

ATTACHMENT (3)

**MASS OF SODIUM TETRABORATE DECAHYDRATE
BUFFER REQUIRED FOR POST-LOCA
CONTAINMENT BUILDING SUMP pH CONTROL**



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CALCULATION TITLE PAGE

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QUALITY ASSURANCE DOCUMENT

This document has been prepared, checked, and reviewed/approved in accordance with the Quality Assurance requirements of 10CFR50 Appendix B, as specified in the MPR Quality Assurance Manual.



RECORD OF REVISIONS

Calculation No. 0090-0148-01	Prepared By 	Checked By 	Page: 2
Revision	Affected Pages	Description	
0	All	Initial Issue	
1	All	<p><u>Summary of Changes from Revision 0:</u></p> <p>Revised Section 1.0 to incorporate new scope.</p> <p>Revised Section 3.0 to discuss new results.</p> <p>Changed Input 14 equilibrium quotients.</p> <p>Revised Section 7.1 to use option I reaction scheme.</p> <p>Revised Sections 7.2, 7.3, and 7.4 to define limiting cases.</p> <p>Revised Sections 7.5.1 to 7.5.3 to describe option I balance equations.</p> <p>Revised Section 7.5.6 to modify validation results.</p> <p>Revised Sections 8.1 and 8.2. Added Section 8.3 to calculate required buffer mass and pH for new limiting cases.</p> <p>Added Section 8.4 for pH as a function of time.</p> <p>Added new references in Section 9.0.</p> <p>Revised/grouped Appendices B and C to incorporate several temperatures.</p> <p>Added new Appendices C, D, E, F, & G.</p> <p>General revisions to incorporate comments provided by CCNPP.</p>	

Note: The revision number found on each individual page of the calculation carries the revision level of the calculation in effect at the time that page was last revised.



RECORD OF REVISIONS

Calculation No. 0090-0148-01	Prepared By <i>Morgan Charvate</i>	Checked By <i>[Signature]</i>	Page: 3
Revision	Affected Pages	Description	
2	All	<p><u>Summary of Changes from Revision 1:</u></p> <p>Changed label of ionic product constant of water 'K_w' in Input 5.</p> <p>Inserted two new temperature points for water density evaluation in Input 7. Removed last three rows.</p> <p>Inserted appropriate units for borated water density expression in Input 8.</p> <p>Changed the temperature values in Inputs 27 and 28.</p> <p>Removed "and Pressurizer water" from first paragraph of Section 7.2.</p> <p>Changed minimum/maximum temperatures for RCS and Pressurizer in Table 7-1.</p> <p>Corrected borated water density units on page 20. Updated the following calculations in Sections 7.3, 7.4, 8.1, 8.2, 8.3, 8.4 and Appendices B, C & D.</p>	
3	1, 3, 5	<p>Updated title/signatures page for Revision 3. Updated this page to indicate changes from Revision 2. Updated Table of Contents (Appendix F title).</p>	
	6, 7	<p>Updated Summary of Results section.</p>	
	15	<p>Changed RCS coolant maximum Boron concentration from 2300 to 2700 ppm (Input 18). This increase will make the determination of the quantity of NaTB bounding for Operational Modes 1 to 4.</p>	
	19	<p>Updated Table 7-1 for RCS/Pressurizer maximum Boron concentration.</p>	
	20 - 25	<p>Calculation updates to maximum Boron in water cases.</p>	
	29 - 31	<p>Calculation updates to mass of buffer and resultant concentrations.</p>	
	33	<p>Updated Table 8-2 for pH as a function of time.</p>	
	Appendices B & C	<p>Updated calculations.</p>	
	F-1	<p>Updated title.</p>	

Note: The revision number found on each individual page of the calculation carries the revision level of the calculation in effect at the time that page was last revised.



Calculation No. 0090-0148-01	Prepared By <i>Monica Charro</i>	Checked By <i>[Signature]</i>	Page: 4 Revision: 2
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Table of Contents

1.0 Purpose	6
2.0 Acceptance Criteria	6
3.0 Summary of Results	6
4.0 Background	7
4.1 General Review of Sodium Tetraborate Decahydrate Qualities	8
5.0 Assumptions	9
6.0 Input	10
7.0 Methodology	16
7.1 Boric Acid and Borax Equilibria	17
7.2 Containment Sump Water Mass	18
7.3 Containment Sump Boron and Boric Acid Concentrations	22
7.4 Acids Produced by Radiolysis	25
7.5 System of Equations	26
7.5.1 Mass Balance	26
7.5.2 Charge Balance	26
7.5.3 Ionic Strength Balance	27
7.5.4 Water Dissociation	27
7.5.5 Determination of pH	27
7.5.6 Chemical Model Validation	28
8.0 Results	29
8.1 Maximum Boric Acid Concentration	29
8.2 Minimum Boric Acid Concentration	31
8.3 Current Design Basis Case	32
8.4 pH vs. Time	33



Calculation No. 0090-0148-01	Prepared By <i>Melissa Christie</i>	Checked By <i>[Signature]</i>	Page: 5 Revision: 3
---------------------------------	--	----------------------------------	------------------------

9.0 References 34

A pH Predictions of Solutions with Boric Acid and Borax DecahydrateA-1

B Containment Sump pH as a Function of Temperature.....B-1

C Containment Sump pH with Borax Decahydrate Buffer – Case IV (no strong acids).....C-1

D Containment Sump pH with Borax Decahydrate Buffer – Case V.....D-1

E Reference 27 – Record for Iodine in Containment.....E-1

F Reference 29 – Record for Radiation Doses F-1

G Reference 22 – Temperature Profile to 30 Days Following LOCA..... G-1



Calculation No.
0090-0148-01

Prepared By

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[Signature]

Page: 6

Revision: 3

1.0 PURPOSE

The purpose of this calculation is to determine the minimum required mass of the buffer Sodium Tetraborate Decahydrate ($\text{Na}_2\text{B}_4\text{O}_7 \cdot 10\text{H}_2\text{O}$), commercially known as Borax Decahydrate, needed to raise the pH of the containment building sump at Calvert Cliffs Nuclear Power Plant (CCNPP) to above or equal to 7.0 following a Loss of Coolant Accident (LOCA). This calculation includes a determination of sump water pH as a function of time during the recirculation phase.

2.0 ACCEPTANCE CRITERIA

1. A minimum sump pH of 7.0 is required to limit radioactive Iodine (I_2) from being released from the irradiated water pool to the containment atmosphere. The higher pH decreases the level of airborne Iodine in containment and reduces the radiological consequences from containment atmosphere leakage following a LOCA. (Reference 1 – B 3.5.5)
2. A maximum sump pH of 8.0 is required to prevent excessive corrosion of materials in the containment building, especially the dissolution of Aluminum which could lead to the formation of chemical precipitates that could increase the head loss of the sump strainers (References 25 and 26).

3.0 SUMMARY OF RESULTS

The analysis calculates that 13,448 lb of Borax Decahydrate is the minimum mass required to raise the containment sump pH following a LOCA to 7.0. This result was obtained for an accident scenario that injects the maximum possible concentration of boric acid into the containment building with the maximum possible amount of water. The resultant concentration of buffer solution using 13,750 lb of Borax Decahydrate in an alternate accident scenario that injects the minimum possible concentration of boric acid delivered by the minimum possible amount of water into containment was determined to produce a final pH of approximately 7.6. The addition of margin to the calculated required minimum mass (13,448 increased to 13,750 lb) provides reasonable conservatism for potential minor changes in plant design. Therefore, it is concluded that 13,750 lb of buffer mass satisfies the acceptance criteria for this evaluation.

It should be noted that the equilibrium pH calculation assumes 100% chemical assay of buffer material present in the containment basement. Plant personnel must determine the chemical assay of buffer material that is to be placed in containment baskets and adjust the mass accordingly. Therefore, the amount of 100% Borax Decahydrate that conservatively meets the criteria for pH control is 13,750 lb.



Calculation No. 0090-0148-01	Prepared By <i>Mama Charvak</i>	Checked By <i>[Signature]</i>	Page: 7 Revision: 3
---------------------------------	------------------------------------	----------------------------------	------------------------

The pH variation as a function of time during the recirculation phase was modeled as a pH variation as a function of sump water temperature. The effect of temperature on the pH of the containment sump water was evaluated using the complete dissolution of the required mass of buffer. The analysis shows that the effect of temperature is not very significant. As calculated, the decrease in temperature from 194°F (1 hour after the accident) to 125°F (30 days after the accident) results in a drop in pH from 7.12 to 7.05 for the highest boric acid case, and 7.61 to 7.60 for the lowest boric acid case.

The calculation determines that the effect of nitric and hydrochloric acids, generated by radiolysis, on the pH or the mass of buffer needed is negligible. Table 8-1 indicates that approximately 3% of the borax decahydrate mass will be used to neutralize the strong acids.

4.0 BACKGROUND

In the event of a Loss of Coolant Accident at Calvert Cliffs Nuclear Power Plant, cooling of the reactor core will be provided by the Safety Injection System (SIS). During the injection mode, the High Pressure Safety Injection (HPSI) pumps and Low Pressure Safety Injection (LPSI) pumps start automatically and take suction from the Refueling Water Tank (RWT). The Containment Spray (CS) pumps will also take suction from the RWT. Coolant lost from the Reactor Coolant System (RCS) rupture will drain to the containment sump and mix with the borated spray water. When the borated water level in the RWT reaches the Recirculation Actuation Signal (RAS) setpoint, the two containment sump isolation valves will open and the LPSI pumps will shut down. As a result, the SIS continues to operate in the recirculation mode with the HPSI and CS pumps taking suction from the containment sump through a set of sump strainers that filter any large pieces of debris.

The water in the RWT contains dissolved boric acid which yields a solution with a pH of approximately 5.0 at 80°F. When the alkaline reactor coolant from the break mixes with spray water, the resulting solution will have a pH of 5.05 (Reference 2 – Section 6.4). The acidic containment spray water will contact most surfaces in the containment building, including the equipment, which will make the metals susceptible to chloride stress corrosion cracking. Furthermore, at low pH levels Iodine may come out of solution as Iodine gas, and eventually be released to the environment, resulting in increased off site radiation exposure (Reference 3).

To achieve passive pH control, CCNPP currently uses trisodium phosphate dodecahydrate (TSP) stored in baskets placed in the containment basement. As the water level in the containment pool rises, the TSP dissolves and flows out of the stainless steel mesh screens on the sides of baskets. Mixing will be achieved as the fluid is recirculated. The TSP increases the pH to greater than or equal to 7.0.



Calculation No.
0090-0148-01

Prepared By

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Page: 8

Revision: 2

The dissolution of TSP into the post-LOCA containment pool and its interaction with other chemicals or corrosion byproducts that may have entered the pool from wetted or submerged surfaces can lead to the formation of precipitates such as calcium phosphate (Reference 4). These precipitates may potentially combine with other types of debris (for example: fiber insulation) accumulated near the sump screens and impede the flow through the sump strainers.

Due to the presence of Calcium-Silicate insulation at CCNPP, a possibility for an alternative buffering agent is being considered to alleviate the impact of chemical precipitate that may be produced from the reaction of the dissolved calcium, silicate, and other species with TSP. Sodium tetraborate (NaTB) decahydrate has been evaluated by the Pressurized Water Reactors Owners Group (PWROG) experimental program, and was demonstrated to have very similar qualities to TSP (Reference 5). The main findings for NaTB properties as a buffering agent are summarized in the following section.

4.1 General Review of Sodium Tetraborate Decahydrate Qualities

The candidate buffering agents selected in Reference 5 were chosen based on a set of criteria that satisfy different conditions that not only reduce precipitate generation but also insure that the candidates have similar performance characteristics to those buffering agents currently in use. It was shown that NaTB is an acceptable alternative to TSP for the following reasons:

1. NaTB exhibited a very similar dissolution time as TSP in water around 67°C (153°F) (Reference 5, Table 5-1).
2. The mass of NaTB required to raise the pH of boric acid solution is comparable to that of TSP (Reference 5, Table 5-2)
3. At increasing temperatures, NaTB exhibited a faster dissolution rate in boric acid solution than TSP (Reference 5, Table 5-3).
4. Buffered solutions of boric acid with NaTB around pH of 8.0, produced less precipitates when dissolved Calcium or Aluminum was added, than with TSP (Reference 5, Tables 5-4/5-5)
5. Buffered solutions of boric acid with NaTB around pH of 8.0 produced comparable Steel corrosion as with TSP. Higher corrosion of Aluminum, however, was recorded for NaTB than for TSP (Reference 5, Table 5-8).

Overall, the above list of conclusions makes NaTB a reasonable alternative buffering agent to TSP for purposes of reducing the risk of producing deleterious chemical precipitates in a design basis accident.



Calculation No. 0090-0148-01	Prepared By <i>Marwan Charaf</i>	Checked By <i>[Signature]</i>	Page: 9 Revision: 2
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5.0 ASSUMPTIONS

The following assumptions are made in this analysis:

1. All chemical species dissolved in the containment sump solution are assumed to be in equilibrium. Therefore, the results for the mass of NaTB required to achieve the target pH are applicable for steady state conditions.
2. The contribution of Hydriodic acid (HI) to lowering the pH of the containment sump pool is assumed to be negligible. Reference 3, Section 2.2.2 states that the total amount of iodine in containment would be of the order of 100 moles with roughly 5% given off as HI. Because of this expected low concentration for iodine ions, they are not accounted for in this analysis.
3. The contribution of Cesium Iodide (CsI) to the containment pool buffer chemistry is assumed to be negligible. Reference 6, Section 3.5 states that 95% of the iodine released should be assumed to be CsI. End-of-Cycle Total Integrated Dose information for Iodine is given in Reference 27 as 14260 grams, or approximately 112 moles. This is comparable to the estimated value given in Assumption 2. Hence, 95% of 112 moles does not yield a significant concentration for iodine or cesium ions in the sump water volume.
4. In a dilute aqueous solution, the addition of a solute makes a negligible change in the volume of the solution. Therefore, in this calculation molality and molarity are assumed to be equivalent. The units for molarity are moles of solute per liter of solution, denoted as 'M'.
5. The total liquid mass in the containment sump at the start of recirculation is determined by adding the amount of water provided by the following sources:
 - a. Reactor Coolant System (RCS)
 - b. Pressurizer Water Volume
 - c. Safety Injection Tanks (SIT)
 - d. Boric Acid Storage Tanks (BAST)
 - e. Refueling Water Tank (RWT)
 - f. Initial Sump Inventory
6. The piping between the various tanks (namely SIT, BAST, and RWT) and the RCS is assumed to hold a negligible amount of water compared to the storage capacity of the tanks.



Calculation No. 0090-0148-01	Prepared By <i>Norma Chaves</i>	Checked By <i>[Signature]</i>	Page: 10 Revision: 2
---------------------------------	------------------------------------	----------------------------------	-------------------------

7. The amount of water in the containment atmosphere is assumed to remain unchanged before and after the accident and thus will not contribute to the liquid mass delivered to the containment sump. This is conservative since the relative humidity inside the containment building will be higher following a LOCA.
8. The initial amount of water in the containment sump is assumed to be 50 gallons from condensation and unidentified leaking water from pipes. This value is higher than the sump level alarm setpoint of 49 gallons (Reference 2, Section 4.3.3). This water is conservatively assumed to be at 0 psig and 70°F, which is below the maximum average ambient air temperature (120°F according to Design Input 23 of Reference 13-part 2). Additionally, this water is assumed to have the same limits of Boron concentration as the RWT (Input 15).
9. The Boron concentration of the water held by the RCS and the Pressurizer is assumed to be the same.
10. The water volume of the condensed steam in the Pressurizer is assumed to be negligible compared to the other water sources.
11. The temperature of the sump water between 19 and 30 days following the accident is linearly extrapolated from the temperature at times less than 19 days provided as design input (Reference 22). The containment pressure at 30 days is assumed to be atmospheric.
12. During the recirculation phase, the containment sump fluid is assumed to be fully mixed with the buffer solution.
13. The pH of the sump water is assumed to be influenced only by the chemistry of boric acid, nitric acid, hydrochloric acid, and borax decahydrate.

6.0 INPUT

1. The approximate effective ionic radii of Hydrogen and Hydroxide ions, H^+ and OH^- , are taken from Reference 7, Table 8.2 in aqueous solution at 25°C. The following values are used in the computation of the ionic activity coefficient: $a_{H^+} = 9.0$ Angstrom, $a_{OH^-} = 3.5$ Angstrom.
2. The individual ionic activity coefficient, γ_i , is estimated from the following equation of the Debye-Hückel theory (Reference 7, Section 8.1):

$$-\log \gamma_i = \frac{Az_i^2 \sqrt{I}}{1 + Ba_i \sqrt{I}}$$



Calculation No.

0090-0148-01

Prepared By

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[Signature]

Page: 11

Revision: 2

where A and B are the Debye-Hückel constants, z is the ionic charge, a is the effective ionic radius, and I is the ionic strength of the solution.

3. The constants 'A' and 'B' for the Debye-Hückel equation from 0°C to 100°C are taken from Reference 7, Table 8-3.

°C	A	B
0	0.4918	0.3248
5	0.4952	0.3256
10	0.4989	0.3264
15	0.5028	0.3273
20	0.5070	0.3282
25	0.5115	0.3291
30	0.5161	0.3301
35	0.5211	0.3312
40	0.5262	0.3323
45	0.5317	0.3334
50	0.5373	0.3346
55	0.5432	0.3358
60	0.5494	0.3371
65	0.5558	0.3384
70	0.5625	0.3397
75	0.5695	0.3411
80	0.5767	0.3426
85	0.5842	0.3440
90	0.5920	0.3456
95	0.6001	0.3471
100	0.6086	0.3488

4. The ionic strength of the solution, 'I', is defined as the summation of the product molarity 'C' times ionic charge 'z' squared for all the ionic species present in the solution (Reference 12, Chapter 6):

$$I = 0.5 \sum_i^n C_i z_i^2$$



Calculation No.

0090-0148-01

Prepared By

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Page: 12

Revision: 2

5. The ionic product constant of water ' K_w ' as a function of temperature is taken from Reference 7, Table 8.5. By definition, $K_w = 10^{(-pK_w)}$.

°C	pK _w
0	14.938
5	14.727
10	14.528
15	14.340
18	14.233
20	14.163
25	13.995
30	13.836
35	13.685
40	13.542
45	13.405
50	13.275
55	13.152
60	13.034
65	12.921
70	12.814
75	12.711
80	12.613
85	12.520
90	12.431
95	12.345
100	12.264
125	11.911
150	11.637
175	11.431
200	11.288
225	11.207
250	11.192
275	11.251
300	11.406

Calculation No.
0090-0148-01

Prepared By

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[Signature]

Page: 13

Revision: 2

6. The molar weights of compounds used in the calculation are given below (Reference 7 for atomic weights):

- a. Boron: $MW_B = 10.81 \text{ g/mol}$
- b. Boric Acid: $MW_{B(OH)_3} = 61.83 \text{ g/mol}$
- c. Borax Decahydrate: $MW_{Na_2B_4O_7 \cdot 10H_2O} = 381.37 \text{ g/mol}$

7. The density of pure water as a function of temperature and pressure is taken from Reference 8. The following values are used in the calculation.

