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TO: T. P. KILLEEN, 730-4B

FROM: J. A. DYER, 773-42A

REVIEWER: T. L. DANIELSON, 773-42A

pH BUFFERING STRATEGY FOR A NON-TIME CRITICAL REMOVAL ACTION AT THE C-AREA GROUNDWATER OPERABLE UNIT

Scope

Area Completion Projects (ACP) will implement a non-time critical (NTC) removal action during 2Q/3Q FY19 at the C-Area Groundwater (CAGW) Operable Unit (OU) to address trichloroethylene (TCE) discharging above the maximum contaminant level (MCL) of 5 µg/L to an unnamed tributary to Castor Creek. ACP requested that SRNL evaluate the proposed pH buffering strategy for the Middle Aquifer Zone (MAZ) of Upper Three Runs Aquifer in support of the planned injection of emulsified vegetable oil and a bioaugmentation culture to facilitate biodegradation of TCE. The evaluation focused on the chemical requirements to buffer the planned 16-foot long x 240-foot wide x 10-foot deep injection zone at pH 7.0 to ensure the viability of the bioaugmented reductive-dechlorination process. Groundwater within the planned injection zone is currently at pH 5.0.

Summary and Recommendations

Summarized in Table 1 is the volume of pH buffer solution necessary to maintain a pH of 7.0 in the injection zone throughout the planned five-year design period for the NTC removal action. Optimistic, best-estimate, and pessimistic cases were considered to acknowledge the significant uncertainties in the input parameters for the pH buffer model. Two different pH buffer solutions were evaluated:

- a proprietary buffer concentrate (CoBupHMg^{TM}) from EOS Remediation LLC that will be diluted in the field at a 4:1 water-to-CoBupHMg^{TM} volume ratio and
- a generic 1.7 wt% NaOH/7.0 wt% $NaHCO_3$ aqueous buffer solution.

Table 1. Recommended pH Buffer Solution Injection Volumes for CAGW NTC Removal Action.

Buffer Solution	Optimistic Case	Best-Estimate Case	Pessimistic Case	Subcontractor Proposed
CoBupHMg™ (gallons concentrate per well)	105	150	205	100
1.7 wt% NaOH/ 7.0 wt% $NaHCO_3$ (gallons solution per well)	3810	5530	7430	1.4

The volume of CoBupHMg™ buffer concentrate per injection well proposed in the CAGW OU NTC Removal Action (100 gallons per well) is comparable to the buffer demand calculated for the optimistic case but is 50% less than the buffer demand for the best-estimate case. Conversely, the calculated volume of a $NaOH/NaHCO_3$ buffer solution is more than three orders-of-magnitude higher than the injection volume proposed in the CAGW OU NTC Removal Action. For example, the CAGW OU NTC Removal Action proposed a dose of 1.4 gallons per well, which may simply raise the pH of the emulsified soybean oil before injection rather than neutralize background acidity in the groundwater and aquifer solids as well as acidity generated by the oxidation and dechlorination reactions.

Based on this evaluation, CoBupHMg™ is the preferred pH buffer solution for the NTC removal action because of its smaller injection volume (even after a 4:1 dilution) and its desirable chemical and physical properties: mobile, slow-release $Mg(OH)_2$ colloids that will migrate radially from the injection well for longer-term groundwater pH adjustment and aquifer buffering.

The pH buffer model indicates that 57% to 66% of the buffer demand will be due to acidity generated through the oxidation of the emulsified soybean oil. Active acidity in the groundwater and reserve acidity in the aquifer sediment each account for approximately 20% of the remaining buffer demand. Acidity generated via dechlorination of TCE is negligible. For this reason, injection of an overly conservative mass of emulsified soybean oil could result in not only excess pH buffer consumption, but also loss of effective porosity for groundwater flow due to the formation of an immiscible oil phase in the aquifer pore space.

<u>Background (SRNS, 2018)</u>

The NTC removal action will employ approximately fifteen direct push technology (DPT) injection points spaced 16 feet apart to create a reactive treatment "barrier" or curtain of emulsified vegetable oil within the MAZ of the Upper Three Runs Aquifer to address the distal portion of the CAGW OU TCE plume before it discharges into an unnamed tributary to Castor

Creek. (Figure 1). The DPT injection points will form two parallel transects perpendicular to groundwater flow from the bluff top to the unnamed tributary to Castor Creek. The TCE concentration in the MAZ groundwater near the planned injection wells is 50 μg/L or less. The EOS_{100}^{TM} emulsified vegetable oil product (EOS Remediation LLC, 2019a) that will be injected will both sequester (absorb) TCE in the injection zone and enhance anaerobic biodegradation of TCE by existing bacteria between the injection area and seepage into the unnamed tributary. The groundwater in the MAZ at this location is approximately pH 5; therefore, a buffer/neutralization agent is needed to raise the pH to 7 to optimize the biotic dehalogenation reaction rate.

