to 1273K and pressure up to 1000 MPa). Most of the work we have done in FY17 has been aimed at getting IAPWS-95 into a modified SUPCRT92. We expect to need this for the next step in our thermodynamic database development focusing on minerals and aqueous species.

The IAPWS-95 model has been around for some time and various code implementations have been produced over the years. A number are listed with links on the IAPWS web site (iapws.org). We could not find an available implementation including source code free of problematic usage restrictions. Consequently, we wrote our own base code implementation following the model description given by Wagner and Pruss (2002) (given in shorter form by IAPWS, 2016). This level of implementation allows calculation of thermophysical properties as a function of temperature and density (as was the case for the earlier equations of state of Keenan et al., (1969) and Haar et al. (1984). The pressure is one of the calculated properties, along with the enthalpy, entropy, Gibbs energy, Helmholtz energy, and still other properties. The base code is incorporated into a single subroutine EVAI95, which calculates all relevant thermophysical

properties using the equations and coefficients given by Pruss and Wagner (2002) and more succinctly summarized by IAPWS (2016).

What has been required is a level of implementation that permits calculation of such properties as a function of other combinations of variables (which are used for example in SUPCRT92):

1. Temperature and pressure. This requires iterating on putative density values until the desired pressure is obtained.
2. Temperature on the liquid-vapor equilibrium (saturation) curve. This requires iterating on the putative saturation pressure and putative vapor and liquid densities until the requisite pressure (satisfying three equations) is obtained. The output includes the thermophysical properties for both vapor and liquid.
3. Pressure on the liquid-vapor equilibrium (saturation) curve. This requires iterating on the putative saturation temperature in addition to the putative pressure and putative vapor and liquid densities. This involves satisfying four equations in four unknowns. This is most easily done by iterating on a putative saturation temperature (running the problem in 2 above), and correcting that to obtain the specified pressure. The output again includes the thermophysical properties for both vapor and liquid.

Iterative calculations are required for cases 1, 2, and 3. These are generally well suited to solution using the Newton-Raphson method or something similar (e.g., secant method). Where there is more than one iteration variable (as in the two saturation curve cases), numerical solution can be simultaneous or nested.

We first looked to see if the base-level implementation of IAPWS-95 represented byEVAI95 could be readily inserted into SUPCRT92, using the requisite SUPCRT92 water routines used to handle iteration needs. This possibility was studied by adding additional write statements to the water module routines and making subsequent step-throughs using a symbolic debugger. We found too much complexity to make this work without substantial rewriting of these subroutines. It was more efficient to create a second-level implementation. That was done in a stand-alone program called H2OI95. The main program for that will be the basis for an interface subroutine in SUPCRT92 that is analogous to the existing SUPCRT92 routine H2O92, which is the principal subroutine for calculating results for water using the Haar et al. (1984) model. We intend to leave the older equation of state model for water in the modified SUPCRT92 as an option.

H2OI95 is now complete as a stand-alone code for evaluating the IAPWS-95 model and producing both thermophysical results and corresponding thermochemical results, the latter being consistent with the recommendations of CODATA (Cox et al., 1989). The code has been extensively validated, as will be noted later in this report. The code operates using a text input file, and it produces both a text output file and a .csv file that can be opened with a spreadsheet or plotting program. We present some examples here.

An input file for calculating the properties of water at 298.15K and 1 bar (0.1 MPa) pressure is:

```
input298

# Calculate results for 298.15K and 1 bar pressure.
# The purpose is to check the consistency of the
# thermochemical results with the CODATA (1989)
# recommendations for the thermochemical properties
# of water.
```

The following strings are write option switches.

#showphi
#showdetails1
#showdetails2
#showdetails3

```
  tempk   press(MPa)
298.150   1.000000000d-01
```

The option switches shown here are commented out. The data header (here the "tempk press(MPa)") determines the problem type (desired temperature and pressure). Only a single data pair is used here, but any number can be included. Partial output from running this input is:

This is liquid.