°F	Pressure (psia)	ρ_w (lb / ft ³)
40	14.7	62.43
70	14.7	62.31
77	14.7	62.25
100	14.7	62.00
120	14.7	61.71
125	14.7	61.63
196	14.7	60.20
103.5	29.7	61.96
115	29.7	61.79
120	264.7	61.76
200	2250	60.55

8. The density of borated water is approximated using the following expression from Reference 9, which incorporates the effect of boric acid concentration ' C_{boric} ' on water density. C_{boric} is evaluated as the ratio of mass of boric acid to mass of fluid:

$$\rho(T, C_{boric}) = \rho_w(T) + 315C_{boric} + 100C_{boric}^2$$

where ρ is the density of borated water, ρ_w is the density of pure water in kg/m^3 , and T is the temperature. Converting to lb/ft^3 :

$$\rho(T, C_{boric}) = \rho_w(T) + 19.665C_{boric} + 6.243C_{boric}^2$$

9. The total gamma dose at the surface of the sump is taken from Reference 29. This value will be used in the calculation of nitric acid (HNO_3) produced from irradiation of water:

$$\gamma_{dose} = 16.84 \text{ MegaRad}$$

Calculation No.
0090-0148-01

Prepared By

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[Signature]

Page: 14

Revision: 2

10. The total gamma and beta doses at the surface of the iodine removal filter are taken from Reference 29. This value will be used in the calculation of the hydrochloric acid (HCl) produced from irradiation of Hypalon cable in containment:

$$\gamma\beta_{dose} = 567.63 \text{MegaRad}$$

11. The mass of chloride bearing cable that contributes to the formation of HCl is taken from Reference 10 as $M_{cable} = 550 \text{ Kg}$ or approximately 1213 Lb. This mass is the maximum for the two units at Calvert Cliffs.

12. The nitric acid generation rate is from Reference 3, Section 2.2.4. The generation rate in moles of HNO_3 is a function of the total gamma dose and volume of sump water:

$$G_{\text{HNO}_3} = 7.3 \times 10^{-6} \frac{\text{mol}}{\text{L} \cdot \text{MegaRad}} \cdot \gamma_{dose}$$

13. The hydrochloric acid generation rate is from Reference 3, Section 2.2.5.2. The generation rate in moles of HCl is a function of the total gamma and beta doses and mass of electrical cable exposed to radiation:

$$G_{\text{HCl}} = 4.6 \times 10^{-4} \frac{\text{mol}}{\text{lb} \cdot \text{MegaRad}} \cdot \gamma\beta_{dose}$$

14. The molal equilibrium quotients ' $Q_{x,y}$ ' for boric acid-borate dissociation schemes are taken from Reference 13, page A-8, and reproduced below as a function of Temperature 'T' in units of Kelvin, and Ionic strength 'I' in units of mole/L:

a. $\log Q_{1,1} = \frac{1573.21}{T} + 28.6059 + 0.012078 \cdot T - 13.2258 \cdot \log(T) + f(I)$

b. $\log Q_{2,1} = \frac{2756.1}{T} - 19.1998 + 0.00033 \cdot T + 5.835 \cdot \log(T) + f(I)$

c. $\log Q_{3,1} = \frac{3339.5}{T} - 8.3178 + 0.00033 \cdot T + 1.497 \cdot \log(T) + f(I)$

d. $\log Q_{4,2} = \frac{12820}{T} - 134.7938 + 0.00033 \cdot T + 42.105 \cdot \log(T) + f(I)$

where $f(I) = (0.325 - 0.00033 \cdot T) \cdot I - 0.0912 \cdot I^{1.5}$



Calculation No. 0090-0148-01	Prepared By <i>Melissa Chambers</i>	Checked By <i>[Signature]</i>	Page: 15 Revision: 3
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15. The minimum RWT Boron concentration considered in this calculation is 2300 ppm, while the maximum RWT Boron concentration is 2700 ppm (Reference 14 – SR 3.5.4.4).
16. The minimum SIT Boron concentration considered in this calculation is 2300 ppm, while the maximum SIT Boron concentration is 2700 ppm (Reference 14 – SR 3.5.1.4).
17. The minimum BAST Boric Acid concentration considered in this calculation is 6.25% by weight. The maximum BAST Boric Acid concentration is 8% by weight (Reference 20).
18. The minimum RCS coolant Boron concentration is 0 ppm (towards the end of the fuel cycle). The maximum RCS coolant Boron concentration is 2700 ppm, based on limit for Boron precipitation in the core following a LOCA (Reference 1 – B 3.5.4).
19. The minimum RWT borated water volume that is injected to the containment sump is 360,000 gallons (Reference 2, Section 6.4.2). The maximum RWT borated water available for injection is taken as 420,000 gallons, which is equivalent to the total tank volume (Reference 2, Table 6-4).
20. The minimum SIT borated water volume considered in this calculation is 1113 ft³, while the maximum SIT borated water volume is 1179 ft³ in each tank (Reference 14 – SR 3.5.1.2). There are four SITs at CCNPP (Reference 31 – Input 3.1).
21. The maximum BAST borated water volume per tank is taken as 1270 ft³ (Reference 13 – Design Input 3 of part 2). The minimum BAST borated water volume is calculated based on the minimum tank level given in Figure 15.1.2-1 of Reference 21 as 107 inches (at 8 w.t.%). The maximum tank level is given as 130 inches (at 6.25 w.t.%). Therefore, the minimum BAST liquid volume is $1270 \text{ ft}^3 \times (107/130) = 1045 \text{ ft}^3$. There are two BASTs at CCNPP.
22. The RCS water volume excluding the Pressurizer is 9576 ft³ (Reference 2, Table 4-1).
23. The minimum Pressurizer water volume considered in this calculation is 600 ft³, while the maximum Pressurizer water volume is 800 ft³ (Reference 2, Table 4-7).
24. The minimum temperature of the RWT is 40°F, while the maximum temperature is 100°F (Reference 1 – B 3.5.4). Atmospheric pressure (Reference 2, Table 6-4) will be used to evaluate the density of water at those temperature extremes.
25. The operating temperature of 120°F and the design pressure of 250 psig for the SIT will be used to evaluate the density of water in the SITs (Reference 2, Table 6-3).
26. The temperature limits of water in the BAST are from Reference 21, Figure 15.1.2-1. The minimum temperature in the BAST is 103.5°F (at 8 w.t.%), and maximum temperature is



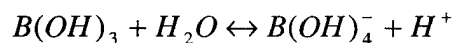
Calculation No. 0090-0148-01	Prepared By <i>Mona Charoub</i>	Checked By <i>[Signature]</i>	Page: 16 Revision: 2
---------------------------------	------------------------------------	----------------------------------	-------------------------

115°F (at 6.25 w.t.%). The design pressure of 15 psig will be used to evaluate the density of water at those temperature extremes (Reference 13 – Design Input 4 of part 2).

27. The RCS normal operating pressure of 2250 psia (Reference 2, Table 4-1) will be used to evaluate the density of coolant at the lowest average coolant temperature of 200°F to cover Operational Modes 1 to 4 (Reference 13 – Design Input 19).
28. The Pressurizer normal operating pressure of 2250 psia (Reference 2, Table 4-7) will be used to evaluate the density of coolant at the lowest average coolant temperature of 200°F (Reference 13 – Design Input 19).
29. The sump water temperature as a function of time following the LOCA is extracted from Reference 22. The input temperatures are graphically shown in Appendix G.
30. In accordance with Reference 29, the Boric Acid Storage Tanks are isolated for the calculation of the lowest possible Boron concentration case in the containment post LOCA sump. This is a conservative approach.

7.0 METHODOLOGY

The solubility of boric acid in water has been studied extensively in the literature. At very low concentrations (≤ 0.025 M), only the mononuclear species produced by the following reaction were found (Reference 15, p. 297):



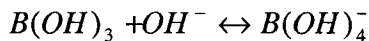
In relatively concentrated solutions (≥ 0.025 M), such as the boric acid concentration expected at CCNPP following a LOCA with several thousand ppm Boron concentration sump water, polymeric ions (Borates containing $B_x(OH)_y$ where $x > 1$) from the acceptance of OH^- ions by $B(OH)_3$ are formed. The determination of the exact structure of those polynuclear species of Boron has been the subject of several experiments (References 11, 16, 17, 18, and 19). All of those studies present data and analyses that support the formation of polyborate ions. Moreover, the data presented in Reference 11 was collected at three different temperatures (50°, 100°, and 200°C). This calculation uses the dissociation schemes identified in Reference 11. A verification of the method was performed by comparing pH predictions with the Reference 11 dissociation scheme to the pH of buffered boric acid/borax solutions from the literature. The results of the comparison are given in Appendix A.

Calculation No. 0090-0148-01	Prepared By <i>Maria Charnot</i>	Checked By <i>[Signature]</i>	Page: 17 Revision: 2
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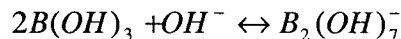
7.1 Boric Acid and Borax Equilibria

The dissolution of Borax Decahydrate whose molecular formula is $\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}$, releases two positively charged Sodium ions, Na^+ , and one doubly negatively charged Tetraborate ion into the solution. However, the tetraborate ion will break down to produce the mononuclear ion $\text{B}(\text{OH})_4^-$, and at equilibrium will only be present to a minute extent (References 15 and 17). Therefore, the boric acid/borax equilibrium equations can be written in the following scheme. The subscripts on the equilibrium quotients $Q_{x,y}$ satisfy the formation of borate ions of the form $\text{B}_x(\text{OH})_{3x+y}^-$. The brackets [] denote the *equilibrium* concentration in mole/L of a given species, so the quotients are assigned based on the thermodynamic equilibrium relationship (Reference 28, pg. 77):

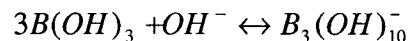
Main Reactions Scheme (Reference 11) – Steps 1, 2, and 3



$$Q_{1,1} = \frac{[\text{B}(\text{OH})_4^-]}{[\text{B}(\text{OH})_3][\text{OH}^-]}$$



$$Q_{2,1} = \frac{[\text{B}_2(\text{OH})_7^-]}{[\text{B}(\text{OH})_3]^2[\text{OH}^-]}$$



$$Q_{3,1} = \frac{[\text{B}_3(\text{OH})_{10}^-]}{[\text{B}(\text{OH})_3]^3[\text{OH}^-]}$$

Step 4 – Option I



$$Q_{4,2} = \frac{[\text{B}_4(\text{OH})_{14}^{-2}]}{[\text{B}(\text{OH})_3]^4[\text{OH}^-]^2}$$

Step 4 – Option II



$$Q_{5,3} = \frac{[\text{B}_5(\text{OH})_{18}^{-3}]}{[\text{B}(\text{OH})_3]^5[\text{OH}^-]^3}$$



Calculation No. 0090-0148-01	Prepared By <i>Maura Chambers</i>	Checked By <i>[Signature]</i>	Page: 18 Revision: 2
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According to Reference 11, the contribution of the (4,2) and the (5,3) species are so similar that replacement of one by the other for modeling the fourth dissociation step has no significant impact on the formation quotients of the other species. This analysis relies on the equilibrium quotients given in Input 14 for the Option I scheme. Furthermore, the methodology is validated in Appendix A, and it is demonstrated that the dissociation scheme with Option I gives very good results in modeling the measured pH values when compared to experimental data. Thus, the calculation of the NaTB mass required to achieve the target pH at CCNPP is conducted using the Option I scheme.

7.2 Containment Sump Water Mass

Table 7-1 below summarizes the different borated water sources identified in the Input Section, their corresponding volumes, temperatures, pressure, and Boron concentrations. Note that only the operating temperature was available for the SIT, and only one volume was considered for the RCS.

The computation of the BAST content of Boron in ppm is obtained from the weight % of boric acid concentration as such:

$$\text{Boron (ppm)} = \text{Mass of Boron} / \text{Mass of Liquid} \times 10^6 = MW_B / MW_{B(OH)_3} \times \text{w.t.\%} \times 10^4,$$

where w.t.% = 6.25 or 8.0 (Input 17). Thus:

$$\text{BAST_MinBoron}_{\text{ppm}} := \frac{10.81 \frac{\text{gm}}{\text{mol}}}{61.83 \frac{\text{gm}}{\text{mol}}} \cdot 6.25 \cdot 10^4$$

$$\text{BAST_MinBoron}_{\text{ppm}} = 10927$$

$$\text{BAST_MaxBoron}_{\text{ppm}} := \frac{10.81 \frac{\text{gm}}{\text{mol}}}{61.83 \frac{\text{gm}}{\text{mol}}} \cdot 8.0 \cdot 10^4$$

$$\text{BAST_MaxBoron}_{\text{ppm}} = 13987$$

The above Boron concentrations are inserted into Table 7-1.



Calculation No. 0090-0148-01	Prepared By <i>Mano Charvot</i>	Checked By <i>[Signature]</i>	Page: 19 Revision: 3
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Table 7-1. Containment Sump Water Sources

Source	Minimum Volume (ft ³)	Maximum Volume (ft ³)	Minimum Temperature (°F)	Maximum Temperature (°F)	Pressure (psia)	Minimum Boron (ppm)	Maximum Boron (ppm)
RWT	48125	56146	40	100	14.7	2300	2700
SIT	1113	1179	120	120	264.7	2300	2700
BAST	1045	1270	103.5	115	29.7	10927	13987
RCS	9576	9576	200	200	2250	0	2700
Pressurizer	600	800	200	200	2250	0	2700
Initial Inventory	6.68	6.68	70	120	14.7	2300	2700

Note: Minimum and maximum volumes are given per each tank for SIT and BAST.

In the following evaluations, the tabulated input from Table 7-1 along with the minimum density of fluid (at maximum temperature), and maximum density (at minimum temperature) based on the corresponding Boron concentration is used to calculate the limiting sump water mass and total Boron content. Furthermore, water sources that will be used or isolated in the most limiting cases are incorporated in the analysis.

INPUT

$$MW_{\text{Boron}} := 10.81 \frac{\text{gm}}{\text{mol}}$$

$$MW_{\text{BoricAcid}} := 61.83 \frac{\text{gm}}{\text{mol}}$$

$$MW_{\text{Borax}} := 381.37 \frac{\text{gm}}{\text{mol}}$$

$$\rho_w := 61.63 \frac{\text{lb}}{\text{ft}^3}$$

Pure Water Density at 125 F & 14.7 psia
(lower bound temperature for long term cooling)

$$\text{Water}_{\text{src}} := \begin{pmatrix} \text{"RWT"} \\ \text{"SIT"} \\ \text{"BAST"} \\ \text{"RCS"} \\ \text{"Pressurizer"} \\ \text{"Initial Inventory"} \end{pmatrix}$$

$$\text{MinWater}_{\text{vol}} := \begin{pmatrix} 48125 \\ 1113 \\ 1045 \\ 9576 \\ 600 \\ 6.68 \end{pmatrix} \text{ft}^3$$

$$\text{MaxWater}_{\text{vol}} := \begin{pmatrix} 56146 \\ 1179 \\ 1270 \\ 9576 \\ 800 \\ 6.68 \end{pmatrix} \text{ft}^3$$



Calculation No.
0090-0148-01

Prepared By

Madison Charoub

Checked By

[Signature]

Page: 20

Revision: 3

at max. temperature
(Input 7)

at min. temperature
(Input 7)

$$\text{MinPureWater}_\rho := \begin{pmatrix} 62.00 \\ 61.76 \\ 61.79 \\ 60.55 \\ 60.55 \\ 61.71 \end{pmatrix} \frac{\text{lb}}{\text{ft}^3}$$

$$\text{MaxPureWater}_\rho := \begin{pmatrix} 62.43 \\ 61.76 \\ 61.96 \\ 60.55 \\ 60.55 \\ 62.31 \end{pmatrix} \frac{\text{lb}}{\text{ft}^3}$$

$$\text{MinBoron}_{\text{ppm}} := \begin{pmatrix} 2300 \\ 2300 \\ 10927 \\ 0 \\ 0 \\ 2300 \end{pmatrix}$$

$$\text{MaxBoron}_{\text{ppm}} := \begin{pmatrix} 2700 \\ 2700 \\ 13987 \\ 2700 \\ 2700 \\ 2700 \end{pmatrix}$$

The isolation of BASTs is considered a Single Point Failure. This gives the lower bound for sump Boron concentration (See Assumption 5 & Input 30).

$$\text{MinFactor} := \begin{pmatrix} 1 \\ 4 \\ 0 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\text{MaxFactor} := \begin{pmatrix} 1 \\ 4 \\ 2 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

COMPUTE

$$\text{MinAcidMassRatio} := \frac{\text{MW}_{\text{BoricAcid}}}{\text{MW}_{\text{Boron}}} \cdot \text{MinBoron}_{\text{ppm}} \cdot 10^{-6}$$

$$\text{MaxAcidMassRatio} := \frac{\text{MW}_{\text{BoricAcid}}}{\text{MW}_{\text{Boron}}} \cdot \text{MaxBoron}_{\text{ppm}} \cdot 10^{-6}$$

$$\text{MinAcidMassRatio} = \begin{pmatrix} 0.0132 \\ 0.0132 \\ 0.0625 \\ 0 \\ 0 \\ 0.0132 \end{pmatrix}$$

$$\text{MaxAcidMassRatio} = \begin{pmatrix} 0.0154 \\ 0.0154 \\ 0.08 \\ 0.0154 \\ 0.0154 \\ 0.0154 \end{pmatrix}$$



Calculation No.
0090-0148-01

Prepared By
Maria Chomicki

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Page: 21
Revision: 3

Borated Water Density as a function of Boric Acid Mass Ratio (Input 8):

$$\text{MinBWater}_\rho := \text{MinPureWater}_\rho + \left(\left(19.665 \text{MinAcidMassRatio} + 6.243 \text{MinAcidMassRatio}^2 \right) \right) \frac{\text{lb}}{\text{ft}^3}$$

$$\text{MaxBWater}_\rho := \text{MaxPureWater}_\rho + \left(\left(19.665 \text{MaxAcidMassRatio} + 6.243 \text{MaxAcidMassRatio}^2 \right) \right) \frac{\text{lb}}{\text{ft}^3}$$

$$\text{MinBWater}_\rho = \begin{pmatrix} 62.26 \\ 62.02 \\ 63.04 \\ 60.55 \\ 60.55 \\ 61.97 \end{pmatrix} \frac{\text{lb}}{\text{ft}^3}$$

$$\text{MaxBWater}_\rho = \begin{pmatrix} 62.74 \\ 62.07 \\ 63.57 \\ 60.86 \\ 60.86 \\ 62.62 \end{pmatrix} \frac{\text{lb}}{\text{ft}^3}$$

$$\text{MinWater}_{\text{mass}} := \left(\text{MinFactor} \cdot \text{MinWater}_{\text{vol}} \cdot \text{MinBWater}_\rho \right)$$

$$\text{MaxWater}_{\text{mass}} := \left(\text{MaxFactor} \cdot \text{MaxWater}_{\text{vol}} \cdot \text{MaxBWater}_\rho \right)$$

$$\text{MinWater}_{\text{mass}} = \begin{pmatrix} 2996252 \\ 276112 \\ 0 \\ 579827 \\ 36330 \\ 414 \end{pmatrix} \text{lb}$$

$$\text{MaxWater}_{\text{mass}} = \begin{pmatrix} 3522329 \\ 292699 \\ 161476 \\ 582749 \\ 48684 \\ 418 \end{pmatrix} \text{lb}$$

Total Sump Water Mass:

$$\sum \text{MinWater}_{\text{mass}} = 3888935 \text{lb}$$

$$\sum \text{MaxWater}_{\text{mass}} = 4608356 \text{lb}$$



Calculation No. 0090-0148-01	Prepared By <i>Manna Charnoff</i>	Checked By <i>[Signature]</i>	Page: 22 Revision: 3
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7.3 Containment Sump Boron and Boric Acid Concentrations

Based on the calculated individual contribution from each borated water source, the collective containment sump Boron concentration can be calculated as:

$$C_{sump} = \frac{\sum_i C_i M_i}{\sum_i M_i}, \text{ where } C_i \text{ and } M_i \text{ are the Boron concentration, and water mass from each}$$

source. Given, the possibility for accident scenarios that generate a combination of minimum Boron/minimum Liquid, minimum Boron/maximum Liquid, maximum Boron/minimum Liquid, or maximum Boron/maximum Liquid, four collective containment sump Boron concentrations are analyzed to determine the range of expected boric acid concentrations that will influence the pH calculation.