According to the underground injection control permit application (SRNS, 2019) for this removal action, the subcontractor proposed the following oil mixture ratios for each injection well location: 275 gallons EOS_{100}™ emulsified oil, 1,375 gallons dechlorinated dilution water, and 150 +/- 50 gallons $CoBupHMg^{TM}$ mixed with 100 to 400 gallons dechlorinated water. More or less buffer may be needed to adjust the final oil mixture to pH 9.0 +/- 0.5 before injection.

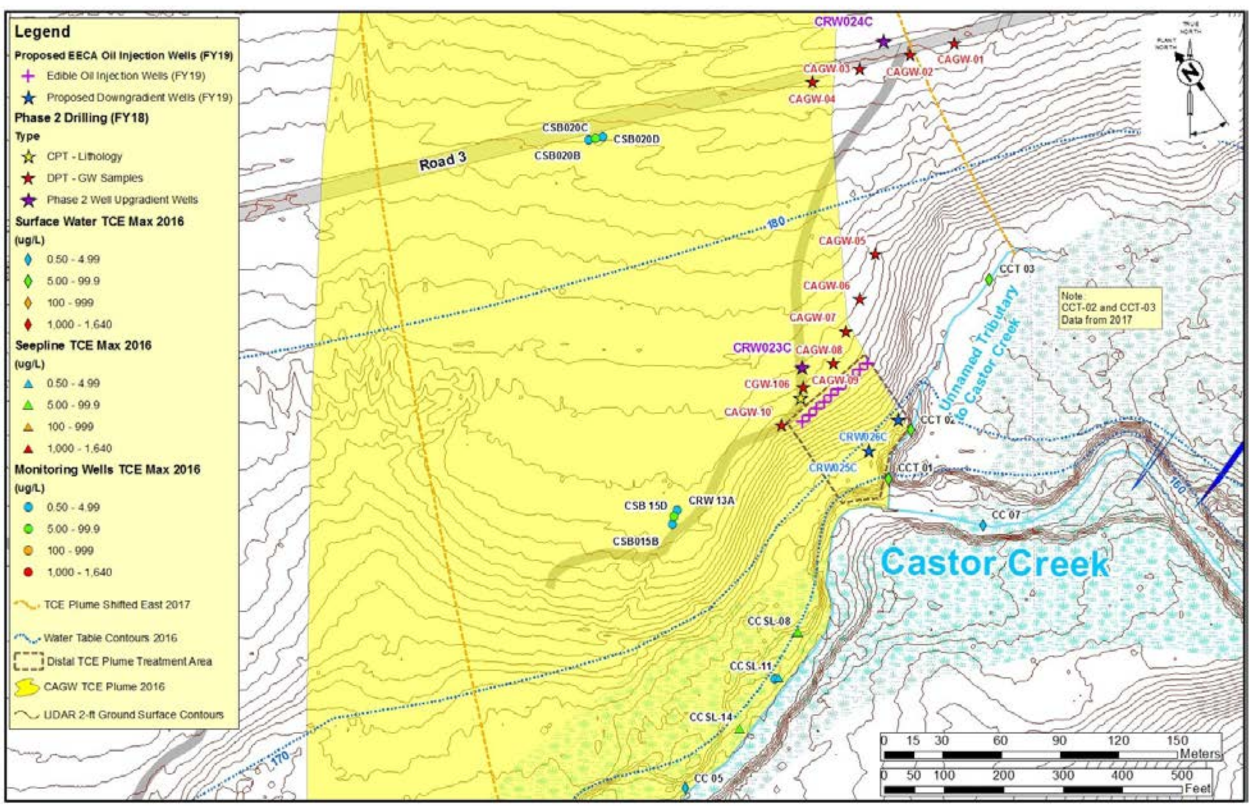

Figure 1. CAGW OU Distal TCE Groundwater Plume Showing Location of Planned Injection Wells (SRNS, 2018).