CALPRE: iter= 0, px= -5.659239016E-03, betamx= 1.05659E+00
CALPRE: iter= 1, px= 1.000118295E-01, betamx= 1.18295E-04
CALPRE: iter= 2, px= 1.000000000E-01, betamx= 4.32196E-12

```
      delta        rho(kg/m3)
0.309641938E+01   0.997047039E+03
```

Thermophysical Results

```
   u(kJ/kg)         h(kJ/kg)         s(kJ/kg/K)
0.104818597E+03   0.104918893E+03   0.367199984E+00
```

```
   a(kJ/kg)          g(kJ/kg)          v(m3/kg)
-0.466207858E+01  -0.456178241E+01   0.100296171E-02
```

```
   cv(kJ/kg/K)       cp(kJ/kg/K)        w(m/s)
0.413756934E+01   0.418131883E+01   0.149669916E+04
```

```
   mu(K/MPa)        dt(kJ/kg/MPa)      bs(K/MPa)
-0.221467031E-03   0.926024267E-06   0.184002805E-04
```

Thermochemical Results

```
   g(kJ/mol)       h(kJ/mol)       s(J/mol/K)
  -237.1403       -285.8300         69.9500
```

```
   a(kJ/mol)       u(kJ/mol)       v(m3/mol)
  -233.4724       -282.1621          0.0000
```

```
  cv(J/mol/K)     cp(J/mol/K)     dt(kJ/mol/Mpa
   4137.5693       4181.3188       1.66826E-08
```

Here CALPRE refers to the subroutine that carries out this kind of calculation. As shown, the calculations only required two iterations. The residual betamx is the relative error in the pressure.

The normal convergence tolerance is 1×10^{-9}, which is very tight, in part to support computer validation. The high precision of the results shown is also intended to support validation. The thermochemical results for enthalpy (h(kJ/mol)) and entropy (s(J/mol/K)) exactly match the recommended CODATA (Cox et al., 1989) values. Here rho is density and delta (δ) is the reduced density (density divided by the critical point density). The other thermophysical and thermochemical results shown use fairly standard symbolic representation (e.g., a is Helmholtz energy, g is Gibbs energy, cp is heat capacity at constant pressure). Explanation of all symbols is given by Wagner and Pruss (2002) and IAPWS (2016). Some of the thermophysical and thermochemical values associated with the same symbol are different not only in units, but also tied to different arbitrary conventions. For example, this is true for the Gibbs energies, enthalpies, Helmholtz energies, internal energies (u), and entropies.

Another type of input file is illustrated by:

        inputdlt

        # Calculate results for specified temperatures and reduced
        # densities. These calculations do not require iteration.

        # The following strings are write option switches.

        #showphi
        #showdetails1
        #showdetails2
        #showdetails3

           tempk   delta
         298.150   1.00d-05
         298.150   1.00d-04
         298.150   1.00d-03
         298.150   1.00d-02
         298.150   1.00d-01
         298.150   2.00d+00
         298.150   4.00d+00
         298.150   5.00d+00
         298.150   6.00d+00

This type of calculation is done by subroutine CALDLT. This option specifies values of temperature and delta (reduced density, noted above). Actual density (rho) can be substituted on the input file in place of reduced density. This option requires no iteration. The delta values of 0.01, 0.1, and 2 each generate the messages:

        WARNING -- PRESSURE IS NOT POSITIVE. PROBABLY IN THE
        UNSTABLE ZONE

        WARNING -- THERMOCHEMICAL ENTROPY VALUE IS NOT POSITIVE.
        PROBABLY IN THE UNSTABLE ZONE

These delta values are "illegal" in the sense that they appear to lie in the "unstable" zone. This lies somewhere between the delta values for saturated vapor and saturated liquid for the given temperature. Between each of those delta values and the "unstable" zone is a "metastable" zone.

Results from the metastable zone may correspond to actual metastable vapor or metastable liquid. However, the IAPWS-95 model was not fitted to any experimental data for metastable fluids, so any results for such represent an extrapolation of the model. This option to specify temperature and density (reduced or actual) is mainly useful for the study of the equation of state model in the so-called two-phase region. An "illegal" delta value may be legally interpreted as the mean delta for a mixture of saturated vapor and saturated liquid. Under this interpretation, one could calculate the relative abundance of the two phases. However, H2OI95 itself does not currently do that.