Calculate Boron Mass in each Case from each source:

$$\begin{aligned} \text{CaseI } B_{mass} &:= \left(\text{MinBoron ppm} \cdot \text{MinWater mass} \right) \cdot 10^{-6} \\ \text{CaseII } B_{mass} &:= \left(\text{MinBoron ppm} \cdot \text{MaxWater mass} \right) \cdot 10^{-6} \\ \text{CaseIII } B_{mass} &:= \left(\text{MaxBoron ppm} \cdot \text{MinWater mass} \right) \cdot 10^{-6} \\ \text{CaseIV } B_{mass} &:= \left(\text{MaxBoron ppm} \cdot \text{MaxWater mass} \right) \cdot 10^{-6} \end{aligned}$$

$$\begin{aligned} \text{CaseI } B_{mass} &= \begin{pmatrix} 6891 \\ 635 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} \text{ lb} & \text{CaseII } B_{mass} &= \begin{pmatrix} 8101 \\ 673 \\ 1764 \\ 0 \\ 0 \\ 1 \end{pmatrix} \text{ lb} \\ \text{CaseIII } B_{mass} &= \begin{pmatrix} 8090 \\ 746 \\ 0 \\ 1566 \\ 98 \\ 1 \end{pmatrix} \text{ lb} & \text{CaseIV } B_{mass} &= \begin{pmatrix} 9510 \\ 790 \\ 2259 \\ 1573 \\ 131 \\ 1 \end{pmatrix} \text{ lb} \end{aligned}$$



Calculation No. 0090-0148-01	Prepared By <i>Marnia Charnick</i>	Checked By <i>[Signature]</i>	Page: 23 Revision: 3
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$$\text{CaseI ppm} := \frac{\sum \text{CaseI Bmass}}{\sum \text{MinWater mass}} \cdot 10^6$$

$$\text{CaseI ppm} = 1936$$

$$\text{CaseII ppm} := \frac{\sum \text{CaseII Bmass}}{\sum \text{MaxWater mass}} \cdot 10^6$$

$$\text{CaseII ppm} = 2287$$

$$\text{CaseIII ppm} := \frac{\sum \text{CaseIII Bmass}}{\sum \text{MinWater mass}} \cdot 10^6$$

$$\text{CaseIII ppm} = 2700$$

$$\text{CaseIV ppm} := \frac{\sum \text{CaseIV Bmass}}{\sum \text{MaxWater mass}} \cdot 10^6$$

$$\text{CaseIV ppm} = 3095$$

Therefore, in summary:

Case I: Minimum Boron concentration delivered via minimum water mass:

$$C_{\text{sump}} = 1936 \text{ ppm.}$$

Case II: Minimum Boron concentration delivered via maximum water mass:

$$C_{\text{sump}} = 2287 \text{ ppm.}$$

Case III: Maximum Boron concentration delivered via minimum water mass:

$$C_{\text{sump}} = 2700 \text{ ppm.}$$

Case IV: Maximum Boron concentration delivered via maximum water mass:

$$C_{\text{sump}} = 3095 \text{ ppm.}$$

Case V: Design Basis for TSP Buffer (Reference 13, considered here for comparison):

$$C_{\text{sump}} = 3105.5 \text{ ppm.}$$

Consequently, the two extremes for Boron concentration (Case I & Case IV), and the current licensing case for TSP (Case V) are used to calculate the un-dissociated Boric acid concentrations which will be used in the pH buffer calculation.

Calculation No.

0090-0148-01

Prepared By

Marwa Charrie

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Page: 24

Revision: 3

Converting from Boron ppm, the concentration of boric acid in moles/L is:

$[B(OH)_3]^0 = (MW_{B(OH)_3} / MW_B \times \text{Boron}_{\text{ppm}} \times 10^{-6}) \times \text{Mass of Liquid} / MW_{B(OH)_3} \times \text{Density of Liquid} / \text{Mass of Liquid}$. Grouping the limiting cases, we get:

$$\text{LimitingCases}_{\text{ppm}} := \begin{pmatrix} \text{CaseI}_{\text{ppm}} \\ \text{CaseIV}_{\text{ppm}} \end{pmatrix}$$

Calculate corresponding Boric acid mass ratio

$$C_{\text{boric_acid}} := \frac{MW_{\text{BoricAcid}}}{MW_{\text{Boron}}} \cdot \text{LimitingCases}_{\text{ppm}} \cdot 10^{-6}$$

$$C_{\text{boric_acid}} = \begin{pmatrix} 0.0111 \\ 0.0177 \end{pmatrix}$$

For conservatism, the long term cooling density is used

$$\rho := \rho_w + \left(\left(19.665 C_{\text{boric_acid}} + 6.243 C_{\text{boric_acid}}^2 \right) \right) \frac{\text{lb}}{\text{ft}^3}$$

$$\rho = \begin{pmatrix} 61.848 \\ 61.98 \end{pmatrix} \frac{\text{lb}}{\text{ft}^3}$$

Un-dissociated Boric acid concentration

$$\text{BOH3} := \left(\left(\frac{\rho}{MW_{\text{Boron}}} \cdot \text{LimitingCases}_{\text{ppm}} \right) \right) \cdot 10^{-6}$$

$$\text{BOH3} = \begin{pmatrix} 0.1774 \\ 0.2843 \end{pmatrix} \frac{\text{mol}}{\text{L}}$$

Calculation No. 0090-0148-01	Prepared By <i>Marwan Charroek</i>	Checked By <i>[Signature]</i>	Page: 25 Revision: 3
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7.4 Acids Produced by Radiolysis

Based on Input 9 and 12, the amount of Nitric acid produced as NO_3^- is calculated for Case I and IV. Similarly, based on Input 10, 11, and 13 the amount of Hydrochloric acid as Cl^- is calculated.

$$\gamma_{\text{dose}} := 16.84$$

$$\gamma\beta_{\text{dose}} := 567.63$$

$$\text{RadWater}_{\text{mass}} := \left(\begin{array}{l} \sum \text{MinWater}_{\text{mass}} \\ \sum \text{MaxWater}_{\text{mass}} \end{array} \right)$$

$$\text{Cable}_{\text{mass}} := 1213 \text{ lb}$$

$$G_{\text{HNO}_3} := 7.3 \cdot 10^{-6} \frac{\text{mol}}{\text{L}} \cdot \frac{\text{RadWater}_{\text{mass}}}{\rho} \cdot \gamma_{\text{dose}}$$

$$G_{\text{HNO}_3} = \left(\begin{array}{l} 218.9 \\ 258.8 \end{array} \right) \text{ mol}$$

$$G_{\text{HCl}} := 4.6 \cdot 10^{-4} \frac{\text{mol}}{\text{lb}} \cdot \text{Cable}_{\text{mass}} \cdot \gamma\beta_{\text{dose}}$$

$$G_{\text{HCl}} = 316.726 \text{ mol}$$

Concentration quantities considering the volume of the water are

$$\text{HCl} := \frac{\frac{G_{\text{HCl}}}{\text{RadWater}_{\text{mass}}}}{\rho}$$

$$\text{HNO}_3 := \frac{\frac{G_{\text{HNO}_3}}{\text{RadWater}_{\text{mass}}}}{\rho}$$

$$\text{HCl} = \left(\begin{array}{l} 1.779 \times 10^{-4} \\ 1.504 \times 10^{-4} \end{array} \right) \frac{\text{mol}}{\text{L}}$$

$$\text{HNO}_3 = \left(\begin{array}{l} 1.229 \times 10^{-4} \\ 1.229 \times 10^{-4} \end{array} \right) \frac{\text{mol}}{\text{L}}$$

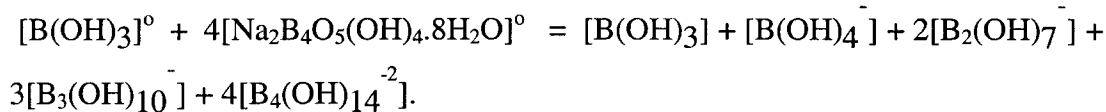
Calculation No. 0090-0148-01	Prepared By <i>Mariam Charoub</i>	Checked By <i>[Signature]</i>	Page: 26 Revision: 2
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7.5 System of Equations

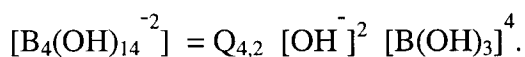
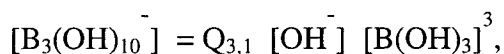
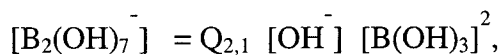
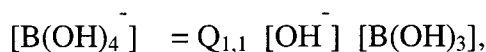
The analysis of the boric acid/borax dissolution and dissociation mechanism is governed by three independent equations which relate the concentrations of the different species in the solution to the pH. The following sections describe the setup of the analytical equations.

7.5.1 Mass Balance

The mass balance for the ionic species is one of the conservation laws that the buffered solution must satisfy (Reference 12, Section 1.5). The dissociation of the initial molecules of boric acid and borax decahydrate produces several ions as discussed in Section 7.1. Therefore, the sum of concentrations of all species of Boron at equilibrium must equal the initial concentration of Boron supplied by both boric acid and sodium tetraborate decahydrate:

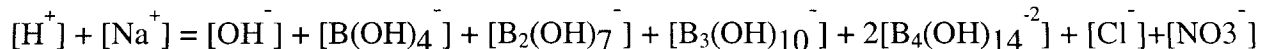


The left-hand side terms are known from the initial concentration of boric acid in the sump, and the mass of borax decahydrate which is a parameter. The terms on the right-hand side are substituted with their corresponding equilibrium quotient expressions, so that only the term $[\text{B}(\text{OH})_3]$ remains in the equation. The substitution involves the following relationships from Section 7.1:



7.5.2 Charge Balance

The charge balance for the ionic species is the second conservation law that the buffered solution must satisfy (Reference 12, Section 1.5). Therefore, electroneutrality of the solution as a whole requires that the sum of all the positive and negative charges add up to zero as such:





Calculation No. 0090-0148-01	Prepared By <i>Alana Chamouk</i>	Checked By <i>[Signature]</i>	Page: 27 Revision: 2
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The concentration of sodium ions is taken to be constant and is determined as twice the concentration of sodium tetraborate decahydrate, since there are two sodium atoms per molecule of sodium tetraborate decahydrate. The concentrations of hydrogen and hydroxide ions are covered in Section 7.5.4 and 7.5.5.

7.5.3 Ionic Strength Balance

The ionic strength I is a measure which counts the ions in solution, with each ionic concentration weighed by the square of its valence (Reference 12, Section 6.1), as formulated in Input 4. Similar to the pH, the Ionic strength is a property of the final equilibrium state of the buffer solution. The ionic strength also comes into play in the activity coefficients of the cations and anions as described by the Debye-Hückel theory (see Input 2). For this reason, in this analysis the ionic strength balance is imposed as a third equation to solve the coupled system of equations, as follows:

$$I = \frac{1}{2} ([H^+] + [Na^+] + [OH^-] + [Cl^-] + [NO_3^-] + [B(OH)_4^-] + [B_2(OH)_7^-] + [B_3(OH)_{10}^-] + 4[B_4(OH)_{14}^{2-}]).$$

7.5.4 Water Dissociation

When accounting for activity corrections in the equilibrium constant for water, the following relationship must be satisfied (Reference 12, Section 6.4):

$$K_w = \gamma_{H^+}[H^+]\gamma_{OH^-}[OH^-].$$

K_w is a function of temperature, and its value at the analysis temperature (see Input 29) is interpolated from the data referenced in Input 5. The activity coefficients for H^+ and OH^- are computed from Inputs 1 and 2.

7.5.5 Determination of pH

By definition, the pH of the solution is

$$pH = -\log(\gamma_{H^+}[H^+]).$$

The pH in this analysis is unknown along with the ionic strength 'I', and the equilibrium concentration of boric acid $[B(OH)_3]$. To start the analysis, a guess is first made for all three variables and the three balance equations are examined to determine the magnitude of the error. The process is iterated until convergence is achieved and a solution pH has been calculated. The mass of sodium tetraborate decahydrate is adjusted until a calculated pH is achieved that satisfies the acceptance criteria.

Calculation No.

0090-0148-01

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Harwan Charoat

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Page: 28

Revision: 2

7.5.6 Chemical Model Validation

As mentioned before, the pH of buffered solutions of boric acid and borax decahydrate has been reported in the literature at varying mixture concentrations. To verify the adequacy of the chemical analysis model described above, the balance equations were solved for a number of input concentrations of initial boric acid and borax. For the eight experimental data points that were modeled, the analytical pH was at most 0.22 units from the experimental pH measurement. In the pH range between 7.0 and 7.5, the model predicted an error of approximately 0.1 pH units. Figure 7-1 below compares the results of the validation to literature data. The details of the validation analysis are given in Appendix A.

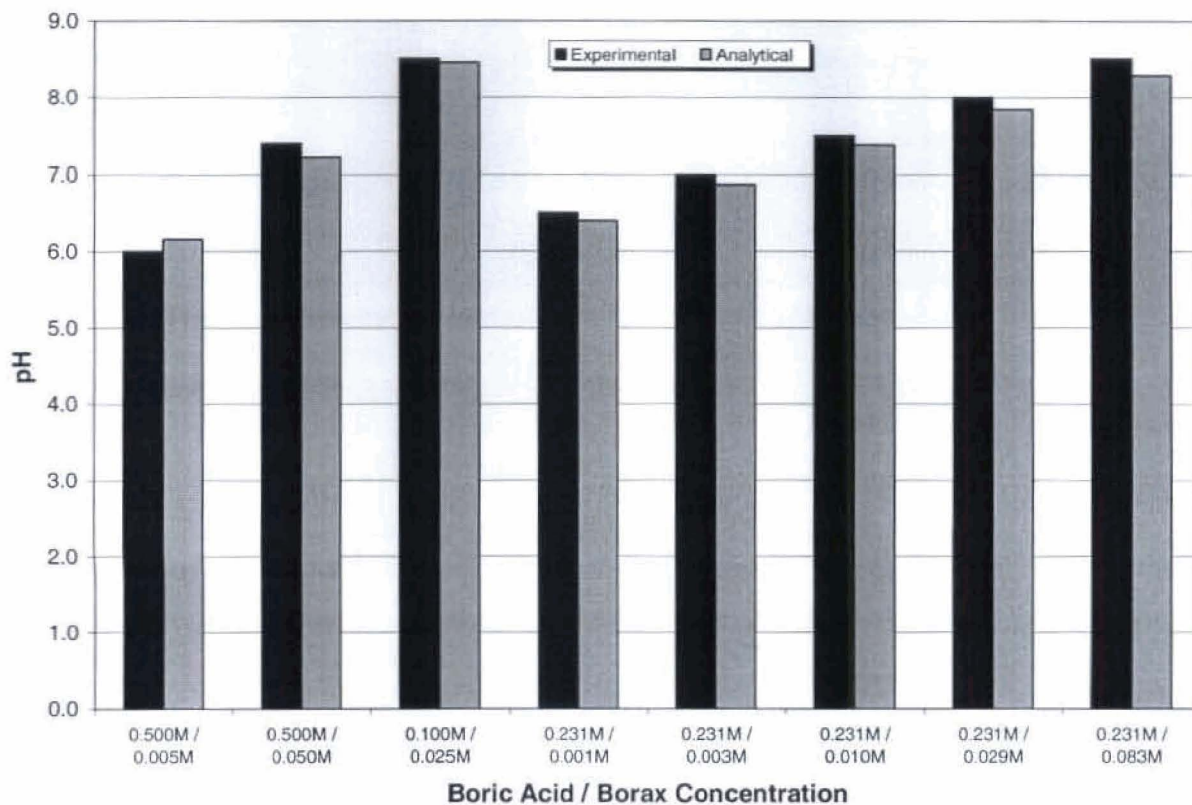


Figure 7-1. Chemical Model Validation Results

Calculation No. 0090-0148-01	Prepared By <i>Maria Chanak</i>	Checked By <i>[Signature]</i>	Page: 29 Revision: 3
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8.0 RESULTS

8.1 Maximum Boric Acid Concentration

Solving for a target pH of 7.0 using the higher initial boric acid concentration of Case IV, the required borax decahydrate concentration that should enter in the containment sump to neutralize the solution is determined to be $[\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}]^0 = 0.0074 \text{ M}$. The calculation steps and the balance equations are given in Appendix B. The borax decahydrate concentration was obtained by trial-and-error to achieve the target pH of 7.0. The absolute mass balance error, the charge balance error, and the ionic strength balance error from the governing equations are each less than 0.0001. The relative errors are also of the same order of magnitude. Therefore, the analytical pH prediction of 7.0 satisfies the first acceptance criterion. This pH value is consistent for 77°F (25°C).

Given the required buffer concentration, the corresponding buffer mass is calculated as such:

[buffer] = moles of borax/liters of solution

where: moles of borax = $\text{Mass}_{\text{Borax}} / \text{MW}_{\text{Borax}}$, and

liters of solution = $(\text{Mass}_{\text{liquid}} + \text{Mass}_{\text{Borax}}) / \text{Density of Sump Liquid}$.

The density of the sump liquid for the buffer mass calculation is determined at the temperature when the recirculation phase starts (at 30 minutes $T = 196^\circ\text{F}$ – Reference 30, and Appendix G). This provides a conservative result since the temperature will decrease at later times. Thus, rearranging to solve for $\text{Mass}_{\text{Borax}}$ using the maximum mass of water from Section 7.2 yields:

$$\text{CaseIV}_{\text{Borax}} := 0.0074 \frac{\text{mol}}{\text{L}} \quad C_{\text{boric_acid}_2} = 0.0177 \quad \text{MW}_{\text{Borax}} = 381.37 \frac{\text{gm}}{\text{mol}}$$

$$\sum \text{MaxWater}_{\text{mass}} = 4608356 \text{ lb} \quad \rho_{\text{ras}} := 60.2 \frac{\text{lb}}{\text{ft}^3} \quad (\text{Input 7})$$

$$\rho_{\text{ras}} := \rho_{\text{w_ras}} + \left(\left[19.665 C_{\text{boric_acid}_2} + 6.243 (C_{\text{boric_acid}_2})^2 \right] \right) \frac{\text{lb}}{\text{ft}^3} \quad (\text{Input 8})$$

$$\rho_{\text{ras}} = 60.55 \frac{\text{lb}}{\text{ft}^3}$$

$$\text{CaseIV}_{\text{BoraxMass}} := \text{CaseIV}_{\text{Borax}} \cdot \frac{\sum \text{MaxWater}_{\text{mass}}}{\rho_{\text{ras}} - \text{CaseIV}_{\text{Borax}} \cdot \text{MW}_{\text{Borax}}} \cdot \text{MW}_{\text{Borax}}$$

$$\text{CaseIV}_{\text{BoraxMass}} = 13448 \text{ lb}$$

Calculation No. 0090-0148-01	Prepared By <i>Maxim Chernov</i>	Checked By <i>[Signature]</i>	Page: 30 Revision: 3
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To determine the corresponding equilibrium Boron concentration that results from the addition of the borax decahydrate buffer, the total mass of Boron must be summed. One mole of NaTB, contains four moles of Boron, and one mole of boric acid contains one mole of Boron. Thus, Concentration of Boron = 4 x Concentration of Borax + 1 x Concentration of Boric Acid.