Modeling Approach

A Base-Add-Design-Tool developed by EOS Remediation LLC (2019b) was employed to calculate the pH buffer solution demand for the planned injection zone. The design tool considers aquifer characteristics, treatment zone dimensions and properties, groundwater geochemistry, initial soil and groundwater contaminant and background ion concentrations, and chemical reagent quantities.

Additional sources of information utilized to develop estimates for the Base-Add-Design-Tool input parameters included:

- Removal site evaluation report, engineering evaluation, and cost analysis (RSER/EE/CA) for the CAGW OU (SRNS, 2018)
- EOS_{100}™ emulsified oil product sheet (EOS Remediation LLC, 2019a)
- CoBupHMg™ buffer product sheet (EOS Remediation LLC, 2019c)
- Underground injection control permit application for this removal action (SRNS, 2019)
- SRS Environmental Restoration Data Management System (ERDMS, 2019)
- Agricultural limestone requirements for target soil pH 7 based on the Moore-Sikora buffer pH test (Sikora and Moore, 2008; Clemson Regulatory Services, 2019)

Optimistic, best-estimate, and pessimistic cases were considered to acknowledge the uncertainties in the model input parameters. Two pH buffer solutions were evaluated:

- a proprietary buffer concentrate (CoBupHMg™) from EOS Remediation LLC that will be diluted in the field at a 4:1 water-to-CoBupHMg™ volume ratio and
- a generic 1.7 wt% NaOH/7.0 wt% $NaHCO_3$ aqueous buffer solution.

ERDMS was mined to arrive at reasonable bounding estimates for geochemical parameters and ion concentrations representative of C-Area groundwater and soil. The Clemson Agricultural Service Lab website (Clemson Regulatory Services, 2019) enabled development of estimates for aquifer buffering capacity.

Key Assumptions

- Treatment requirements: 16-foot long x 240-foot wide x 10-foot deep treatment zone and a five-year design period for all uncertainty cases and pH buffers.
- Aquifer characteristics: 0.017 ft/ft hydraulic gradient; 13 ft/day hydraulic conductivity; 2.15 g/cm^3 specific gravity; 25% effective porosity.

- Total inorganic carbon (TIC) concentration was back-calculated using a limited set of coupled pH and total carbonate alkalinity measurements found in ERDMS for C-Area groundwater. Estimated TIC concentrations were 10, 20, and 30 mg/L for the optimistic, best-estimate, and pessimistic cases, respectively.
- Aquifer buffering capacity was estimated using recommended lime application rates from the Clemson Agricultural Service Lab (Clemson Regulatory Services, 2019) to raise soil pH from 5.0 to 7.0 assuming soil buffer pH values of 7.85, 7.75, and 7.65 for the optimistic, best-estimate, and pessimistic cases, respectively. To enable input to the Base-Add-Design-Tool model, the lime application rates from Clemson were transformed into equivalent aquifer buffering capacities rounded to 7, 10, and 15 meq/kg per pH unit for the optimistic, best-estimate, and pessimistic cases, respectively. Appendix A shows the derivation of the equivalent aquifer buffering capacities for the three uncertainty cases.
- Assumed concentrations dissolved oxygen, nitrate, ferric to ferrous iron reduction, and sulfate are summarized Table 2. Mineral acidity (strong acids) is zero because groundwater and soil pH is greater than 4.5.
- Groundwater and soil TCE concentrations were fixed at 100 μg/L (two times maximum distal plume concentration of 50 μg/L) and 0.5 mg/kg, respectively.

Table 2. Assumed Base-Add-Design-Tool Geochemical Parameters.

Parameter	Optimistic Case	Best-Estimate Case	Pessimistic Case
Dissolved Oxygen (mg/L)	2	3	6
Nitrate (mg/L)	3.0	1.5	1.0
Ferric to Ferrous reduction (mg/L)	10.0	5.0	2.0
Sulfate (mg/L)	0.5	1.0	2.0

<u>Results</u>

Figure B-1, Figure B-2, and Figure B-3 in Appendix B present the Base-Add-Design-Tool results for the CoBupHMg™ buffer solution for the best estimate, optimistic, and pessimistic cases, respectively. Each figure includes the buffer calculation sheet from the Base-Add-Design-Tool Microsoft Excel file as well as a table of post-processing calculations that transform the total base demand from OH^- equivalents to gallons of pH buffer solution per injection well.

Similarly, Figure C-1, Figure C-2, and Figure C-3 in Appendix C present the Base-Add-Design-Tool results for the NaOH/$NaHCO_3$ buffer solution.