The main "saturation curve" option is illustrated by the following input file:

```
inputsct

# Calculate results for specified temperatures along the
# saturation curve, using the "psat" option. The purpose
# is to compare results with those given in Table 13.1
# of Wagner and Pruss (2002).

# The following strings are write option switches.

#showphi
#showdetails1
#showdetails2
#showdetails3

   tempk    psat
 273.160
 274.000
 280.000
 300.000
 320.000
 340.000
 360.000
 380.000
 400.000
 420.000
 440.000
 460.000
 480.000
 500.000
 520.000
 540.000
 560.000
 580.000
 600.000
 620.000
 640.000
 647.096
```

This "psat" option utilizes specified temperature values (the last value is 647.096K is the critical point temperature). The saturation pressure and the properties of both saturated vapor and

saturated liquid are calculated. In H2OI95, the iterative calculation here is done by simultaneously solving three equations in three unknowns. Two of the equations represent the pressure obtained from the equation of state model, once for putative delta of vapor, once for putative delta of liquid. The third equation is a form of the Maxwell equation, which gives the pressure as a function of both delta values. One can write the equation for equilibrium between vapor and liquid as

$$g_V = g_L \tag{1}$$

Where g_V is the Gibbs energy of the vapor and g_L is the Gibbs energy of the liquid. Applying the general relation $g=a+pv$, where a is Helmholtz energy, p is pressure, and v is volume to both vapor and liquid, substituting into equation (1) and recognizing that one is looking for a single pressure, one may obtain:

$$p = \frac{(a_L - a_V)}{(v_V - v_L)} \tag{2}$$

Here the Helmholtz energies come from evaluation of the basic equation of state model and the volumes derive from the respective delta values ($v=1/\delta$). The pressure so calculated is the "Maxwell pressure." There are other forms of the Maxwell equation, but this is the one that we use. Note that use of this equation prevents convergence to a numerical solution in which $v_V=v_L$. Direct use of equation (1) does not provide this.

This saturation curve option is initialized with estimates of the saturation pressure and saturation densities of vapor and liquid using equations (2.5, 2.6, and 2.7) given by Wagner and Pruss (2002) in their development of IAPWS-95. These equations are technically not part of the IAPWS-95 model, but they produce accurate starting estimates. Convergence is illustrated by the following snippet of standard output:

```
        CALSCT: Temp(K) =  400.0000        tau   = 0.161774000E+01

        CALSCT: iter=  0, psat= 2.457652635E-01, betamx= 1.25696E-02
        CALSCT: iter=  1, psat= 2.457693473E-01, betamx= 6.81047E-08
        CALSCT: iter=  2, psat= 2.457693456E-01, betamx= 3.36587E-12

        CALSCT key results:

        Vapor

              delta        rho(kg/m3)
           0.425281845E-02   0.136940754E+01

        Liquid

              delta        rho(kg/m3)
           0.291144733E+01   0.937486039E+03
```

Here CALSCT is the subroutine that carries out this type of calculation. The final value of psat is the calculated saturation pressure. The full fluid properties output is on the output file (not shown here) and the corresponding .csv files (also not shown here).

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We note that there are convergence issues between the triple point temperature (273.16K) and 298.15K and between 647.082K and the critical point temperature (647.096K). In the first instance, the convergence criterion is increased from 1×10^{-9} to 1×10^{-8}. In the second instance, the convergence criterion is increased to 1×10^{-7}. In addition, between 647.090K and the critical point temperature, iteration is otherwise stopped after five iterations. These accommodations were found necessary during testing, as at some point further iteration would fail to result in any improvement. Basically, this is a characteristic of the equation of state itself in these regions, not something showing a need for an improved numerical method. In examining the treatment of this kind of problem in SUPCRT92 (which uses a different equation of state model), we found a similar accommodation. Junglas (2008) offers the only known previous attempt at numerical study of making such calculations on the saturation curve using IAPWS-95. He showed that problems can arise due to the sometimes very non-cubic behavior of the model, especially approaching the critical temperature. Because of these issues and necessary special accommodations, CALSCT is the most complex subroutine in H2OI95.