The limiting total Boron concentration given in Appendix B as part of the pH calculation occurs for Case IV conditions (for pH =7.0 to 7.1). Simplifying:

$$\begin{aligned} \text{TotalBoron}_{\text{conc}} &:= E_{\text{Boron}} \\ \text{TotalBoron}_{\text{conc}} &= 0.3139 \frac{\text{mol}}{\text{L}} \\ \text{TotalBoron}_{\text{ppm}} &:= \frac{\text{TotalBoron}_{\text{conc}} \cdot \text{MW}_{\text{Boron}}}{\rho_{\text{ras}}} \cdot 10^6 \\ \text{TotalBoron}_{\text{ppm}} &= 3498 \end{aligned}$$

Appendix C provides a similar pH calculation for Case IV without the contribution of the radiolysis generated acids. The results are reported here to aid in the surveillance testing of the buffering agent.

$$\begin{aligned} \text{CaseIV_noa}_{\text{Borax}} &:= 0.0072 \frac{\text{mol}}{\text{L}} \\ \text{CaseIV_noa}_{\text{BoraxMass}} &:= \text{CaseIV_noa}_{\text{Borax}} \cdot \frac{\sum \text{MaxWater}_{\text{mass}}}{\rho_{\text{ras}} - \text{CaseIV_noa}_{\text{Borax}} \cdot \text{MW}_{\text{Borax}}} \cdot \text{MW}_{\text{Borax}} \\ \text{CaseIV_noa}_{\text{BoraxMass}} &= 13083 \text{ lb} \end{aligned}$$

Table 8-1 below summarizes the mass of buffer needed to neutralize the different acids, and provides the units in grams per liter.

$$\begin{aligned} \text{CaseIV}_{\text{Borax}} \cdot \text{MW}_{\text{Borax}} &= 2.822 \frac{\text{gm}}{\text{L}} \\ \text{CaseIV_noa}_{\text{Borax}} \cdot \text{MW}_{\text{Borax}} &= 2.746 \frac{\text{gm}}{\text{L}} \end{aligned}$$



Calculation No. 0090-0148-01	Prepared By <i>Marwan Charred</i>	Checked By <i>[Signature]</i>	Page: 31 Revision: 3
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Table 8-1. Borax Decahydrate Concentration and Mass for pH = 7.0

Acid Type	NaTB Quantity Required to Neutralize		
	mol/L	g/L	lb
Boric	0.0072	2.74	13,083
Radiolysis Generated	0.0002 ⁽¹⁾	0.08	365
<i>Total</i>	0.0074	2.82	13,448

Note (1): Effective concentration estimated as 'Total' minus 'Boric'.

8.2 Minimum Boric Acid Concentration

To insure that the predicted amount of buffer does not violate the second acceptance criterion under less acidic sump conditions, the pH for Case I using the above buffer mass must be calculated. First, the initial concentration of borax decahydrate in the Case I water volume must be determined. For conservatism, the higher density of water at 125°F is used. The mass of Borax is conservatively rounded up to establish an upper bound:

$$\text{Deploy BoraxMass} := 13750\text{lb} \quad \sum \text{MinWater}_{\text{mass}} = 3888935\text{lb} \quad \rho_1 = 61.848 \frac{\text{lb}}{\text{ft}^3}$$

$$\text{CaseI Borax} := \frac{\text{Deploy BoraxMass} \cdot \rho_1}{\text{MW Borax} \left(\text{Deploy BoraxMass} + \sum \text{MinWater}_{\text{mass}} \right)}$$

$$\text{CaseI Borax} = 0.0092 \frac{\text{mol}}{\text{L}}$$

The above initial buffer concentration is entered into the pH calculation in Appendix B. The results indicate that the pH is 7.6 at a temperature of 77°F (25°C). Therefore, the calculated buffer mass of 13,750 lb results in a containment sump pH that satisfies the second acceptance criterion.

Calculation No. 0090-0148-01	Prepared By <i>Norman Charouk</i>	Checked By <i>[Signature]</i>	Page: 32 Revision: 2
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8.3 Current Design Basis Case

To compare the mass of NaTB from Case IV required to achieve a final sump pH equal to 7.0 to that of TSP, the current licensing basis case is used to calculate the mass of NaTB for the latter conditions of boric acid concentration and sump water mass. Solving for a target pH of 7.0 using the initial boric acid concentration of Case V, the required borax decahydrate concentration that should enter in the containment sump to neutralize the solution is determined to be $[\text{Na}_2\text{B}_4\text{O}_5(\text{OH})_4 \cdot 8\text{H}_2\text{O}]^0 = 0.0075 \text{ M}$. Fluid properties are evaluated at 25°C (77°F) to reflect the conditions used in Reference 13, Part 1, neglecting the participation of nitric and hydrochloric acids. The input boric acid concentration is calculated in this section. The pH calculation steps and the balance equations are given in Appendix D. The borax decahydrate concentration was obtained by trial-and-error to achieve the target pH. The absolute mass balance error, the charge balance error, and the ionic strength balance error is each less than 0.00001.

$$\text{CaseV ppm} := 3105.5$$

Reference 13,
pg. 18 of Calc. No.
000811-86-C93-02

$$M_{\text{SUMP}} := 4503500 \text{ lb}$$

Boric Acid mass ratio is

$$C_{\text{BA}} := \text{CaseV ppm} \cdot \frac{\text{MW}_{\text{BoricAcid}}}{\text{MW}_{\text{Boron}}} \cdot 10^{-6}$$

$$C_{\text{BA}} = 0.01776$$

$$\rho_{\text{W77F}} := 62.251 \frac{\text{lb}}{\text{ft}^3}$$

pure water density

$$\rho_{\text{sump77}} := \rho_{\text{W77F}} + \left(19.665 C_{\text{BA}} + 6.243 C_{\text{BA}}^2 \right) \frac{\text{lb}}{\text{ft}^3}$$

borated water density

$$\rho_{\text{sump77}} = 62.602 \frac{\text{lb}}{\text{ft}^3}$$

Initial Boric Acid Concentration is

$$\text{InitBoricAcid} := \frac{\rho_{\text{sump77}}}{\text{MW}_{\text{Boron}}} \cdot \text{CaseV ppm} \cdot 10^{-6}$$

$$\text{InitBoricAcid} = 0.2881 \frac{\text{mol}}{\text{L}}$$

input to pH calc - Appendix D

$$\text{CaseV}_{\text{Borax}} := 0.0075 \frac{\text{mol}}{\text{L}}$$

output from pH calc - Appendix D

$$\text{CaseV}_{\text{BoraxMass}} := \text{CaseV}_{\text{Borax}} \cdot \frac{M_{\text{SUMP}}}{\rho_{\text{sump77}} - \text{CaseV}_{\text{Borax}} \cdot \text{MW}_{\text{Borax}}} \cdot \text{MW}_{\text{Borax}}$$

$$\text{CaseV}_{\text{BoraxMass}} = 12882 \text{ lb}$$

Calculation No.
0090-0148-01

Prepared By
Melissa Charney

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Page: 33
Revision: 3

8.4 pH vs. Time

The containment sump pH as a function of time is calculated for the recirculation phase in a postulated LOCA. The recirculation phase begins roughly 30 minutes from the start of the accident (Reference 30). It is assumed that borax granular material would have already dissolved due to the relatively elevated temperature of the water and the rising pool level. The analysis performed in this section, assumes that the buffer mass obtained in Section 8.1 is fully dissolved and mixed with the fluid (Assumption 12). Therefore, the effect of the sump water temperature on the pH can be evaluated. In order to minimize the sump pH transient, Case IV sump conditions with the full acid load of the radiolysis generated acids, which in reality are produced over time, are considered at the start of the transient. In order to maximize the sump pH transient, the production of radiolysis generated acids in Case I sump conditions is considered to occur 12 hours after the start of the transient, with the maximum attainable concentrations released into the water.

The sump water temperatures are selected from Input 29. The following set of times and temperatures are evaluated for the pH transient calculations. The pH computations for Case I and Case IV transients are performed in Appendix B, and the results are summarized in Table 8-2.

Table 8-2. Sump water temperature and pH as a function of time

Hour	°F	°K	pH (Case IV) ⁽¹⁾	pH (Case I) ⁽²⁾
1	194.34	363.34	7.12	7.61
2	193.19	362.70	7.12	7.61
3	190.03	360.95	7.11	7.61
4	186.46	358.96	7.11	7.61
8	177.12	353.77	7.10	7.61
12	169.76	349.68	7.09	7.60
24	154.89	341.42	7.08	7.60
125	160.79	344.70	7.08	7.60
242	153.42	340.61	7.07	7.60
361	145.11	335.99	7.07	7.60
720	125.70	325.20	7.05	7.60

Note (1): Strong acids included in the pH calculation at each time.

Note (2): Strong acids included in the pH calculation from 12 hours.



Calculation No. 0090-0148-01	Prepared By <i>Alwan Charvat</i>	Checked By <i>[Signature]</i>	Page: 34 Revision: 2
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As shown in the above table, the initial higher temperature of the sump water will result in a slightly larger value for the equilibrium pH than at lower temperatures. This can be explained from the dynamics of the equilibrium quotient relationships of Section 7.1. Since 'Q_{xy}' is inversely proportional to temperature (See Input 14), the decrease of water temperature with time leads to higher values for Q_{xy}, thus an increase in the equilibrium concentrations of some dissociated borates in the temperature range of interest. In simple terms, the concentration of positively charged hydrogen ions must increase to maintain electro-neutrality with the negatively charged borate ions, effectively reducing the pH as temperature declines.

In conclusion, the temperature impact on the pH of the sump water is negligible. The results obtained in Sections 8.1 and 8.2 are conservative since the mass or concentration of sodium tetraborate decahydrate fulfills the requirement of pH greater than or equal to 7.0 at ambient temperature. Moreover, at the highest temperature shortly after the initiation of recirculation, the resultant pH is below the upper limit of pH = 8.0.

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Calculation No.

0090-0148-01

Prepared By

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Page: 35

Revision: 2

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Calculation No.

0090-0148-01

Prepared By

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Page: 36

Revision: 2

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Calculation No.

0090-0148-01

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Page: A-1

Revision: 2

A

pH Predictions of Solutions with Boric Acid and Borax Decahydrate

The chemical analysis methodology described in Section 7 was used to predict the theoretical pH value of buffer systems of boric acid and borax decahydrate whose pH was known experimentally. Table A-1 below summarizes the results of the validation analyses. Note that the Reference 5 borax decahydrate concentration was given in g/L (See Figure A-1), so it was converted to molar units and reported in Table A-1.

Table A-1. Results of Validation Using Option I Dissociation Scheme at 298°K (25°C / 77°F)

[Boric Acid] / [Borax]	pH (measured)	pH (calculated)	Reference
0.500M / 0.005M	6.0	6.16	23, Table I
0.500M / 0.050M	7.4	7.21	23, Table I
0.100M / 0.025M	8.5	8.45	24, pg. 682
0.231M / 0.001M	6.5	6.40	5, Figure 5-1
0.231M / 0.003M	7.0	6.87	5, Figure 5-1
0.231M / 0.010M	7.5	7.38	5, Figure 5-1
0.231M / 0.029M	8.0	7.84	5, Figure 5-1
0.231M / 0.083M	8.5	8.28	5, Figure 5-1

The worksheet in this appendix presents the analysis steps undertaken to validate the chemical dissociation methodology. The inputs of this model correspond to the data points in Table A-1. The exact values for pH, equilibrium $B(OH)_3$ concentration, and ionic strength obtained from the iterative program are used to compute the error in the balance equations. The dissociation scheme with option I is used. Individually, the mass balance error, the charge balance error, and the ionic strength balance error is less than 0.0001. The relative errors are also of the same order of magnitude.

Calculation No.
0090-0148-01

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Page: A-2
Revision: 2

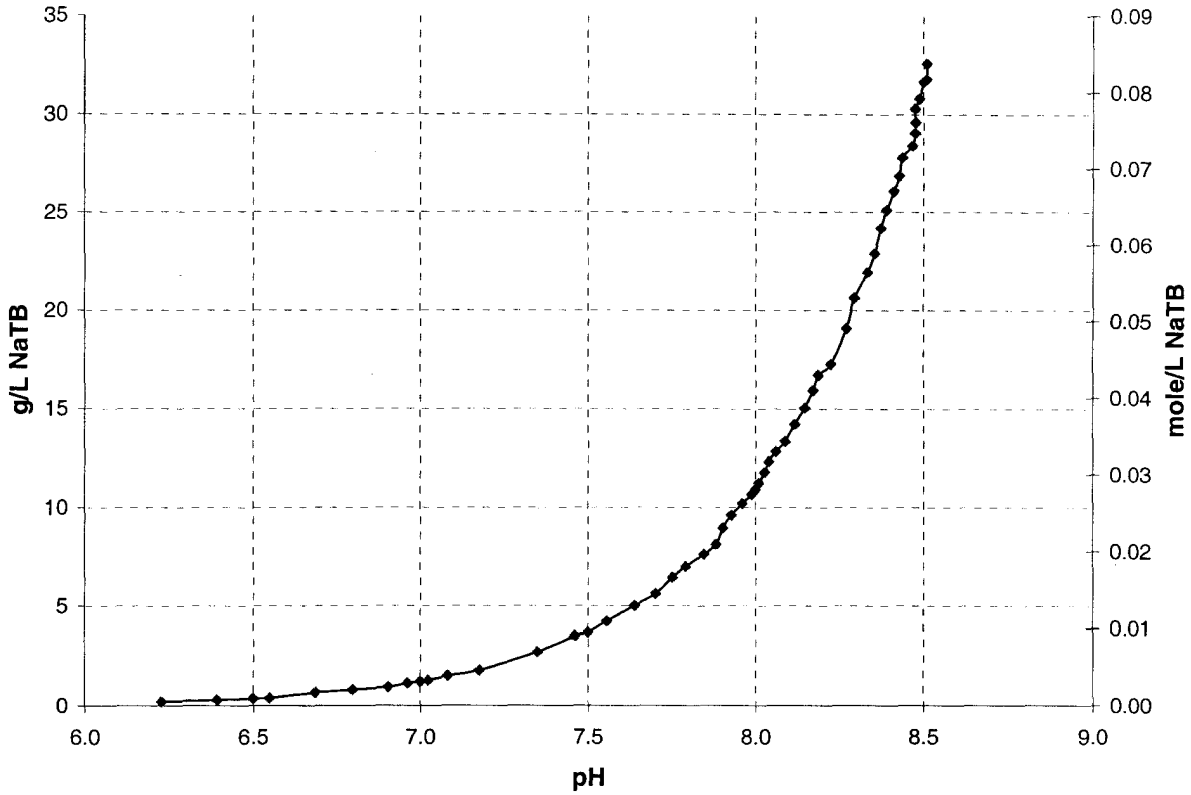


Figure A-1. Adjustment of pH with addition of sodium tetraborate decahydrate to 2500 ppm Boron solution (reproduced from Reference 5)



Calculation No. 0090-0148-01	Prepared By <i>Marcus Charnot</i>	Checked By <i>[Signature]</i>	Page: A-3 Revision: 2
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INPUT

Room Temperature

$$T_k := 298.15 \text{ K}$$

Initial Concentrations (Each row represents a validation case):

$$\text{BoricAcid} := \begin{pmatrix} 0.5 \\ 0.5 \\ 0.1 \\ 0.231 \\ 0.231 \\ 0.231 \\ 0.231 \\ 0.231 \\ 0.231 \end{pmatrix} \frac{\text{mol}}{\text{L}}$$

$$\text{Borax} := \begin{pmatrix} 0.005 \\ 0.05 \\ 0.025 \\ 0.001 \\ 0.003 \\ 0.010 \\ 0.029 \\ 0.083 \end{pmatrix} \frac{\text{mol}}{\text{L}}$$

$$\text{Na} := 2 \cdot \text{Borax}$$

Sodium ion concentration

$$\text{Na} = \begin{pmatrix} 0.01 \\ 0.1 \\ 0.05 \\ 0.002 \\ 0.006 \\ 0.02 \\ 0.058 \\ 0.166 \end{pmatrix} \frac{\text{mol}}{\text{L}}$$

Remove units on variables

$$\text{BoricAcid} := \text{BoricAcid} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{Borax} := \text{Borax} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{Na} := \text{Na} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{TK} := \frac{T_k}{\text{K}}$$

Initial Total Boron Concentration

$$\text{EQ}_{\text{Boron}} := 4 \cdot \text{Borax} + \text{BoricAcid}$$

$$\text{EQ}_{\text{Boron}} = \begin{pmatrix} 0.52 \\ 0.7 \\ 0.2 \\ 0.235 \\ 0.243 \\ 0.271 \\ 0.347 \\ 0.563 \end{pmatrix}$$

Calculation No. 0090-0148-01	Prepared By <i>Melvin Charvat</i>	Checked By <i>[Signature]</i>	Page: A-4 Revision: 2
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CONSTANTS

$a_H := 9$	effective ionic radius of H+
$a_{OH} := 3.5$	effective ionic radius of OH-
$DH_A := .5115$	Debye-Huckel Constants
$DH_B := .3291$	
$K_w := 1.0116 \cdot 10^{-14}$	water equilibrium constant

GUESSES

pH :=	Ionic strength :=	BOH ₃ :=	(6.15629)	(0.01005)	(0.49115)
			7.21160	0.10486	0.42228
			8.44780	0.05431	0.10236
			6.40220	0.00201	0.22977
			6.87007	0.00606	0.22740
			7.38344	0.02058	0.21987
			7.84066	0.06228	0.20417
			8.27814)	(0.19123)	(0.17920)

COMPUTE

$$\gamma_H := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic_strength}}\right)}{1 + DH_B \cdot a_H \cdot \sqrt{\text{Ionic_strength}}}}$$

$$\gamma_{OH} := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic_strength}}\right)}{1 + DH_B \cdot a_{OH} \cdot \sqrt{\text{Ionic_strength}}}}$$