References

Clemson Regulatory Services (2019) Agricultural Service Lab - Soil Testing. Clemson, SC. https://www.clemson.edu//public/regulatory/ag-srvc-lab/soil-testing/index.html

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SRNS (2019) Underground Injection Control Permit Application for the Implementation of the Non-Time Critical Removal Action at the C-Area Groundwater Operable Unit (U). SRNS-RP-2019-00030, Rev. 0. Savannah River Nuclear Solutions, Aiken, SC.

Appendix A. Calculations for Aquifer Buffer Capacity

Clemson Regulatory Services (2019) provides tables of recommended ground, agricultural limestone application rates to raise the soil pH of the surface eight inches to a target pH as a function of the current soil pH, target soil pH, and Moore-Sikora buffer pH (Sikora and Moore, 2008). Table A-1 displays the recommended agricultural limestone application rates for a target pH of 7.0 (Clemson Regulatory Services, 2019). Data in Table A-1 were normalized to a soil depth of one foot, rather than eight inches.

Soil buffer pH values of 7.85, 7.75, and 7.65 were chosen for the optimistic, best-estimate, and pessimistic cases, respectively. To enable input to the Base-Add-Design-Tool model, the lime application rates from Clemson were transformed into equivalent aquifer buffering capacities rounded to 7, 10, and 15 meq/kg per pH unit increase for the optimistic, best-estimate, and pessimistic cases, respectively. Conversion calculations are shown below.

Table A-1. Agricultural Limestone Requirement (ton/acre/foot depth) for Target pH 7.0 based on Moore-Sikora Buffer pH Test (Clemson Regulatory Services, 2019).

Buffer pH	Soil pH										
	6.4	6.2	6	5.8	5.6	5.4	5.2	5	4.9	4.7	4.5
7.95	0.30	0.30	0.38	0.38	0.45	0.45	0.45	0.45	0.45	0.53	0.53
7.9	0.53	0.68	0.75	0.75	0.83	0.90	0.90	0.98	0.98	0.98	1.05
7.85	0.83	0.98	1.05	1.20	1.28	1.28	1.35	1.43	1.43	1.50	1.50
7.8	1.13	1.28	1.43	1.58	1.65	1.73	1.80	1.88	1.95	1.95	2.03
7.75	1.43	1.65	1.80	1.95	2.10	2.18	2.25	2.33	2.40	2.48	2.55
7.7	1.65	1.95	2.18	2.33	2.48	2.63	2.70	2.85	2.85	3.00	3.08
7.65	1.95	2.25	2.55	2.78	2.93	3.08	3.15	3.30	3.38	3.45	3.60
7.6	2.25	2.63	2.93	3.15	3.30	3.53	3.68	3.75	3.83	3.98	4.05
7.55	2.48	2.93	3.23	3.53	3.75	3.90	4.13	4.28	4.28	4.43	4.58
7.5	2.78	3.23	3.60	3.90	4.13	4.35	4.58	4.73	4.80	4.95	5.10
7.45	3.08	3.60	3.98	4.28	4.58	4.80	5.03	5.18	5.25	5.40	5.63
7.4	3.38	3.90	4.35	4.73	5.03	5.25	5.48	5.63	5.78	5.93	6.15
7.35	3.60	4.20	4.73	5.10	5.40	5.70	5.93	6.15	6.23	6.45	6.60
7.3	3.90	4.58	5.10	5.48	5.85	6.15	6.38	6.60	6.68	6.90	7.13
7.25	4.20	4.88	5.40	5.85	6.23	6.53	6.83	7.05	7.20	7.43	7.50
7.2	4.43	5.18	5.78	6.23	6.68	6.98	7.28	7.50	7.50	7.50	7.50
7.15	4.73	5.55	6.15	6.68	7.05	7.43	7.50	7.50	7.50	7.50	7.50
7.1	5.03	5.85	6.53	7.05	7.50	7.50	7.50	7.50	7.50	7.50	7.50
7.05	5.33	6.15	6.90	7.43	7.50	7.50	7.50	7.50	7.50	7.50	7.50
7	5.55	6.53	7.20	7.50	7.50	7.50	7.50	7.50	7.50	7.50	7.50