The other saturation curve option is that in which the pressure is specified instead of the temperature. An input file illustrating this is:

```
inputscp

# Calculate the saturation temperature and corresponding
# results for specified pressure values. This is an example
# of the "tsat" option. Pressure must be specified in MPa,
# not bars.

# The following strings are write option switches.

#showphi
#showdetails1
#showdetails2
#showdetails3

  press(MPa)    tsat
  0.0100
  0.0500
  0.1000
  0.5000
  1.0000
  5.0000
 10.0000
 15.0000
 20.0000
```

This "tsat" option is implemented by making "psat" calculations for putative temperature values, and correcting the putative temperature to produce the specified pressure (this is a nested iteration approach). Correction of the temperature is done using the secant method, as the normal equation of state outputs do not include enough information to calculate a true Jacobian (which in this case is just a scalar). An advantage of this nested approach is that the calculation for any putative temperature utilizes coding in subroutine CALSTC that deals with the previously described issues regarding convergence in certain ranges of temperature.

A partial standard output snippet shows that convergence of the secant method is rapid:

CALSCP: press = 0.100000000E-01 MPa

CALSCP: iter= 0, tempk= 318.9556, betamx= 3.68669E-05
CALSCP: iter= 1, tempk= 320.9556, betamx= 1.06816E-01
CALSCP: iter= 2, tempk= 318.9563, betamx= 1.58835E-06
CALSCP: iter= 3, tempk= 318.9563, betamx= 2.51858E-11

CALSCP key results:

Temp(K)   press(MPa)
318.9563   0.100000000E-01

Vapor

delta   rho(kg/m3)
0.211694790E-03   0.681657223E-01

Liquid

delta   rho(kg/m3)
0.307401638E+01   0.989833275E+03

Here CALSCP is the subroutine that carries out this type of calculation. Iteration in CALSTC done for each CALSCP iteration is not shown here.

When calculation is made for specified temperature and pressure problem where the temperature is less than the critical temperature and the pressure is less than the critical pressure, a CALSCT calculation is first made to determine the saturation properties of vapor and liquid. This allows a determination of whether the stable fluid is vapor or liquid. This then determines whether the initial starting value for the reduced density is a vapor-like density or a liquid-like density. To obtain results for a stable fluid, it is necessary to get this right. In general, starting with a liquid-like density value will lead to a computed solution corresponding to liquid, while starting with a vapor-like value will lead to a computed solution corresponding to vapor. In the first example discussed in this report in which the properties of water at 298.15K and 1 bar were calculated, it was determined that the stable fluid was liquid. A liquid-like density was used as the starting estimate, and the expected results for the liquid were obtained. If this calculation were repeated starting with a vapor-like density, results for the vapor (metastable in this case) would likely be obtained.

This illustrates a peculiar characteristic of IAPWS-95 and similar equations of state based on model equations for the Helmholtz energy as a function of temperature and density. When solving iterative problems for specified temperature and pressure, specified temperature on the saturation curve, or specified pressure on the saturation curve, there may be multiple numerical solutions. A true cubic equation of state would offer more than one solution; however, equations of state like those for IAPWS-95 and the older IAPS-84 are more chaotic (see Junglas, 2008, for illustrations in the case of IAPWS-95). For some temperatures below the critical point, instead of an unstable region sandwiched between two metastable regions bounded on sides by stable vapor and stable liquid, there may be a complex of interspersed regions with characteristics of unstable

and metastable regions. The physical meaning of this is uncertain. It is important for most practical calculations to stay out of such chaotic space. This is achieved by making a reasonable choice of starting estimates and using under-relaxation techniques to avoid entering such space when making iterative corrections. In general, one is mainly interested in achieving results for stable phases. Both SUPCRT92 and H2OI95 are set up to do this without any special effort on the part of the user (appropriate starting estimates are provided in software). By modifying starting estimates in the source code of either code, it is possible to seek results for metastable fluids. It is also possible to seek results for metastable fluids using options in which temperature and reduced or actual density are specified.