Calculation No. 0090-0148-01	Prepared By <i>Marcus Christoff</i>	Checked By <i>[Signature]</i>	Page: A-5 Revision: 2
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$$\gamma_H = \begin{pmatrix} 0.913 \\ 0.823 \\ 0.85 \\ 0.954 \\ 0.928 \\ 0.888 \\ 0.845 \\ 0.799 \end{pmatrix} \quad \gamma_{OH} = \begin{pmatrix} 0.9 \\ 0.757 \\ 0.805 \\ 0.951 \\ 0.919 \\ 0.865 \\ 0.796 \\ 0.71 \end{pmatrix}$$

$$H_{plus} := \frac{10^{-pH}}{\gamma_H}$$

$$OH_{minus} := \frac{K_w}{H_{plus} \cdot \gamma_H \cdot \gamma_{OH}}$$

$$H_{plus} = \begin{pmatrix} 7.643 \times 10^{-7} \\ 7.464 \times 10^{-8} \\ 4.195 \times 10^{-9} \\ 4.15 \times 10^{-7} \\ 1.453 \times 10^{-7} \\ 4.656 \times 10^{-8} \\ 1.709 \times 10^{-8} \\ 6.596 \times 10^{-9} \end{pmatrix} \quad OH_{minus} = \begin{pmatrix} 1.612 \times 10^{-8} \\ 2.174 \times 10^{-7} \\ 3.522 \times 10^{-6} \\ 2.685 \times 10^{-8} \\ 8.159 \times 10^{-8} \\ 2.828 \times 10^{-7} \\ 8.807 \times 10^{-7} \\ 2.703 \times 10^{-6} \end{pmatrix}$$

Calculation No.
0090-0148-01

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Mawra Charout

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Page: A-6

Revision: 2

$$\log Q_{11} := \left[\frac{1573.21}{TK} + 28.6059 + 0.012078TK - 13.2258 \log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots \right. \\ \left. + -0.0912 \text{Ionic_strength}^{1.5} \right]$$

$$Q_{11} := 10^{\log Q_{11}}$$

$$\log Q_{21} := \left[\frac{2756.1}{TK} - 19.1998 + 0.00033TK + 5.835 \log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots \right. \\ \left. + -0.0912 \text{Ionic_strength}^{1.5} \right]$$

$$Q_{21} := 10^{\log Q_{21}}$$

$$\log Q_{31} := \left[\frac{3339.5}{TK} - 8.3178 + 0.00033TK + 1.497 \log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots \right. \\ \left. + -0.0912 \text{Ionic_strength}^{1.5} \right]$$

$$Q_{31} := 10^{\log Q_{31}}$$

$$\log Q_{42} := \left[\frac{12820}{TK} - 134.7938 + 0.00033TK + 42.105 \log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots \right. \\ \left. + -0.0912 \text{Ionic_strength}^{1.5} \right]$$

$$Q_{42} := 10^{\log Q_{42}}$$



Calculation No. 0090-0148-01	Prepared By <i>Maswa Charant</i>	Checked By <i>[Signature]</i>	Page: A-7 Revision: 2
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$$Q_{11} = \begin{pmatrix} 5.746 \times 10^4 \\ 5.995 \times 10^4 \\ 5.865 \times 10^4 \\ 5.723 \times 10^4 \\ 5.734 \times 10^4 \\ 5.775 \times 10^4 \\ 5.886 \times 10^4 \\ 6.207 \times 10^4 \end{pmatrix}$$

$$Q_{21} = \begin{pmatrix} 3.829 \times 10^4 \\ 3.996 \times 10^4 \\ 3.909 \times 10^4 \\ 3.814 \times 10^4 \\ 3.822 \times 10^4 \\ 3.849 \times 10^4 \\ 3.923 \times 10^4 \\ 4.136 \times 10^4 \end{pmatrix}$$

$$Q_{31} = \begin{pmatrix} 4.872 \times 10^6 \\ 5.084 \times 10^6 \\ 4.974 \times 10^6 \\ 4.853 \times 10^6 \\ 4.863 \times 10^6 \\ 4.897 \times 10^6 \\ 4.992 \times 10^6 \\ 5.263 \times 10^6 \end{pmatrix}$$

$$Q_{42} = \begin{pmatrix} 3.1 \times 10^{12} \\ 3.235 \times 10^{12} \\ 3.165 \times 10^{12} \\ 3.087 \times 10^{12} \\ 3.094 \times 10^{12} \\ 3.116 \times 10^{12} \\ 3.176 \times 10^{12} \\ 3.349 \times 10^{12} \end{pmatrix}$$



Calculation No.
 0090-0148-01

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Maria Charrat

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Page: A-8
 Revision: 2

$$BOH4 := \overrightarrow{(Q_{11} \cdot OH_{\text{minus}} \cdot BOH_3)}$$

$$B2OH7 := \overrightarrow{(Q_{21} \cdot OH_{\text{minus}} \cdot BOH_3^2)}$$

$$B3OH10 := \overrightarrow{(Q_{31} \cdot OH_{\text{minus}} \cdot BOH_3^3)}$$

$$B4OH14 := \overrightarrow{(Q_{42} \cdot OH_{\text{minus}}^2 \cdot BOH_3^4)}$$

$$BOH4 = \begin{pmatrix} 4.548 \times 10^{-4} \\ 5.504 \times 10^{-3} \\ 2.115 \times 10^{-2} \\ 3.531 \times 10^{-4} \\ 1.064 \times 10^{-3} \\ 3.59 \times 10^{-3} \\ 1.058 \times 10^{-2} \\ 3.007 \times 10^{-2} \end{pmatrix}$$

$$B2OH7 = \begin{pmatrix} 1.489 \times 10^{-4} \\ 1.549 \times 10^{-3} \\ 1.443 \times 10^{-3} \\ 5.407 \times 10^{-5} \\ 1.612 \times 10^{-4} \\ 5.261 \times 10^{-4} \\ 1.44 \times 10^{-3} \\ 3.591 \times 10^{-3} \end{pmatrix}$$

$$B3OH10 = \begin{pmatrix} 9.304 \times 10^{-3} \\ 8.323 \times 10^{-2} \\ 1.879 \times 10^{-2} \\ 1.581 \times 10^{-3} \\ 4.665 \times 10^{-3} \\ 1.472 \times 10^{-2} \\ 3.741 \times 10^{-2} \\ 8.188 \times 10^{-2} \end{pmatrix}$$

$$B4OH14 = \begin{pmatrix} 4.685 \times 10^{-5} \\ 4.861 \times 10^{-3} \\ 4.309 \times 10^{-3} \\ 6.206 \times 10^{-6} \\ 5.507 \times 10^{-5} \\ 5.822 \times 10^{-4} \\ 4.28 \times 10^{-3} \\ 2.524 \times 10^{-2} \end{pmatrix}$$



Calculation No.
0090-0148-01

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Page: A-9
Revision: 2

MASS BALANCE ERROR

$$\text{Sum Boron} := \text{BOH}_3 + \text{BOH}_4 + 2 \cdot \text{B}_2\text{OH}_7 + 3 \cdot \text{B}_3\text{OH}_{10} + 4 \cdot \text{B}_4\text{OH}_{14}$$

$$\text{MBE} := \text{EQ}_{\text{Boron}} - \text{Sum}_{\text{Boron}}$$

$$\text{MBE} = \begin{pmatrix} -8.463 \times 10^{-7} \\ -9.471 \times 10^{-6} \\ 7.949 \times 10^{-6} \\ 1.294 \times 10^{-6} \\ -2.466 \times 10^{-6} \\ 2.602 \times 10^{-6} \\ 5.869 \times 10^{-8} \\ -3.346 \times 10^{-5} \end{pmatrix}$$

$$\text{Sum}_{\text{Boron}} = \begin{pmatrix} 0.520001 \\ 0.700009 \\ 0.199992 \\ 0.234999 \\ 0.243002 \\ 0.270997 \\ 0.347 \\ 0.563033 \end{pmatrix}$$

CHARGE BALANCE ERROR

$$\text{Pos}_{\text{charge}} := \text{H}_{\text{plus}} + \text{Na}$$

$$\text{Neg}_{\text{charge}} := \text{OH}_{\text{minus}} + \text{BOH}_4 + \text{B}_2\text{OH}_7 + \text{B}_3\text{OH}_{10} + 2 \cdot \text{B}_4\text{OH}_{14}$$


$$\text{CBE} := \text{Pos}_{\text{charge}} - \text{Neg}_{\text{charge}}$$

$$\text{CBE} = \begin{pmatrix} -2.557 \times 10^{-7} \\ -2.738 \times 10^{-6} \\ 1.848 \times 10^{-6} \\ -7.811 \times 10^{-8} \\ -4.614 \times 10^{-7} \\ 2.805 \times 10^{-7} \\ -3.838 \times 10^{-7} \\ -1.298 \times 10^{-5} \end{pmatrix}$$

$$\text{Pos}_{\text{charge}} = \begin{pmatrix} 0.01 \\ 0.1 \\ 0.05 \\ 0.002 \\ 0.006 \\ 0.02 \\ 0.058 \\ 0.166 \end{pmatrix}$$

$$\text{Neg}_{\text{charge}} = \begin{pmatrix} 0.010001 \\ 0.100003 \\ 0.049998 \\ 0.002 \\ 0.006001 \\ 0.02 \\ 0.058 \\ 0.166013 \end{pmatrix}$$



Calculation No. 0090-0148-01	Prepared By <i>Marwa Charrouf</i>	Checked By 	Page: A-10 Revision: 2
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IONIC STRENGTH BALANCE ERROR

$$\text{Sum}_{\text{Ions}} := \frac{1}{2} \cdot (\text{Na} + \text{H}_{\text{plus}} + \text{OH}_{\text{minus}} + \text{BOH4} + \text{B2OH7} + \text{B3OH10} + 4 \cdot \text{B4OH14})$$

$$\text{SBE} := \text{Ionic}_{\text{strength}} - \text{Sum}_{\text{Ions}}$$

$$\text{SBE} = \begin{pmatrix} 2.255 \times 10^{-6} \\ -2.361 \times 10^{-6} \\ 1.665 \times 10^{-6} \\ 3.34 \times 10^{-6} \\ 4.557 \times 10^{-6} \\ -2.089 \times 10^{-6} \\ -3.389 \times 10^{-7} \\ -1.242 \times 10^{-5} \end{pmatrix}$$

$$\text{Sum}_{\text{Ions}} = \begin{pmatrix} 0.010048 \\ 0.104862 \\ 0.054308 \\ 0.002007 \\ 0.006055 \\ 0.020582 \\ 0.06228 \\ 0.191242 \end{pmatrix}$$



Calculation No.
0090-0148-01

Prepared By
Marina Chernov

Checked By
[Signature]

Page: B-1
Revision: 3

B

Containment Sump pH as a Function of Temperature

This appendix implements the methodology discussed in Section 7.5. The temperature of the fluid determines the constants to be used. The input concentrations are obtained from Sections 7.3 and 7.4. The two limiting cases for boric acid concentration are analyzed via a horizontal array containing two elements, while vertical arrays are used for the temperature variation, whereby each pH column representing a boric acid concentration.

INPUT

Temperature Array

$$T_k := \begin{pmatrix} 363.34 \\ 362.70 \\ 360.95 \\ 358.96 \\ 353.77 \\ 349.68 \\ 341.42 \\ 344.70 \\ 340.61 \\ 335.99 \\ 325.20 \\ 298.15 \end{pmatrix} K$$

Initial **Case IV** and **Case I** Concentrations:

$$\text{Boric Acid} := (0.2843 \quad 0.1774) \frac{\text{mol}}{\text{L}}$$

$$\text{Borax} := (0.0074 \quad 0.0092) \frac{\text{mol}}{\text{L}}$$

Sodium ion concentration

$$\text{Na} := 2 \cdot \text{Borax}$$

$$\text{Na} = (0.015 \quad 0.018) \frac{\text{mol}}{\text{L}}$$

Chloride ion concentration

$$\text{Cl} := (1.504 \cdot 10^{-4} \quad 1.779 \cdot 10^{-4}) \frac{\text{mol}}{\text{L}}$$

Nitrate ion concentration

$$\text{NO}_3 := (1.229 \cdot 10^{-4} \quad 1.229 \cdot 10^{-4}) \frac{\text{mol}}{\text{L}}$$

Initial Total Boron Concentration

$$\text{EQ}_{\text{Boron}} := 4 \cdot \text{Borax} + \text{Boric Acid}$$

$$\text{EQ}_{\text{Boron}} = (0.3139 \quad 0.2142)$$

Remove units on variables

$$\text{Boric Acid} := \text{Boric Acid} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{Borax} := \text{Borax} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{Na} := \text{Na} \cdot \frac{\text{L}}{\text{mol}} \quad \text{Cl} := \text{Cl} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{TK} := \frac{T_k}{K} \quad \text{NO}_3 := \text{NO}_3 \cdot \frac{\text{L}}{\text{mol}}$$



Calculation No. 0090-0148-01	Prepared By <i>Marwa Chemsak</i>	Checked By <i>[Signature]</i>	Page: B-2 Revision: 3
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CONSTANTS

$a_{H^+} := 9$ effective ionic radius of H^+
 $a_{OH^-} := 3.5$ effective ionic radius of OH^-

Debye-Huckel Constants at each temperature

water equilibrium constant at each temperature

$DH_A :=$ (0.5923
0.5913
0.5886
0.5855
0.5776
0.5717
0.5602
0.5647
0.5591
0.5530
0.5397
0.5115)

$DH_B :=$ (0.3457
0.3455
0.3449
0.3443
0.3428
0.3416
0.3393
0.3401
0.3390
0.3378
0.3351
0.3291)

$K_w :=$ (3.735 10⁻¹³
3.639 10⁻¹³
3.387 10⁻¹³
3.122 10⁻¹³
2.503 10⁻¹³
2.084 10⁻¹³
1.409 10⁻¹³
1.652 10⁻¹³
1.354 10⁻¹³
1.072 10⁻¹³
5.963 10⁻¹⁴
1.011610⁻¹⁴)

GUESSES

$pH :=$ (7.11927 7.61491
7.11809 7.61481
7.11482 7.61455
7.11051 7.61370
7.09966 7.61207
7.09182 7.60203
7.07618 7.60170
7.08246 7.60184
7.07462 7.60167
7.06587 7.60169
7.04618 7.60273
7.00780 7.61179)

Ionic strength := (0.01485 0.01849
0.01485 0.01849
0.01485 0.01849
0.01486 0.01850
0.01486 0.01851
0.01487 0.01852
0.01488 0.01855
0.01487 0.01853
0.01488 0.01855
0.01489 0.01857
0.01491 0.01863
0.01504 0.01900)

$BOH_3 :=$ (0.28101 0.17983
0.28094 0.17975
0.28076 0.17952
0.28055 0.17926
0.28000 0.17856
0.27957 0.17854
0.27872 0.17737
0.27906 0.17784
0.27863 0.17726
0.27816 0.17659
0.27710 0.17498
0.27484 0.17104)

Calculation No.
0090-0148-01

Prepared By
Maria Charro

Checked By
[Signature]

Page: B-3
Revision: 3

COMPUTE

$$\gamma_{H_CaseIV} := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic_strength}^{(1)}}\right)}{1+DH_B \cdot a_H \cdot \sqrt{\text{Ionic_strength}^{(1)}}}$$

$$\gamma_{OH_CaseIV} := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic_strength}^{(1)}}\right)}{1+DH_B \cdot a_{OH} \cdot \sqrt{\text{Ionic_strength}^{(1)}}}$$

$$\gamma_{H_CaseI} := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic_strength}^{(2)}}\right)}{1+DH_B \cdot a_H \cdot \sqrt{\text{Ionic_strength}^{(2)}}}$$

$$\gamma_{OH_CaseI} := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic_strength}^{(2)}}\right)}{1+DH_B \cdot a_{OH} \cdot \sqrt{\text{Ionic_strength}^{(2)}}}$$

- 0.886
- 0.887
- 0.887
- 0.888
- 0.889
- 0.89
- 0.892
- 0.891
- 0.892
- 0.893
- 0.895
- 0.899

- 0.865
- 0.865
- 0.866
- 0.866
- 0.868
- 0.869
- 0.872
- 0.871
- 0.872
- 0.873
- 0.876
- 0.881

- 0.878
- 0.878
- 0.878
- 0.879
- 0.88
- 0.881
- 0.883
- 0.883
- 0.883
- 0.885
- 0.887
- 0.891

- 0.853
- 0.853
- 0.854
- 0.854
- 0.856
- 0.857
- 0.86
- 0.859
- 0.86
- 0.861
- 0.864
- 0.869

$$H_{plus_CaseIV} := \frac{10^{-pH^{(1)}}}{\gamma_{H_CaseIV}}$$

$$H_{plus_CaseI} := \frac{10^{-pH^{(2)}}}{\gamma_{H_CaseI}}$$

$$OH_{minus_CaseIV} := \frac{K_w}{H_{plus_CaseIV} \cdot \gamma_{H_CaseIV} \cdot \gamma_{OH_CaseIV}}$$

$$OH_{minus_CaseI} := \frac{K_w}{H_{plus_CaseI} \cdot \gamma_{H_CaseI} \cdot \gamma_{OH_CaseI}}$$



Calculation No. 0090-0148-01	Prepared By <i>Monica Chamick</i>	Checked By <i>[Signature]</i>	Page: B-4 Revision: 3
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$$H_{\text{plus_CaseIV}} = \begin{pmatrix} 8.572 \times 10^{-8} \\ 8.593 \times 10^{-8} \\ 8.654 \times 10^{-8} \\ 8.736 \times 10^{-8} \\ 8.943 \times 10^{-8} \\ 9.097 \times 10^{-8} \\ 9.41 \times 10^{-8} \\ 9.283 \times 10^{-8} \\ 9.442 \times 10^{-8} \\ 9.624 \times 10^{-8} \\ 1.005 \times 10^{-7} \\ 1.092 \times 10^{-7} \end{pmatrix}$$

$$OH_{\text{minus_CaseIV}} = \begin{pmatrix} 5.682 \times 10^{-6} \\ 5.519 \times 10^{-6} \\ 5.095 \times 10^{-6} \\ 4.647 \times 10^{-6} \\ 3.627 \times 10^{-6} \\ 2.962 \times 10^{-6} \\ 1.927 \times 10^{-6} \\ 2.294 \times 10^{-6} \\ 1.844 \times 10^{-6} \\ 1.429 \times 10^{-6} \\ 7.573 \times 10^{-7} \\ 1.169 \times 10^{-7} \end{pmatrix}$$

$$H_{\text{plus_CaseI}} = \begin{pmatrix} 2.765 \times 10^{-8} \\ 2.765 \times 10^{-8} \\ 2.765 \times 10^{-8} \\ 2.769 \times 10^{-8} \\ 2.775 \times 10^{-8} \\ 2.837 \times 10^{-8} \\ 2.833 \times 10^{-8} \\ 2.834 \times 10^{-8} \\ 2.832 \times 10^{-8} \\ 2.829 \times 10^{-8} \\ 2.815 \times 10^{-8} \\ 2.743 \times 10^{-8} \end{pmatrix}$$

$$OH_{\text{minus_CaseI}} = \begin{pmatrix} 1.805 \times 10^{-5} \\ 1.757 \times 10^{-5} \\ 1.633 \times 10^{-5} \\ 1.502 \times 10^{-5} \\ 1.197 \times 10^{-5} \\ 9.724 \times 10^{-6} \\ 6.551 \times 10^{-6} \\ 7.691 \times 10^{-6} \\ 6.293 \times 10^{-6} \\ 4.975 \times 10^{-6} \\ 2.765 \times 10^{-6} \\ 4.76 \times 10^{-7} \end{pmatrix}$$