Optimistic Case

$$\frac{1.43\text{ ton}}{\text{acre}\cdot\text{ft}}\,\frac{2000\text{ lb}}{\text{ton}}\,\frac{1\text{ acre}}{43{,}560\text{ ft}^2}\,\frac{1\text{ ft}^3\text{soil}}{100\text{ lb soil}}\,\frac{1000\text{ g}}{\text{kg}}\,\frac{1\text{ gmole CaCO}_3}{100\text{ g CaCO}_3}\,\frac{2\text{ equiv.}}{\text{gmole CaCO}_3}\,\frac{1000\text{ meq}}{\text{equiv.}}\,\frac{1}{2\text{ pH units increase}}$$

$$=\frac{6.6\text{ meq}}{\text{kg}\cdot\text{pH unit}}\approx\frac{\mathbf{7\ meq}}{\mathbf{kg\cdot pH\ unit}}$$

Best-Estimate Case

$$\frac{2.33\text{ ton}}{\text{acre}\cdot\text{ft}}\,\frac{2000\text{ lb}}{\text{ton}}\,\frac{1\text{ acre}}{43{,}560\text{ ft}^2}\,\frac{1\text{ ft}^3\text{soil}}{100\text{ lb soil}}\,\frac{1000\text{ g}}{\text{kg}}\,\frac{1\text{ gmole CaCO}_3}{100\text{ g CaCO}_3}\,\frac{2\text{ equiv.}}{\text{gmole CaCO}_3}\,\frac{1000\text{ meq}}{\text{equiv.}}\,\frac{1}{2\text{ pH units increase}}$$

$$=\frac{10.7\text{ meq}}{\text{kg}\cdot\text{pH unit}}\approx\frac{\mathbf{10\ meq}}{\mathbf{kg\cdot pH\ unit}}$$

Pessimistic Case

$$\frac{3.30\text{ ton}}{\text{acre}\cdot\text{ft}}\,\frac{2000\text{ lb}}{\text{ton}}\,\frac{1\text{ acre}}{43560\text{ ft}^2}\,\frac{1\text{ ft}^3\text{soil}}{100\text{ lb soil}}\,\frac{1000\text{ g}}{\text{kg}}\,\frac{1\text{ gmole CaCO}_3}{100\text{ g CaCO}_3}\,\frac{2\text{ equiv}}{\text{gmole CaCO}_3}\,\frac{1000\text{ meq}}{\text{equiv}}\,\frac{1}{2\text{ pH units increase}}$$

$$=\frac{15.2\text{ meq}}{\text{kg}\cdot\text{pH unit}}\approx\frac{\mathbf{15\ meq}}{\mathbf{kg\cdot pH\ unit}}$$

Appendix B. Results of Base-Add-Design-Tool Calculations for CoBupHMg™ Buffer Solution

Site Information				
Facility Name:	SRS			
Site Name:	CAGW OU - Best Estimate Case			
Owner:	DOE			
Aquifer Characteristics				
Description:	Silty fine-Medium Grain Sand			
Hydraulic Gradient:	0.017	m/m	0	ft/ft
Hydraulic Conductivity:	3.96	m/d	13	ft/d
Sediment Specific Gravity:	2.15	g/cm^3		
Porosity:	0.25	mL/cm^3		
Bulk Density:	1.61	g/cm^3	100	lb/ft^3
Treatment Zone				
Design Period:	5.0	yr		
Width:	73.2	m	240	ft
Length:	4.9	m	16	ft
Vertical Thickness:	3.1	m	10	ft
Volume:	1,088	m^3	38,427	ft^3
Treated Soil:	1,754,626	Kg	3,860,170	lb
Pore Volume:	272,035	L	71,864	gal
GW Flux:	5,472,703	L/yr	1,445,740	gal/yr
Total GW Vol.:	27,635,550	L	7,300,563	gal
Hydraulic Retention Time:	0.05	yr		
Geochemistry				
Target pH:	7.0	SU	α =	0.18
Background pH:	5.0	SU	α =	0.96
Total Inorganic Carbon:	20	mg/L		
Background CO_2 Acidity:	1.3	meq/L		
Background CO_2 Alkalinity:	0.0	meq/L		
Mineral Acidity:	0.0	meq/L		
Total GW Acidity	1	meq/L		
Aquifer Buffering Capac.:	10.0	meq/Kg/pH		
Base to raise starting pH	35,093	OH^- eq		

Initial GW and Soil Concentrations			
Average Conc.	GW	Soil	GW+Soil
Units	(mg/L)	(mg/Kg)	(Kg)
PCE	0.0	0.0	0
TCE	0.1	0.5	4
DCE	0.0	0.0	0
VC	0.0	0.0	0
Oxygen	3.0	NA	83
Nitrate	1.5	NA	41
Fe(III) --> Fe(II)	5.0	0.0	138
Sulfate	1.0	NA	28