H2OI95 has been validated in several ways. Pruss and Wagner (2002) give three tables showing results to high precision. These are intended to facilitate validation of computer implementation. These tables are repeated in IAPWS (2016), where the second part of the first such table from Pruss and Wagner (2002) has been deleted, apparently because some of the values originally given in the older document are incorrect. Results from H2OI95 otherwise match perfectly with the tables in the 2016 document. For example, we obtained results matching Table 6 of the 2016 document using the following input file

inputt6

Compare results with Table 6 of IAPWS (2016), "Revised Release
on the IAPWS Formulation 1995 for the Thermodynamic Properties
of Ordinary Water Substance for General and Scientific Use".
This document is available from the iapws.org web site as
document IAPWS R6-95 (IAPWS95-2016.pdf). The purpose is to
validate the calculation of the phi functions. The line below
with "showphi" causes the phi functions to be written on the
output. Results are obtained from specified temperature and
density values. Density must be specified in kg/m3.

The following strings are write option switches.

showphi
#showdetails1
#showdetails2
#showdetails3

    tempk   rho(kg/m3)
   500.000   0.8380250d+03

This input file uses the "showphi" option to show the "phi" functions that are at the heart of the IAPWS-95 model (all thermophysical properties such as pressure, enthalpy, and entropy are calculated from these functions). The key results obtained running H2OI95 were:

phi functions

phi0 = 0.204797733E+01   phir = -0.342693206E+01
phi0d = 0.384236747E+00   phird = -0.364366650E+00
phi0dd = -0.147637878E+00   phirdd = 0.856063701E+00
phi0t = 0.904611106E+01   phirt = -0.581403435E+01
phi0tt = -0.193249185E+01   phirtt = -0.223440737E+01

$$phi0dt = 0.000000000E+00 \quad phirdt = -0.112176915E+01$$

Shi and Mao (2012) wrote an IAPWS-95 implementation to make saturation curve calculations at specified temperatures. The intended application was interpretation of fluid inclusions in minerals. Their numerical method omits the use of a Maxwell equation and uses two equations and two unknowns (the vapor and liquid delta values). One of the equations is based on direct equality of the Gibbs energies of vapor and liquid (equation 1 in this report). This is less rigorous than our approach, but given that they use the same starting approximations as we do, and those approximations being very good, there is no problem with their calculated results, which H2OI95 matches. Without the accurate starting estimates, their method would be more prone to arriving at numerically correct but otherwise wrong results, such as arriving at the same point in P-T-δ space for both vapor and liquid (meaning "vapor" has become liquid or vice versa). Even our approach including a form of the Maxwell equation can lead to undesired results. For example, with certain starting estimates, one can obtain a solution at some low pressure (very obviously not the saturation pressure), at which metastable liquid and stable vapor have matching Gibbs energies. Thus, using accurate starting estimates remains critical to obtaining desired results on the saturation curve.

We have also compared calculation of thermophysical properties with the NIST on-line calculator (http://webbook.nist.gov/chemistry/fluid/), which is useful for this purpose because it can be run to give results to high precision (nine significant figures).

We note that we have added some additional improvements to SUPCRT92, notably fixing the "saturation curve" option that often crashed the program. We found that it had been modified to a "1 bar-saturation curve" option in which 1 bar was a minimal pressure. The code would crash if a flag was not reset after doing a calculation for 1 bar. The reset would occur only if a calculation was made for a pressure above 1 bar. The basic problem was that a single flag was being used for two purposes. We separated that into two flags, and set up a true "saturation curve" option, a "1 bar-saturation curve" option, and a "1 atm-saturation curve" option. These options are explicitly shown to the user.

4. Planned FY18 Efforts

We will be creating the interface subroutine to link the modified SUPCRT92 to H2OI95. This may be completed before the end of 2017. We will release the stand-alone H2OI95 including source code with minimal restrictions (such as a BSD 3-clause license) and make the code available for download. We will write the longer institutional report on H2OI95 and revise the Part 2 paper for submittal to a suitable journal. We still need to integrate our modified SUPCRT92 with the SUPCRTBL of Zimmer et al. (2016). We will similarly release this and make it available for download. We will then return to the focus on developing a new thermodynamic database for aqueous species, gases, and minerals. We will be watching for potentially impactful developments by others, including the new paper by Miron et al. (2017) and the forthcoming NEA Ancillary Data volume.

5. Acknowledgments

6. References

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