Calculation No. 0090-0148-01	Prepared By <i>Maria Chavez</i>	Checked By <i>[Signature]</i>	Page: B-5 Revision: 3
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$$\log Q_{11_CaseIV} := \left[\begin{array}{l} \frac{1573.21}{TK} + 28.6059 + 0.012078TK - 13.2258 \log(TK) \dots \\ + (0.325 - 0.00033TK) \cdot \text{Ionic_strength}^{(1)} \dots \\ + -0.0912 \left(\text{Ionic_strength}^{(1)} \right)^{1.5} \end{array} \right]$$

$$Q_{11_CaseIV} := 10^{\log Q_{11_CaseIV}}$$

$$\log Q_{11_CaseI} := \left[\begin{array}{l} \frac{1573.21}{TK} + 28.6059 + 0.012078TK - 13.2258 \log(TK) \dots \\ + (0.325 - 0.00033TK) \cdot \text{Ionic_strength}^{(2)} \dots \\ + -0.0912 \left(\text{Ionic_strength}^{(2)} \right)^{1.5} \end{array} \right]$$

$$Q_{11_CaseI} := 10^{\log Q_{11_CaseI}}$$

$$\log Q_{21_CaseIV} := \left[\begin{array}{l} \frac{2756.1}{TK} - 19.1998 + 0.00033TK + 5.835 \log(TK) \dots \\ + (0.325 - 0.00033TK) \cdot \text{Ionic_strength}^{(1)} \dots \\ + -0.0912 \left(\text{Ionic_strength}^{(1)} \right)^{1.5} \end{array} \right]$$

$$Q_{21_CaseIV} := 10^{\log Q_{21_CaseIV}}$$

$$\log Q_{21_CaseI} := \left[\begin{array}{l} \frac{2756.1}{TK} - 19.1998 + 0.00033TK + 5.835 \log(TK) \dots \\ + (0.325 - 0.00033TK) \cdot \text{Ionic_strength}^{(2)} \dots \\ + -0.0912 \left(\text{Ionic_strength}^{(2)} \right)^{1.5} \end{array} \right]$$

$$Q_{21_CaseI} := 10^{\log Q_{21_CaseI}}$$

Calculation No. 0090-0148-01	Prepared By <i>Mona Chomik</i>	Checked By <i>[Signature]</i>	Page: B-6 Revision: 3
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$$\log Q_{31_CaseIV} := \left[\begin{aligned} &\frac{3339.5}{TK} - 8.3178 + 0.00033TK + 1.497 \log(TK) \dots \\ &+ (0.325 - 0.00033TK) \cdot \text{Ionic_strength}^{(1)} \dots \\ &+ -0.0912 \left(\text{Ionic_strength}^{(1)} \right)^{1.5} \end{aligned} \right]$$

$$Q_{31_CaseIV} := 10^{\log Q_{31_CaseIV}}$$

$$\log Q_{31_CaseI} := \left[\begin{aligned} &\frac{3339.5}{TK} - 8.3178 + 0.00033TK + 1.497 \log(TK) \dots \\ &+ (0.325 - 0.00033TK) \cdot \text{Ionic_strength}^{(2)} \dots \\ &+ -0.0912 \left(\text{Ionic_strength}^{(2)} \right)^{1.5} \end{aligned} \right]$$

$$Q_{31_CaseI} := 10^{\log Q_{31_CaseI}}$$

$$\log Q_{42_CaseIV} := \left[\begin{aligned} &\frac{12820}{TK} - 134.7938 + 0.00033TK + 42.105 \log(TK) \dots \\ &+ (0.325 - 0.00033TK) \cdot \text{Ionic_strength}^{(1)} \dots \\ &+ -0.0912 \left(\text{Ionic_strength}^{(1)} \right)^{1.5} \end{aligned} \right]$$

$$Q_{42_CaseIV} := 10^{\log Q_{42_CaseIV}}$$

$$\log Q_{42_CaseI} := \left[\begin{aligned} &\frac{12820}{TK} - 134.7938 + 0.00033TK + 42.105 \log(TK) \dots \\ &+ (0.325 - 0.00033TK) \cdot \text{Ionic_strength}^{(2)} \dots \\ &+ -0.0912 \left(\text{Ionic_strength}^{(2)} \right)^{1.5} \end{aligned} \right]$$

$$Q_{42_CaseI} := 10^{\log Q_{42_CaseI}}$$



Calculation No. 0090-0148-01	Prepared By <i>Marwa Charouf</i>	Checked By <i>[Signature]</i>	Page: B-7 Revision: 3
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$$Q_{11_CaseIV} = \begin{pmatrix} 2.917 \times 10^3 \\ 2.985 \times 10^3 \\ 3.181 \times 10^3 \\ 3.424 \times 10^3 \\ 4.167 \times 10^3 \\ 4.889 \times 10^3 \\ 6.849 \times 10^3 \\ 5.977 \times 10^3 \\ 7.087 \times 10^3 \\ 8.642 \times 10^3 \\ 1.41 \times 10^4 \\ 5.76 \times 10^4 \end{pmatrix}$$

$$Q_{11_CaseI} = \begin{pmatrix} 2.921 \times 10^3 \\ 2.989 \times 10^3 \\ 3.186 \times 10^3 \\ 3.429 \times 10^3 \\ 4.173 \times 10^3 \\ 4.897 \times 10^3 \\ 6.86 \times 10^3 \\ 5.987 \times 10^3 \\ 7.099 \times 10^3 \\ 8.657 \times 10^3 \\ 1.412 \times 10^4 \\ 5.771 \times 10^4 \end{pmatrix}$$

$$Q_{21_CaseIV} = \begin{pmatrix} 2.805 \times 10^3 \\ 2.861 \times 10^3 \\ 3.024 \times 10^3 \\ 3.223 \times 10^3 \\ 3.822 \times 10^3 \\ 4.392 \times 10^3 \\ 5.889 \times 10^3 \\ 5.231 \times 10^3 \\ 6.067 \times 10^3 \\ 7.213 \times 10^3 \\ 1.107 \times 10^4 \\ 3.838 \times 10^4 \end{pmatrix}$$

$$Q_{21_CaseI} = \begin{pmatrix} 2.809 \times 10^3 \\ 2.866 \times 10^3 \\ 3.029 \times 10^3 \\ 3.228 \times 10^3 \\ 3.828 \times 10^3 \\ 4.399 \times 10^3 \\ 5.899 \times 10^3 \\ 5.239 \times 10^3 \\ 6.077 \times 10^3 \\ 7.225 \times 10^3 \\ 1.109 \times 10^4 \\ 3.846 \times 10^4 \end{pmatrix}$$

$$Q_{31_CaseIV} = \begin{pmatrix} 6.744 \times 10^4 \\ 6.978 \times 10^4 \\ 7.668 \times 10^4 \\ 8.545 \times 10^4 \\ 1.14 \times 10^5 \\ 1.441 \times 10^5 \\ 2.352 \times 10^5 \\ 1.93 \times 10^5 \\ 2.471 \times 10^5 \\ 3.291 \times 10^5 \\ 6.643 \times 10^5 \\ 4.884 \times 10^6 \end{pmatrix}$$

$$Q_{31_CaseI} = \begin{pmatrix} 6.754 \times 10^4 \\ 6.989 \times 10^4 \\ 7.68 \times 10^4 \\ 8.559 \times 10^4 \\ 1.142 \times 10^5 \\ 1.443 \times 10^5 \\ 2.356 \times 10^5 \\ 1.933 \times 10^5 \\ 2.475 \times 10^5 \\ 3.296 \times 10^5 \\ 6.654 \times 10^5 \\ 4.894 \times 10^6 \end{pmatrix}$$

Calculation No. 0090-0148-01	Prepared By <i>Marina Charouf</i>	Checked By <i>[Signature]</i>	Page: B-8 Revision: 3
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$$\begin{array}{l}
 Q_{42_CaseIV} = \begin{pmatrix} 2.599 \times 10^8 \\ 2.783 \times 10^8 \\ 3.364 \times 10^8 \\ 4.189 \times 10^8 \\ 7.551 \times 10^8 \\ 1.224 \times 10^9 \\ 3.428 \times 10^9 \\ 2.258 \times 10^9 \\ 3.808 \times 10^9 \\ 7.03 \times 10^9 \\ 3.255 \times 10^{10} \\ 3.107 \times 10^{12} \end{pmatrix}
 \end{array}
 \qquad
 \begin{array}{l}
 Q_{42_CaseI} = \begin{pmatrix} 2.603 \times 10^8 \\ 2.788 \times 10^8 \\ 3.37 \times 10^8 \\ 4.195 \times 10^8 \\ 7.563 \times 10^8 \\ 1.226 \times 10^9 \\ 3.434 \times 10^9 \\ 2.261 \times 10^9 \\ 3.814 \times 10^9 \\ 7.042 \times 10^9 \\ 3.261 \times 10^{10} \\ 3.113 \times 10^{12} \end{pmatrix}
 \end{array}$$

$$BOH4_CaseIV := \overrightarrow{(Q_{11_CaseIV} \cdot OH_{minus_CaseIV} \cdot BOH_3^{(1)})}$$

$$BOH4_CaseI := \overrightarrow{(Q_{11_CaseI} \cdot OH_{minus_CaseI} \cdot BOH_3^{(2)})}$$

$$B2OH7_CaseIV := \overrightarrow{[Q_{21_CaseIV} \cdot OH_{minus_CaseIV} \cdot (BOH_3^{(1)})^2]}$$

$$B2OH7_CaseI := \overrightarrow{[Q_{21_CaseI} \cdot OH_{minus_CaseI} \cdot (BOH_3^{(2)})^2]}$$

$$B3OH10_CaseIV := \overrightarrow{[Q_{31_CaseIV} \cdot OH_{minus_CaseIV} \cdot (BOH_3^{(1)})^3]}$$

$$B3OH10_CaseI := \overrightarrow{[Q_{31_CaseI} \cdot OH_{minus_CaseI} \cdot (BOH_3^{(2)})^3]}$$

$$B4OH14_CaseIV := \overrightarrow{[Q_{42_CaseIV} \cdot OH_{minus_CaseIV}^2 \cdot (BOH_3^{(1)})^4]}$$

$$B4OH14_CaseI := \overrightarrow{[Q_{42_CaseI} \cdot OH_{minus_CaseI}^2 \cdot (BOH_3^{(2)})^4]}$$



Calculation No.

0090-0148-01

Prepared By

Merina Charro

Checked By

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Page: B-9

Revision: 3

BOH4_CaseIV = $\left(\begin{array}{l} 4.656 \times 10^{-3} \\ 4.628 \times 10^{-3} \\ 4.551 \times 10^{-3} \\ 4.463 \times 10^{-3} \\ 4.231 \times 10^{-3} \\ 4.048 \times 10^{-3} \\ 3.678 \times 10^{-3} \\ 3.826 \times 10^{-3} \\ 3.642 \times 10^{-3} \\ 3.435 \times 10^{-3} \\ 2.959 \times 10^{-3} \\ 1.85 \times 10^{-3} \end{array} \right)$

BOH4_CaseI = $\left(\begin{array}{l} 9.479 \times 10^{-3} \\ 9.443 \times 10^{-3} \\ 9.343 \times 10^{-3} \\ 9.23 \times 10^{-3} \\ 8.92 \times 10^{-3} \\ 8.501 \times 10^{-3} \\ 7.971 \times 10^{-3} \\ 8.189 \times 10^{-3} \\ 7.918 \times 10^{-3} \\ 7.605 \times 10^{-3} \\ 6.833 \times 10^{-3} \\ 4.698 \times 10^{-3} \end{array} \right)$

B2OH7_CaseIV = $\left(\begin{array}{l} 1.258 \times 10^{-3} \\ 1.246 \times 10^{-3} \\ 1.215 \times 10^{-3} \\ 1.179 \times 10^{-3} \\ 1.087 \times 10^{-3} \\ 1.017 \times 10^{-3} \\ 8.814 \times 10^{-4} \\ 9.344 \times 10^{-4} \\ 8.687 \times 10^{-4} \\ 7.976 \times 10^{-4} \\ 6.436 \times 10^{-4} \\ 3.389 \times 10^{-4} \end{array} \right)$

B2OH7_CaseI = $\left(\begin{array}{l} 1.639 \times 10^{-3} \\ 1.627 \times 10^{-3} \\ 1.594 \times 10^{-3} \\ 1.558 \times 10^{-3} \\ 1.461 \times 10^{-3} \\ 1.364 \times 10^{-3} \\ 1.216 \times 10^{-3} \\ 1.274 \times 10^{-3} \\ 1.202 \times 10^{-3} \\ 1.121 \times 10^{-3} \\ 9.386 \times 10^{-4} \\ 5.356 \times 10^{-4} \end{array} \right)$



Calculation No.
0090-0148-01

Prepared By

Morgan Charnock

Checked By

[Signature]

Page: B-10

Revision: 3

B3OH10_CaseIV = $\left(\begin{array}{l} 8.502 \times 10^{-3} \\ 8.54 \times 10^{-3} \\ 8.647 \times 10^{-3} \\ 8.769 \times 10^{-3} \\ 9.08 \times 10^{-3} \\ 9.324 \times 10^{-3} \\ 9.81 \times 10^{-3} \\ 9.623 \times 10^{-3} \\ 9.857 \times 10^{-3} \\ 1.012 \times 10^{-2} \\ 1.07 \times 10^{-2} \\ 1.185 \times 10^{-2} \end{array} \right)$

B3OH10_CaseI = $\left(\begin{array}{l} 7.088 \times 10^{-3} \\ 7.133 \times 10^{-3} \\ 7.258 \times 10^{-3} \\ 7.403 \times 10^{-3} \\ 7.784 \times 10^{-3} \\ 7.986 \times 10^{-3} \\ 8.611 \times 10^{-3} \\ 8.364 \times 10^{-3} \\ 8.675 \times 10^{-3} \\ 9.03 \times 10^{-3} \\ 9.857 \times 10^{-3} \\ 1.166 \times 10^{-2} \end{array} \right)$

B4OH14_CaseIV = $\left(\begin{array}{l} 5.23 \times 10^{-5} \\ 5.281 \times 10^{-5} \\ 5.427 \times 10^{-5} \\ 5.603 \times 10^{-5} \\ 6.106 \times 10^{-5} \\ 6.561 \times 10^{-5} \\ 7.679 \times 10^{-5} \\ 7.205 \times 10^{-5} \\ 7.805 \times 10^{-5} \\ 8.594 \times 10^{-5} \\ 1.101 \times 10^{-4} \\ 2.423 \times 10^{-4} \end{array} \right)$

B4OH14_CaseI = $\left(\begin{array}{l} 8.863 \times 10^{-5} \\ 8.986 \times 10^{-5} \\ 9.338 \times 10^{-5} \\ 9.768 \times 10^{-5} \\ 1.102 \times 10^{-4} \\ 1.178 \times 10^{-4} \\ 1.458 \times 10^{-4} \\ 1.338 \times 10^{-4} \\ 1.491 \times 10^{-4} \\ 1.695 \times 10^{-4} \\ 2.337 \times 10^{-4} \\ 6.038 \times 10^{-4} \end{array} \right)$



Calculation No. 0090-0148-01	Prepared By <i>Marianne Charvat</i>	Checked By <i>[Signature]</i>	Page: B-11 Revision: 3
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REGROUP

$BOH4 := (BOH4_CaseIV \ BOH4_CaseI)$

$H_{plus} := (H_{plus_CaseIV} \ H_{plus_CaseI})$

$B2OH7 := (B2OH7_CaseIV \ B2OH7_CaseI)$

$OH_{minus} := (OH_{minus_CaseIV} \ OH_{minus_CaseI})$

$B3OH10 := (B3OH10_CaseIV \ B3OH10_CaseI)$

$B4OH14 := (B4OH14_CaseIV \ B4OH14_CaseI)$

MASS BALANCE ERROR

$SumIV_{Boron} := BOH_3^{(1)} + BOH4_{1,1} + 2 \cdot B2OH7_{1,1} + 3 \cdot B3OH10_{1,1} + 4 \cdot B4OH14_{1,1}$

$SumI_{Boron} := BOH_3^{(2)} + BOH4_{1,2} + 2 \cdot B2OH7_{1,2} + 3 \cdot B3OH10_{1,2} + 4 \cdot B4OH14_{1,2}$

$MBE_{IV} := EQ_{Boron_{1,1}} - SumIV_{Boron}$

$MBE_I := EQ_{Boron_{1,2}} - SumI_{Boron}$

$MBE_{IV} =$	$\begin{pmatrix} 2.069 \times 10^{-6} \\ 7.349 \times 10^{-6} \\ 2.99 \times 10^{-6} \\ -1.391 \times 10^{-6} \\ 1.109 \times 10^{-5} \\ 1.325 \times 10^{-5} \\ 9.719 \times 10^{-7} \\ -1.2 \times 10^{-5} \\ 6.911 \times 10^{-6} \\ 3.431 \times 10^{-6} \\ 1.124 \times 10^{-6} \\ 5.379 \times 10^{-6} \end{pmatrix}$	$MBE_I =$	$\begin{pmatrix} -5.887 \times 10^{-6} \\ -6.172 \times 10^{-6} \\ 5.018 \times 10^{-8} \\ -5.975 \times 10^{-6} \\ 6.288 \times 10^{-6} \\ 2.413 \times 10^{-6} \\ 1.166 \times 10^{-5} \\ -4.353 \times 10^{-6} \\ -1.56 \times 10^{-6} \\ -5.84 \times 10^{-6} \\ 2.83 \times 10^{-6} \\ 6.277 \times 10^{-6} \end{pmatrix}$	$SumIV_{Boron} =$	$\begin{pmatrix} 0.313898 \\ 0.313893 \\ 0.313897 \\ 0.313901 \\ 0.313889 \\ 0.313887 \\ 0.313899 \\ 0.313912 \\ 0.313893 \\ 0.313897 \\ 0.313899 \\ 0.313895 \end{pmatrix}$	$SumI_{Boron} =$	$\begin{pmatrix} 0.214206 \\ 0.214206 \\ 0.2142 \\ 0.214206 \\ 0.214194 \\ 0.214198 \\ 0.214188 \\ 0.214204 \\ 0.214202 \\ 0.214206 \\ 0.214197 \\ 0.214194 \end{pmatrix}$
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Calculation No. 0090-0148-01	Prepared By <i>Narva Charoie</i>	Checked By <i>[Signature]</i>	Page: B-12 Revision: 3
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CHARGE BALANCE ERROR

$$\text{PosIV}_{\text{charge}} := \text{H}_{\text{plus}}_{1,1} + \text{Na}_{1,1}$$

$$\text{PosI}_{\text{charge}} := \text{H}_{\text{plus}}_{1,2} + \text{Na}_{1,2}$$

$$\text{NegIV}_{\text{charge}} := \text{OH}_{\text{minus}}_{1,1} + \text{BOH4}_{1,1} + \text{B2OH7}_{1,1} + \text{B3OH10}_{1,1} + 2 \cdot \text{B4OH14}_{1,1} + \text{Cl}_{1,1} + \text{NO3}_{1,1}$$

$$\text{NegI}_{\text{charge}} := \text{OH}_{\text{minus}}_{1,2} + \text{BOH4}_{1,2} + \text{B2OH7}_{1,2} + \text{B3OH10}_{1,2} + 2 \cdot \text{B4OH14}_{1,2}$$

$$\text{NegI}_{12\text{Hr}}_{\text{charge}} := \text{OH}_{\text{minus}}_{1,2} + \text{BOH4}_{1,2} + \text{B2OH7}_{1,2} + \text{B3OH10}_{1,2} + 2 \cdot \text{B4OH14}_{1,2} + \text{Cl}_{1,2} + \text{NO3}_{1,2}$$

$$\text{CBE}_{\text{IV}} := \text{PosIV}_{\text{charge}} - \text{NegIV}_{\text{charge}}$$

$$\text{CBE}_{\text{I}} := \text{PosI}_{\text{charge}} - \text{NegI}_{\text{charge}}$$

$$\text{CBE}_{12\text{Hr}} := \text{PosI}_{\text{charge}} - \text{NegI}_{12\text{Hr}}_{\text{charge}}$$

$$\text{CBE}_{\text{I}_{s12i}} := \text{CBE}_{12\text{Hr}}_{s12i}$$

$$s12i := 6..12$$

$$\text{CBE}_{\text{IV}} = \begin{pmatrix} -1.176 \times 10^{-7} \\ 1.015 \times 10^{-6} \\ 1.105 \times 10^{-6} \\ -9.196 \times 10^{-7} \\ 2.958 \times 10^{-6} \\ 3.511 \times 10^{-6} \\ 1.69 \times 10^{-6} \\ -3.153 \times 10^{-6} \\ 1.209 \times 10^{-6} \\ -1.782 \times 10^{-7} \\ -8.326 \times 10^{-7} \\ 4.805 \times 10^{-7} \end{pmatrix}$$

$$\text{CBE}_{\text{I}} = \begin{pmatrix} -1.624 \times 10^{-6} \\ -4.421 \times 10^{-7} \\ 1.039 \times 10^{-6} \\ -1.434 \times 10^{-6} \\ 3.355 \times 10^{-6} \\ 3.098 \times 10^{-6} \\ 3.392 \times 10^{-6} \\ -2.974 \times 10^{-6} \\ 3.388 \times 10^{-7} \\ -1.12 \times 10^{-6} \\ -2.5 \times 10^{-7} \\ 7.955 \times 10^{-7} \end{pmatrix}$$

$$\begin{matrix} \text{PosIV}_{\text{charge}} = & \begin{pmatrix} 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \\ 0.0148 \end{pmatrix} \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \\ \text{PosI}_{\text{charge}} = & \begin{pmatrix} 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \end{pmatrix} \end{matrix}$$