	Amount Added		Amount Consumed
Reagents	Kg	lb	
Acetic Acid	0		100%
Lactic Acid	0		100%
Glucose	0		100%
Soybean Oil	14,482	31,860.5	50%
Caustic Soda	0		100%
Caustic Potash	0		100%
Soda Ash	0		100%
Baking Soda	0	0.0	100%
Hydrated Lime	0		100%
Magnesium Hydroxide	5,326	11,716.4	100%

Base Demand Summary	OH^- eq
Influent Acidity	35,642
Base to raise starting pH	35,093
Acidity from Dechlorination	85
Acidity from Added Substrate	380,777
Acidity from e^- accept / donors	-268,898
Total Base Demand	182,698
Total Base Added	182,698
Fraction of Base Demand Met	100%

Calculate Volume of CoBupHMg Required per Injection Well

Number of Injection Wells: 15

Total Equivalents OH- Required	Equivalents OH- per lb CoBupHMg Concentrate	lb Buffer Conc./Gal.	lb Buffer Conc./ 5-Gal. Container	Actual Gallons Conc./Well	# 5-Gal. Containers Conc./Well
182,698	7	11.44	50	152	35

Figure B-1. Results of Base-Add-Design-Tool Calculations for CoBupHMg™ Buffer Solution – Best-Estimate Case.

Site Information					
Facility Name:	SRS				
Site Name:	CAGW OU - Optimistic Case				
Owner:	DOE				
Aquifer Characteristics					
Description:	Silty fine-Medium Grain Sand				
Hydraulic Gradient:	0.017	m/m	0	ft/ft
Hydraulic Conductivity:	3.96	m/d	13	ft/d
Sediment Specific Gravity:	2.15	g/cm^3		
Porosity:	0.25	mL/cm^3		
Bulk Density:	1.61	g/cm^3	100	lb/ft^3

Initial GW and Soil Concentrations			
Average Conc.	GW	Soil	GW+Soil
Units	(mg/L)	(mg/Kg)	(Kg)
PCE	0.0	0.0	0
TCE	0.1	0.5	4
DCE	0.0	0.0	0
VC	0.0	0.0	0
Oxygen	2.0	NA	55
Nitrate	3.0	NA	83
Fe(III) --> Fe(II)	10.0	0.0	276
Sulfate	0.5	NA	14

Treatment Zone				
Design Period:	5.0	yr		
Width:	73.2	m	240	ft
Length:	4.9	m	16	ft
Vertical Thickness:	3.1	m	10	ft
Volume:	1,088	m^3	38,427	ft^3
Treated Soil:	1,754,626	Kg	3,860,170	lb
Pore Volume:	272,035	L	71,864	gal
GW Flux:	5,472,703	L/yr	1,445,740	gal/yr
Total GW Vol.:	27,635,550	L	7,300,563	gal
Hydraulic Retention Time:	0.05	yr		

Reagents	Amount Added Kg	Amount Added lb	Amount Consumed
Acetic Acid	0		100%
Lactic Acid	0		100%
Glucose	0		100%
Soybean Oil	14,482	31,860.5	40%
Caustic Soda	0		100%
Caustic Potash	0		100%
Soda Ash	0		100%
Baking Soda	0	0.0	100%
Hydrated Lime	0		100%
Magnesium Hydroxide	3,665	8,063.6	100%

Geochemistry				
Target pH:	7.0	SU	α =	0.18
Background pH:	5.0	SU	α =	0.96
Total Inorganic Carbon:	10	mg/L		
Background CO_2 Acidity:	0.6	meq/L		
Background CO_2 Alkalinity:	0.0	meq/L		
Mineral Acidity:	0.0	meq/L		
Total GW Acidity	1	meq/L		
Aquifer Buffering Capac.:	7.0	meq/Kg/pH		
Base to raise starting pH	24,565	OH^- eq		

Base Demand Summary	OH^- eq
Influent Acidity	17,821
Base to raise starting pH	24,565
Acidity from Dechlorination	85
Acidity from Added Substrate	304,621
Acidity from e^- accept / donors	-221,354
Total Base Demand	125,738
Total Base Added	125,738
Fraction of Base Demand Met	100%

Calculate Volume of CoBupHMg Required per Injection Well

Number of Injection Wells: 15

Total Equivalents OH- Required	Equivalents OH- per lb CoBupHMg Concentrate	lb Buffer Conc./Gal.	lb Buffer Conc./ 5-Gal. Container	Actual Gallons Conc./Well	# 5-Gal. Containers Conc./Well
125,738	7	11.44	50	105	24

Figure B-2. Results of Base-Add-Design-Tool Calculations for CoBupHMg™ Buffer Solution – Optimistic Case.

Site Information				
Facility Name:	SRS			
Site Name:	CAGW OU - Pessimistic Case			
Owner:	DOE			
Aquifer Characteristics				
Description:	Silty fine-Medium Grain Sand			
Hydraulic Gradient:	0.017	m/m	0	ft/ft
Hydraulic Conductivity:	3.96	m/d	13	ft/d
Sediment Specific Gravity:	2.15	g/cm^3		
Porosity:	0.25	mL/cm^3		
Bulk Density:	1.61	g/cm^3	100	lb/ft^3
Treatment Zone				
Design Period:	5.0	yr		
Width:	73.2	m	240	ft
Length:	4.9	m	16	ft
Vertical Thickness:	3.1	m	10	ft
Volume:	1,088	m^3	38,427	ft^3
Treated Soil:	1,754,626	Kg	3,860,170	lb
Pore Volume:	272,035	L	71,864	gal
GW Flux:	5,472,703	L/yr	1,445,740	gal/yr
Total GW Vol.:	27,635,550	L	7,300,563	gal
Hydraulic Retention Time:	0.05	yr		
Geochemistry				
Target pH:	7.0	SU	α =	0.18
Background pH:	5.0	SU	α =	0.96
Total Inorganic Carbon:	30	mg/L		
Background CO_2 Acidity:	1.9	meq/L		
Background CO_2 Alkalinity:	0.0	meq/L		
Mineral Acidity:	0.0	meq/L		
Total GW Acidity	2	meq/L		
Aquifer Buffering Capac.:	15.0	meq/Kg/pH		
Base to raise starting pH	52,639	OH^- eq		

Initial GW and Soil Concentrations			
Average Conc.	GW	Soil	GW+Soil
Units	(mg/L)	(mg/Kg)	(Kg)
PCE	0.0	0.0	0
TCE	0.1	0.5	4
DCE	0.0	0.0	0
VC	0.0	0.0	0
Oxygen	6.0	NA	166
Nitrate	1.0	NA	28
Fe(III) --> Fe(II)	2.0	0.0	55
Sulfate	2.0	NA	55

	Amount Added		Amount Consumed
Reagents	Kg	lb	
Acetic Acid	0		100%
Lactic Acid	0		100%
Glucose	0		100%
Soybean Oil	14,482	31,860.5	60%
Caustic Soda	0		100%
Caustic Potash	0		100%
Soda Ash	0		100%
Baking Soda	0	0.0	100%
Hydrated Lime	0		100%
Magnesium Hydroxide	7,154	15,737.7	100%

Base Demand Summary	OH^- eq
Influent Acidity	53,462
Base to raise starting pH	52,639
Acidity from Dechlorination	85
Acidity from Added Substrate	456,932
Acidity from e^- accept / donors	-317,715
Total Base Demand	245,403
Total Base Added	245,403
Fraction of Base Demand Met	100%

Calculate Volume of CoBupHMg Required per Injection Well

Number of Injection Wells: 15

Total Equivalents OH- Required	Equivalents OH- per lb CoBupHMg Concentrate	lb Buffer Conc./Gal.	lb Buffer Conc./ 5-Gal. Container	Actual Gallons Conc./Well	# 5-Gal. Containers Conc./Well
245,403	7	11.44	50	204	47

Figure B-3. Results of Base-Add-Design-Tool Calculations for CoBupHMg™ Buffer Solution – Pessimistic Case.

Appendix C. Results of Base-Add-Design-Tool Calculations for NaOH/$NaHCO_3$ Buffer Solution