Calculation No. 0090-0148-01	Prepared By <i>Maman Charney</i>	Checked By <i>[Signature]</i>	Page: B-13 Revision: 3
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$$\begin{array}{ccc}
 \begin{array}{c} (0.0148) \\ 0.014799 \\ 0.014799 \\ 0.014801 \\ 0.014797 \\ 0.014797 \\ 0.014798 \\ 0.014803 \\ 0.014799 \\ 0.0148 \\ 0.014801 \\ (0.0148) \end{array} & \text{Neg}_{IV}\text{charge} = & \begin{array}{c} (0.0184) \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0181 \\ 0.0181 \\ 0.0181 \\ 0.0181 \\ 0.0181 \\ 0.0181 \\ (0.0181) \end{array} & \text{Neg}_{I_12\text{Hr}}\text{charge} = & \begin{array}{c} (0.0187) \\ 0.0187 \\ 0.0187 \\ 0.0187 \\ 0.0187 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ 0.0184 \\ (0.0184) \end{array}
 \end{array}$$

IONIC STRENGTH BALANCE ERROR

$$\text{SumIV}_{\text{Ions}} := \frac{1}{2} \cdot \left(\text{Na}_{1,1} + \text{H}_{\text{plus}}_{1,1} + \text{OH}_{\text{minus}}_{1,1} + \text{BOH4}_{1,1} + \text{B2OH7}_{1,1} + \text{B3OH10}_{1,1} \dots \right. \\
 \left. + 4 \cdot \text{B4OH14}_{1,1} + \text{Cl}_{1,1} + \text{NO3}_{1,1} \right)$$

$$\text{SumI}_{\text{Ions}} := \frac{1}{2} \cdot \left(\text{Na}_{1,2} + \text{H}_{\text{plus}}_{1,2} + \text{OH}_{\text{minus}}_{1,2} + \text{BOH4}_{1,2} + \text{B2OH7}_{1,2} + \text{B3OH10}_{1,2} + 4 \cdot \text{B4OH14}_{1,2} \right)$$

$$\text{SumI}_{12\text{HrIons}} := \frac{1}{2} \cdot \left(\text{Na}_{1,2} + \text{H}_{\text{plus}}_{1,2} + \text{OH}_{\text{minus}}_{1,2} + \text{BOH4}_{1,2} + \text{B2OH7}_{1,2} + \text{B3OH10}_{1,2} \dots \right. \\
 \left. + 4 \cdot \text{B4OH14}_{1,2} + \text{Cl}_{1,2} + \text{NO3}_{1,2} \right)$$

$\text{SBE}_{IV} := \text{Ionic}_{\text{strength}}^{(1)} - \text{SumIV}_{\text{Ions}}$	SumIV _{Ions} =	SumI _{Ions} =	(0.014852)	(0.018489)
$\text{SBE}_I := \text{Ionic}_{\text{strength}}^{(2)} - \text{SumI}_{\text{Ions}}$			0.014852	0.01849
$\text{SBE}_{I_12\text{Hr}} := \text{Ionic}_{\text{strength}}^{(2)} - \text{SumI}_{12\text{HrIons}}$			0.014854	0.018493
			0.014857	0.018498
			0.01486	0.018509
			0.014864	0.018366
			0.014876	0.018394
			0.014874	0.018385
			0.014878	0.018399
			0.014886	0.01842
			0.014911	0.018483
			(0.015042)	(0.018853)



Calculation No.

0090-0148-01

Prepared By

Marva Charrat

Checked By

[Signature]

Page: B-14

Revision: 3

$$SBE_{IV} = \begin{pmatrix} -2.449 \times 10^{-6} \\ -2.391 \times 10^{-6} \\ -3.805 \times 10^{-6} \\ 3.419 \times 10^{-6} \\ 3.331 \times 10^{-7} \\ 6.053 \times 10^{-6} \\ 3.964 \times 10^{-6} \\ -3.722 \times 10^{-6} \\ 2.456 \times 10^{-6} \\ 3.87 \times 10^{-6} \\ -5.983 \times 10^{-7} \\ -2.12 \times 10^{-6} \end{pmatrix}$$

$$SumI_{12HrIons} = \begin{pmatrix} 0.01864 \\ 0.018641 \\ 0.018643 \\ 0.018649 \\ 0.018659 \\ 0.018516 \\ 0.018544 \\ 0.018535 \\ 0.018549 \\ 0.01857 \\ 0.018634 \\ 0.019003 \end{pmatrix}$$

$$SBE_I = \begin{pmatrix} 5.304 \times 10^{-7} \\ -1.122 \times 10^{-7} \\ -2.891 \times 10^{-6} \\ 1.579 \times 10^{-6} \\ 1.493 \times 10^{-6} \\ 3.7 \times 10^{-6} \\ 5.832 \times 10^{-6} \\ -5.323 \times 10^{-6} \\ 1.034 \times 10^{-6} \\ -7.218 \times 10^{-8} \\ -3.861 \times 10^{-6} \\ -3.444 \times 10^{-6} \end{pmatrix}$$

Calculation No.

0090-0148-01

Prepared By

Marcus Chernick

Checked By

[Signature]

Page: C-1

Revision: 3

C

Containment Sump pH with Borax Decahydrate Buffer – Case IV (no strong acids)

This appendix implements the methodology discussed in Section 7.5. The temperature of the fluid determines the constants to be used. Input concentrations are obtained from Section 7.3.

INPUT

Temperature

$$T_k := 298.15 \text{ K}$$

Initial Concentrations:

$$\text{Boric}_{\text{Acid}} := 0.2843 \frac{\text{mol}}{\text{L}}$$

Corresponding to 3095 ppm Boron

$$\text{Borax} := 0.0072 \frac{\text{mol}}{\text{L}}$$

$$\text{Na} := 2 \cdot \text{Borax}$$

Sodium ion concentration

$$\text{Na} = 0.0144 \frac{\text{mol}}{\text{L}}$$

$$\text{Cl} := 0.0 \frac{\text{mol}}{\text{L}}$$

Chloride ion concentration set to zero

$$\text{NO}_3 := 0.0 \frac{\text{mol}}{\text{L}}$$

Nitrate ion concentration set to zero

Remove units on variables

$$\text{Boric}_{\text{Acid}} := \text{Boric}_{\text{Acid}} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{Borax} := \text{Borax} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{Na} := \text{Na} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{TK} := \frac{T_k}{\text{K}}$$

$$\text{Cl} := \text{Cl} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{NO}_3 := \text{NO}_3 \cdot \frac{\text{L}}{\text{mol}}$$

Initial Total Boron Concentration

$$\text{EQ}_{\text{Boron}} := 4 \cdot \text{Borax} + \text{Boric}_{\text{Acid}}$$

$$\text{EQ}_{\text{Boron}} = 0.3131$$

Calculation No.

0090-0148-01

Prepared By

Manwa Carroll

Checked By

[Signature]

Page: C-2

Revision: 3

CONSTANTS

$a_H := 9$ effective ionic radius of H+

$a_{OH} := 3.5$ effective ionic radius of OH-

$DH_A := .5115$
Debye-Huckel Constants

$DH_B := .3291$

$K_w := 1.0116 \cdot 10^{-14}$ water equilibrium constant

GUESS

pH := 7.00675

Ionic strength := 0.01464

BOH₃ := 0.27439

COMPUTE

$$\gamma_H := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic_strength}}\right)}{1 + DH_B \cdot a_H \cdot \sqrt{\text{Ionic_strength}}}}$$

$$\gamma_H = 0.9$$

$$H_{\text{plus}} := \frac{10^{-\text{pH}}}{\gamma_H}$$

$$OH_{\text{minus}} := \frac{K_w}{H_{\text{plus}} \cdot \gamma_H \cdot \gamma_{OH}}$$

$$\gamma_{OH} := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic_strength}}\right)}{1 + DH_B \cdot a_{OH} \cdot \sqrt{\text{Ionic_strength}}}}$$

$$\gamma_{OH} = 0.882$$

$$H_{\text{plus}} = 1.093 \times 10^{-7}$$

$$OH_{\text{minus}} = 1.164 \times 10^{-7}$$

Calculation No.

0090-0148-01

Prepared By

Alana Chernov

Checked By

[Signature]

Page: C-3

Revision: 3

$$\log Q_{11} := \frac{1573.21}{TK} + 28.6059 + 0.012078TK - 13.2258\log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots$$

$$+ -0.0912\text{Ionic_strength}^{1.5}$$

$$Q_{11} := 10^{\log Q_{11}}$$

$$Q_{11} = 5.758 \times 10^4$$

$$\log Q_{21} := \frac{2756.1}{TK} - 19.1998 + 0.00033TK + 5.835\log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots$$

$$+ -0.0912\text{Ionic_strength}^{1.5}$$

$$Q_{21} := 10^{\log Q_{21}}$$

$$Q_{21} = 3.838 \times 10^4$$

$$\log Q_{31} := \frac{3339.5}{TK} - 8.3178 + 0.00033TK + 1.497\log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots$$

$$+ -0.0912\text{Ionic_strength}^{1.5}$$

$$Q_{31} := 10^{\log Q_{31}}$$

$$Q_{31} = 4.883 \times 10^6$$

$$\log Q_{42} := \frac{12820}{TK} - 134.7938 + 0.00033TK + 42.105\log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots$$

$$+ -0.0912\text{Ionic_strength}^{1.5}$$

$$Q_{42} := 10^{\log Q_{42}}$$

$$Q_{42} = 3.107 \times 10^{12}$$

$$\text{BOH4} := Q_{11} \cdot \text{OH}_{\text{minus}} \cdot \text{BOH}_3$$

$$\text{BOH4} = 1.84 \times 10^{-3}$$

$$\text{B2OH7} := Q_{21} \cdot \text{OH}_{\text{minus}} \cdot \text{BOH}_3^2$$

$$\text{B2OH7} = 3.364 \times 10^{-4}$$

$$\text{B3OH10} := Q_{31} \cdot \text{OH}_{\text{minus}} \cdot \text{BOH}_3^3$$

$$\text{B3OH10} = 1.175 \times 10^{-2}$$

$$\text{B4OH14} := Q_{42} \cdot \text{OH}_{\text{minus}}^2 \cdot \text{BOH}_3^4$$

$$\text{B4OH14} = 2.387 \times 10^{-4}$$



Calculation No.

0090-0148-01

Prepared By

Monica Chastock

Checked By

[Signature]

Page: C-4

Revision: 3

MASS BALANCE ERROR

$$\text{Sum}_{\text{Boron}} := \text{BOH}_3 + \text{BOH}_4 + 2 \cdot \text{B}_2\text{OH}_7 + 3 \cdot \text{B}_3\text{OH}_{10} + 4 \cdot \text{B}_4\text{OH}_{14}$$

$$\text{Sum}_{\text{Boron}} = 0.3131$$

$$\text{EQ}_{\text{Boron}} - \text{Sum}_{\text{Boron}} = 4.0282 \times 10^{-6}$$

CHARGE BALANCE ERROR

$$\text{Pos}_{\text{charge}} := \text{H}_{\text{plus}} + \text{Na}$$

$$\text{Pos}_{\text{charge}} = 0.0144$$

$$\text{Neg}_{\text{charge}} := \text{OH}_{\text{minus}} + \text{BOH}_4 + \text{B}_2\text{OH}_7 + \text{B}_3\text{OH}_{10} + 2 \cdot \text{B}_4\text{OH}_{14} + \text{Cl} + \text{NO}_3$$

$$\text{Neg}_{\text{charge}} = 0.0144$$

$$\text{Pos}_{\text{charge}} - \text{Neg}_{\text{charge}} = 2.18 \times 10^{-7}$$

IONIC STRENGTH BALANCE ERROR

$$\text{Sum}_{\text{Ions}} := \frac{1}{2} (\text{Na} + \text{H}_{\text{plus}} + \text{OH}_{\text{minus}} + \text{BOH}_4 + \text{B}_2\text{OH}_7 + \text{B}_3\text{OH}_{10} + 4 \cdot \text{B}_4\text{OH}_{14} + \text{Cl} + \text{NO}_3)$$

$$\text{Sum}_{\text{Ions}} = 0.01464$$

$$\text{Ionic}_{\text{strength}} - \text{Sum}_{\text{Ions}} = 1.25 \times 10^{-6}$$

Calculation No.

0090-0148-01

Prepared By

Alwan Charroff

Checked By

[Signature]

Page: D-1

Revision: 2

D

Containment Sump pH with Borax Decahydrate Buffer – Case V

This appendix implements the methodology discussed in Section 7.5. The temperature of the fluid determines the constants to be used. Input concentrations are obtained from Section 8.3.

INPUT

25C Temperature

$$T_k := 298.15 \text{ K}$$

Initial Concentrations:

$$\text{Boric}_{\text{Acid}} := 0.2881 \frac{\text{mol}}{\text{L}}$$

Corresponding to 3105.5 ppm Boron

$$\text{Borax} := 0.0075 \frac{\text{mol}}{\text{L}}$$

$$\text{Na} := 2 \cdot \text{Borax}$$

Sodium ion concentration

$$\text{Na} = 0.015 \frac{\text{mol}}{\text{L}}$$

Chloride ion concentration set to zero

$$\text{Cl} := 0.0 \frac{\text{mol}}{\text{L}}$$

$$\text{NO}_3 := 0.0 \frac{\text{mol}}{\text{L}}$$

Nitrate ion concentration set to zero

Remove units on variables

$$\text{Boric}_{\text{Acid}} := \text{Boric}_{\text{Acid}} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{Borax} := \text{Borax} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{Na} := \text{Na} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{TK} := \frac{T_k}{\text{K}}$$

$$\text{Cl} := \text{Cl} \cdot \frac{\text{L}}{\text{mol}}$$

$$\text{NO}_3 := \text{NO}_3 \cdot \frac{\text{L}}{\text{mol}}$$

Initial Total Boron Concentration

$$\text{EQ}_{\text{Boron}} := 4 \cdot \text{Borax} + \text{Boric}_{\text{Acid}}$$

$$\text{EQ}_{\text{Boron}} = 0.3181$$

Calculation No.
0090-0148-01

Prepared By

Mervin Charo

Checked By

[Signature]

Page: D-2

Revision: 2

CONSTANTS

$a_H := 9$ effective ionic radius of H+

$a_{OH} := 3.5$ effective ionic radius of OH-

$DH_A := .5115$ Debye-Huckel Constants

$DH_B := .3291$

$K_w := 1.0116 \cdot 10^{-14}$ water equilibrium constant

GUESS

pH := 7.00888

Ionic strength := 0.01525

BOH₃ := 0.27771

COMPUTE

$$\gamma_H := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic strength}}\right)}{1 + DH_B \cdot a_H \cdot \sqrt{\text{Ionic strength}}}}$$

$$\gamma_H = 0.899$$

$$H_{\text{plus}} := \frac{10^{-\text{pH}}}{\gamma_H}$$

$$OH_{\text{minus}} := \frac{K_w}{H_{\text{plus}} \cdot \gamma_H \cdot \gamma_{OH}}$$

$$\gamma_{OH} := 10^{\frac{-\left(DH_A \cdot \sqrt{\text{Ionic strength}}\right)}{1 + DH_B \cdot a_{OH} \cdot \sqrt{\text{Ionic strength}}}}$$

$$\gamma_{OH} = 0.88$$

$$H_{\text{plus}} = 1.09 \times 10^{-7}$$

$$OH_{\text{minus}} = 1.173 \times 10^{-7}$$

Calculation No.
0090-0148-01

Prepared By
Manan Chavak

Checked By
[Signature]

Page: D-3
Revision: 2

$$\log Q_{11} := \frac{1573.21}{TK} + 28.6059 + 0.012078TK - 13.2258\log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots$$

$$+ -0.0912\text{Ionic_strength}^{1.5}$$

$$Q_{11} := 10^{\log Q_{11}}$$

$$Q_{11} = 5.76 \times 10^4$$

$$\log Q_{21} := \frac{2756.1}{TK} - 19.1998 + 0.00033TK + 5.835\log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots$$

$$+ -0.0912\text{Ionic_strength}^{1.5}$$

$$Q_{21} := 10^{\log Q_{21}}$$

$$Q_{21} = 3.839 \times 10^4$$

$$\log Q_{31} := \frac{3339.5}{TK} - 8.3178 + 0.00033TK + 1.497\log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots$$

$$+ -0.0912\text{Ionic_strength}^{1.5}$$

$$Q_{31} := 10^{\log Q_{31}}$$

$$Q_{31} = 4.885 \times 10^6$$

$$\log Q_{42} := \frac{12820}{TK} - 134.7938 + 0.00033TK + 42.105\log(TK) + (0.325 - 0.00033TK) \cdot \text{Ionic_strength} \dots$$

$$+ -0.0912\text{Ionic_strength}^{1.5}$$

$$Q_{42} := 10^{\log Q_{42}}$$

$$Q_{42} = 3.108 \times 10^{12}$$

$$\text{BOH4} := Q_{11} \cdot \text{OH}_{\text{minus}} \cdot \text{BOH}_3$$

$$\text{BOH4} = 1.876 \times 10^{-3}$$

$$\text{B2OH7} := Q_{21} \cdot \text{OH}_{\text{minus}} \cdot \text{BOH}_3^2$$

$$\text{B2OH7} = 3.472 \times 10^{-4}$$

$$\text{B3OH10} := Q_{31} \cdot \text{OH}_{\text{minus}} \cdot \text{BOH}_3^3$$

$$\text{B3OH10} = 1.227 \times 10^{-2}$$

$$\text{B4OH14} := Q_{42} \cdot \text{OH}_{\text{minus}}^2 \cdot \text{BOH}_3^4$$

$$\text{B4OH14} = 2.542 \times 10^{-4}$$



Calculation No.

0090-0148-01

Prepared By

Alana Charrouf

Checked By

[Signature]

Page: D-4

Revision: 2

MASS BALANCE ERROR

$$\text{Sum}_{\text{Boron}} := \text{BOH}_3 + \text{BOH}_4 + 2 \cdot \text{B}_2\text{OH}_7 + 3 \cdot \text{B}_3\text{OH}_{10} + 4 \cdot \text{B}_4\text{OH}_{14}$$

$$\text{Sum}_{\text{Boron}} = 0.3181$$

$$\text{EQ}_{\text{Boron}} - \text{Sum}_{\text{Boron}} = -3.6339 \times 10^{-6}$$

CHARGE BALANCE ERROR

$$\text{Pos}_{\text{charge}} := \text{H}_{\text{plus}} + \text{Na}$$

$$\text{Pos}_{\text{charge}} = 0.015$$

$$\text{Neg}_{\text{charge}} := \text{OH}_{\text{minus}} + \text{BOH}_4 + \text{B}_2\text{OH}_7 + \text{B}_3\text{OH}_{10} + 2 \cdot \text{B}_4\text{OH}_{14} + \text{Cl} + \text{NO}_3$$

$$\text{Neg}_{\text{charge}} = 0.015$$

$$\text{Pos}_{\text{charge}} - \text{Neg}_{\text{charge}} = -3.624 \times 10^{-7}$$

IONIC STRENGTH BALANCE ERROR

$$\text{Sum}_{\text{Ions}} := \frac{1}{2} \cdot (\text{Na} + \text{H}_{\text{plus}} + \text{OH}_{\text{minus}} + \text{BOH}_4 + \text{B}_2\text{OH}_7 + \text{B}_3\text{OH}_{10} + 4 \cdot \text{B}_4\text{OH}_{14} + \text{Cl} + \text{NO}_3)$$

$$\text{Sum}_{\text{Ions}} = 0.01525$$

$$\text{Ionic}_{\text{strength}} - \text{Sum}_{\text{Ions}} = -4.496 \times 10^{-6}$$



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320 King Street
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Calculation No.

0090-0148-01

Prepared By

Anna ChomE

Checked By

[Signature]

Page: E-1

Revision: 2

E

Reference 27 – Record for Iodine in Containment

From: Massari, John
Sent: Wednesday, July 16, 2008 5:54 PM
To: 'Kinsey, Steve'; KINSEY, STEPHEN P
Cc: Swailes, John
Subject: Iodine in Containment

Steve,

Here's the info you wanted on mass of iodine released to containment post-LOCA. The core inventories (in moles) come from the SAS2H/ORIGEN case CDCB.out in calculation CA06358 if you need a reference. I've covered both TID-14484 (current) and AST (NRC approved but not implemented until 2010 RFO) methods, and included decay and BOC/EOC effects to give you an idea of the range during the cycle. Decay actually doesn't do much for you since the bulk of the iodine is stable I-127 and long-lived I-129. What's not considered is removal mechanisms that don't lead to the sump such as iodine filters or plate-out in the unsprayed region.

John

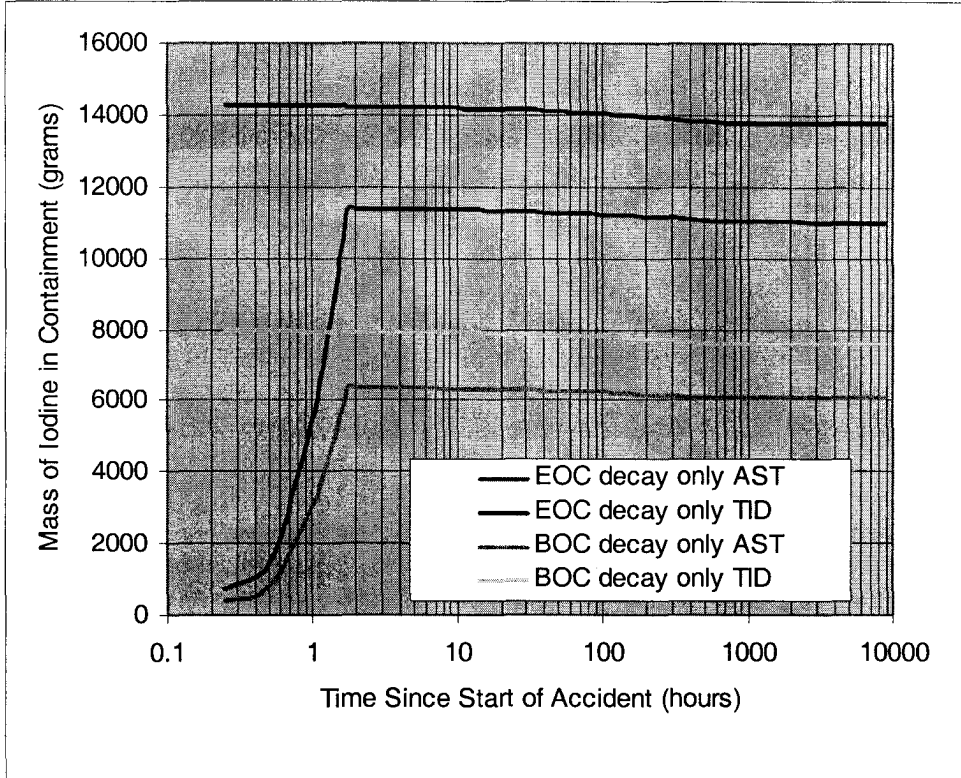


Calculation No.
0090-0148-01

Prepared By
Maria Charvat

Checked By
[Signature]

Page: E-2
Revision: 2



<<Iodine in containment for sump pH.xls>>



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Calculation No. 0090-0148-01	Prepared By <i>John Massari</i>	Checked By <i>Steve Kinsey</i>	Page: F-1 Revision: 3
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F

Reference 29 – Record for Radiation Doses

From: Massari, John [mailto:John.Massari@constellation.com]
Sent: Thu 2008-07-24 17:04
To: Kinsey, Steve
Cc: Wilson, William J; Swailes, John; Massoud, Mahmoud; Furio, Patricia S
Subject: RE: Buffer Calc

Steve,

I can confirm the first 2 bullets and I've added in the adjusted doses for the last one below and the associated references needed.

Mahmoud, please add in the 30-day sump temperature.

John

-----Original Message-----

From: Kinsey, Steve [mailto:skinsey@mpr.com]
Sent: Thursday, July 24, 2008 2:55 PM
To: Massari, John
Cc: Wilson, William J; Swailes, John; Massoud, Mahmoud; Furio, Patricia S
Subject: Buffer Calc

Dear Mr. Massari:

Please confirm the design inputs below by return email as discussed today in our 12:30 PM Conference. There are four items for you to address. Please confirm the first two items. Please fill in information on the last two items

- * RCS boron concentration to use in the calculation.
The upper bound of the RCS concentration during power operations is less than the minimum shutdown boron concentration. Therefore, the bounding maximum RCS boron concentration is the 2300 ppm minimum boron concentration required in the RWT.
The lower bound RCS boron concentration is 0 ppm boron.
These limits will be used to evaluate the required sodium tetraborate decahydrate to achieve pH>7.0 in the ECCS sump pool post LOCA and post RAS.
- * BAST boric acid load not delivered to the ECCS sump pool.
MPR will use a minimum boric acid load which does not include the contents of the BAST to develop the upper bound on pH for the total NaTB load.
- * Sump Water Temperature at 30 Days
The sump water temperature at 30 days is {Please fill in}
MPR is adding a pH versus Time section to the calculation which will provide Licensing with needed input for the Buffer LAR. pH is affected



Calculation No. 0090-0148-01	Prepared By <i>Marnon Charvat</i>	Checked By <i>[Signature]</i>	Page: F-2 Revision: 2
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MPR is adding a pH versus Time section to the calculation which will Provide Licensing with needed input for the Buffer LAR. pH is affected by temperature. The sump water temperature varies with time. Therefore, the sump pH will Vary with time. The current design calculation, CA06774, Revision 1 provides sump water temperature to 1,000,000 seconds or about 11 days. The pH versus Time results will be based on the temperature provided here.

* The dose rate for HCl and H2NO3 formation
The new dose adjustments for determining radiologically generated acids are {Please fill in}
The dose calculation changed about 2004 but was not carried into CA04602, Revision 0.
The new generation rates will be based on the adjustments that you provide here.

Sump Surface (50' from filter)

	18-m cycle 1-year intetrated doses			M 18m-24m		M 24m VAP		24m VAP w/ App K adjusted		
	beta + gamma	beta	gamma	beta	gamma	beta	gamma	beta+gamma	beta	gamma
Airborne	141.5	133.9	7.6	1	1	1.0327	1.0178	146.01	138.28	7.74
Plateout	88.57	88	0.57	1	1	1.0097	1.0097	89.43	88.85	0.58
Filter	0.45	0	0.45	1	1	1	1.0097	0.45	0.00	0.45
Sump	8	0	8	1	1	1	1.0096	8.08	0.00	8.08
Total	238.52	221.9	16.62					243.97	227.13	16.84

Filter Housing Surface

	18-m cycle 1-year intetrated doses			M 18m-24m		M 24m VAP		24m VAP w/ App K adjusted		
	beta + gamma	beta	gamma	beta	gamma	beta	gamma	beta+gamma	beta	gamma
Airborne	141.5	133.9	7.6	1	1	1.0327	1.0178	146.01	138.28	7.74
Plateout	88.57	88	0.57	1	1	1.0097	1.0097	89.43	88.85	0.58
Filter	321	0	321	1	1	1	1.0097	324.11	0.00	324.11
Sump	8	0	8	1	1	1	1.0096	8.08	0.00	8.08
Total	559.07	221.9	337.17					567.63	227.13	340.50

18-month cycle 1y int. doses from CA03879 (Bechtel Calc M-81-27 sh. 26, 32, 33)
18m to 24m-cycle multiplier for 1y int. dose from NEU-93-335 (Bechtel M-91-44 sh 48b & 48c)
App K + VAP 1y int. dose multiplier from CA06188 p. 48



MPR Associates, Inc.
320 King Street
Alexandria, VA 22314

Calculation No.

0090-0148-01

Prepared By

Marwan Charroub

Checked By

Steve Kinsey

Page: G-1

Revision: 2

G

Reference 22 – Temperature Profile to 30 Days Following LOCA

From: Massoud, Mahmoud

Sent: Thursday, July 24, 2008 10:43 AM

To: KINSEY, STEPHEN P; Swailes, John; Massari, John; 'Kinsey, Steve'

Subject: RE: Data File

Gentlemen

I've attached the result of extended GOTHIC analysis. The analysis runs for an additional 660,000 seconds (about 8 days). The code predicts that the sump water temperature at 19.2 days would be about 140 F.

Although I extended the decay heat to beyond 1 month, the code did not run to 2,592,000 seconds due to the lack of sufficient data for the containment air coolers.

-Mahmoud

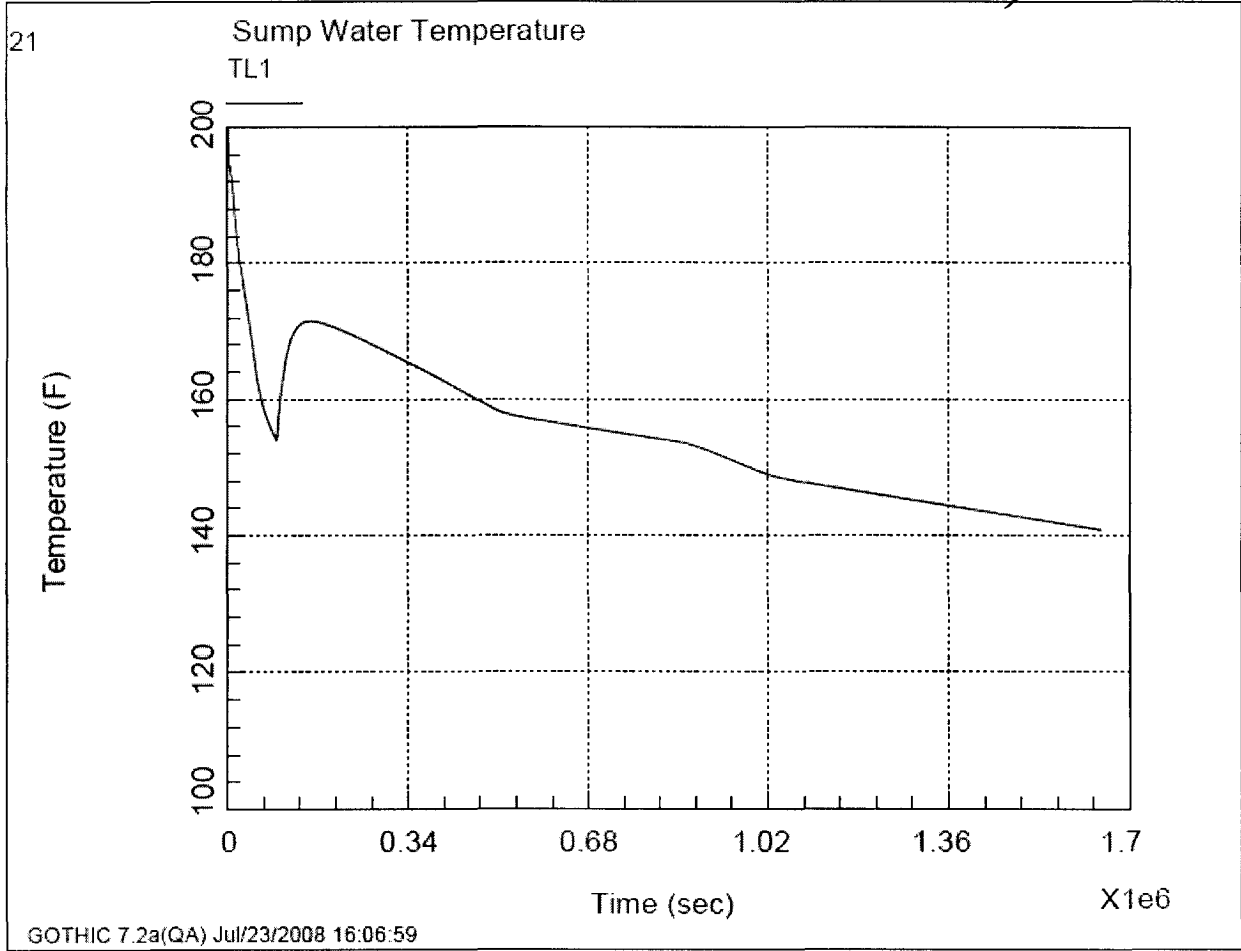


Calculation No.
0090-0148-01

Prepared By
Marwan Charab

Checked By
[Signature]

Page: G-2
Revision: 2



END OF EMAIL MESSAGE

Extrapolation

The above temperature profile is used for a linear least-squares polynomial fit supplying the data only from 10 days to 19 days. The figure below shows the original temperature profile with the superimposed linear fit extending to 30 days. The extrapolated temperature value at 30 days is 125.763 °F.



Calculation No.
0090-0148-01

Prepared By
Marwan Charaf

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[Signature]

Page: G-3
Revision: 2

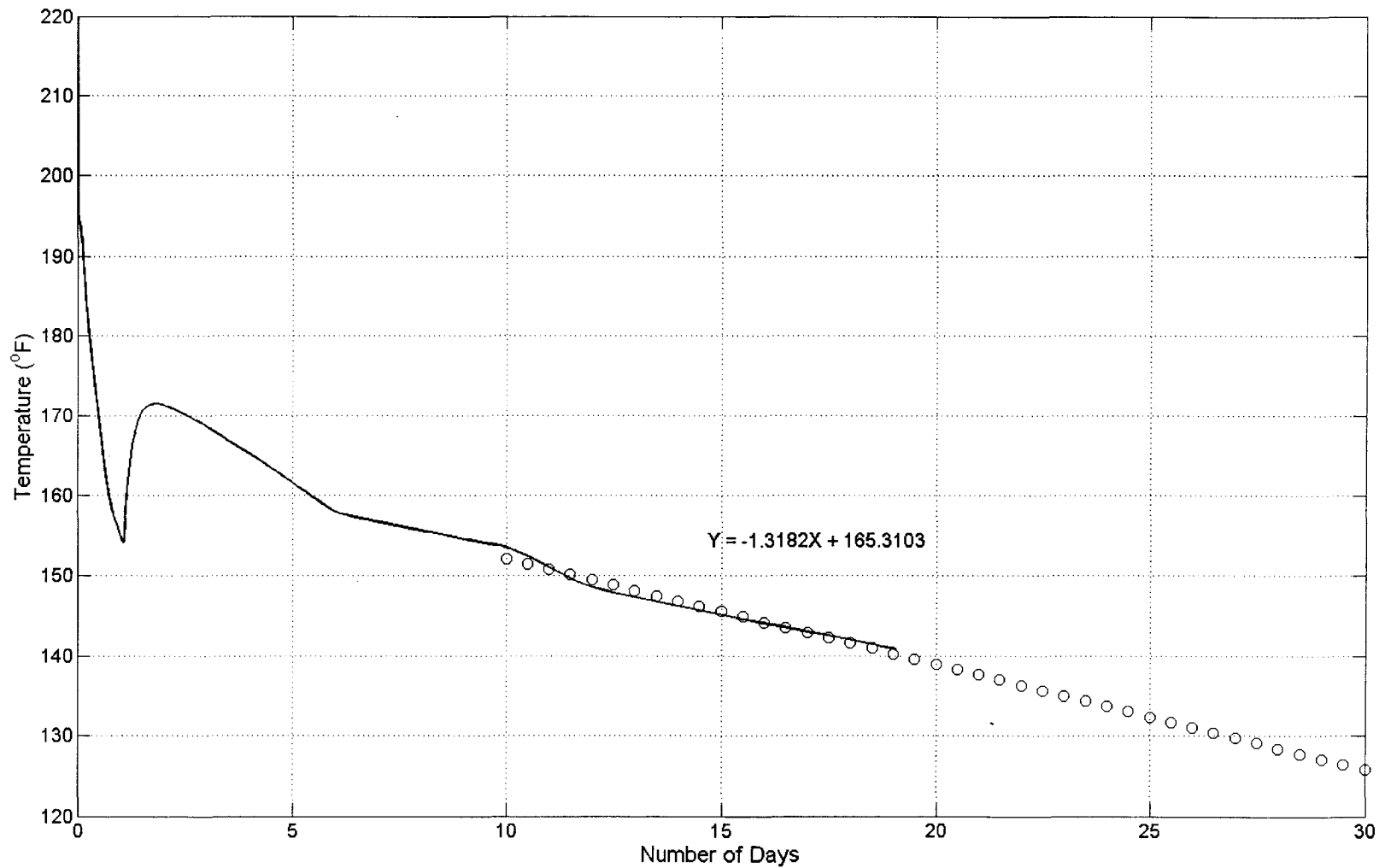


Figure G-1. Sump Water Temperature Extrapolated to 30 Days