Site Information				
Facility Name:	SRS			
Site Name:	CAGW OU - Best Estimate Case			
Owner:	DOE			
Aquifer Characteristics				
Description:	Silty fine-Medium Grain Sand			
Hydraulic Gradient:	0.017	m/m	0	ft/ft
Hydraulic Conductivity:	3.96	m/d	13	ft/d
Sediment Specific Gravity:	2.15	g/cm^3		
Porosity:	0.25	mL/cm^3		
Bulk Density:	1.61	g/cm^3	100	lb/ft^3
Treatment Zone				
Design Period:	5.0	yr		
Width:	73.2	m	240	ft
Length:	4.9	m	16	ft
Vertical Thickness:	3.1	m	10	ft
Volume:	1,088	m^3	38,427	ft^3
Treated Soil:	1,754,626	Kg	3,860,170	lb
Pore Volume:	272,035	L	71,864	gal
GW Flux:	5,472,703	L/yr	1,445,740	gal/yr
Total GW Vol.:	27,635,550	L	7,300,563	gal
Hydraulic Retention Time:	0.05	yr		
Geochemistry				
Target pH:	7.0	SU	α =	0.18
Background pH:	5.0	SU	α =	0.96
Total Inorganic Carbon:	20	mg/L		
Background CO_2 Acidity:	1.3	meq/L		
Background CO_2 Alkalinity:	0.0	meq/L		
Mineral Acidity:	0.0	meq/L		
Total GW Acidity	1	meq/L		
Aquifer Buffering Capac.:	10.0	meq/Kg/pH		
Base to raise starting pH	35,093	OH^- eq		

Initial GW and Soil Concentrations			
Average Conc.	GW	Soil	GW+Soil
Units	(mg/L)	(mg/Kg)	(Kg)
PCE	0.0	0.0	0
TCE	0.1	0.5	4
DCE	0.0	0.0	0
VC	0.0	0.0	0
Oxygen	3.0	NA	83
Nitrate	1.5	NA	41
Fe(III) --> Fe(II)	5.0	0.0	138
Sulfate	1.0	NA	28

Reagents	Amount Added Kg	Amount Added lb	Amount Consumed
Acetic Acid	0		100%
Lactic Acid	0		100%
Glucose	0		100%
Soybean Oil	14,482	31,860.5	50%
Caustic Soda	5,373	11,821.4	100%
Caustic Potash	0		100%
Soda Ash	0		100%
Baking Soda	22,126	48,677.2	100%
Hydrated Lime	0		100%
Magnesium Hydroxide	0		100%

Base Demand Summary	OH^- eq
Influent Acidity	35,642
Base to raise starting pH	35,093
Acidity from Dechlorination	85
Acidity from Added Substrate	380,777
Acidity from e^- accept / donors	-268,898
Total Base Demand	182,698
Total Base Added	182,698
Fraction of Base Demand Met	100%

Calculate Volume of NaHCO3/NaOH Buffer Solution Required per Injection Well

Number of Injection Wells: 15

Total Mass NaHCO3 Required (lb)	Total Mass NaOH Required (lb)	Wt% NaOH	Wt% NaHCO3	Total Mass Buffer Solution (lb)	lb Buffer Soln./Gal.	Gallons of Buffer/Well
48,677	11,821	1.7	7.0	695388	8.382	5531

Figure C-1. Results of Base-Add-Design-Tool Calculations for NaOH/$NaHCO_3$ Buffer Solution – Best-Estimate Case.

Site Information				
Facility Name:	SRS			
Site Name:	CAGW OU - Optimistic Case			
Owner:	DOE			
Aquifer Characteristics				
Description:	Silty fine-Medium Grain Sand			
Hydraulic Gradient:	0.017	m/m	0	ft/ft
Hydraulic Conductivity:	3.96	m/d	13	ft/d
Sediment Specific Gravity:	2.15	g/cm^3		
Porosity:	0.25	mL/cm^3		
Bulk Density:	1.61	g/cm^3	100	lb/ft^3

Treatment Zone				
Design Period:	5.0	yr		
Width:	73.2	m	240	ft
Length:	4.9	m	16	ft
Vertical Thickness:	3.1	m	10	ft
Volume:	1,088	m^3	38,427	ft^3
Treated Soil:	1,754,626	Kg	3,860,170	lb
Pore Volume:	272,035	L	71,864	gal
GW Flux:	5,472,703	L/yr	1,445,740	gal/yr
Total GW Vol.:	27,635,550	L	7,300,563	gal
Hydraulic Retention Time:	0.05	yr		

Geochemistry				
Target pH:	7.0	SU	α =	0.18
Background pH:	5.0	SU	α =	0.96
Total Inorganic Carbon:	10	mg/L		
Background CO_2 Acidity:	0.6	meq/L		
Background CO_2 Alkalinity:	0.0	meq/L		
Mineral Acidity:	0.0	meq/L		
Total GW Acidity	1	meq/L		
Aquifer Buffering Capac.:	7.0	meq/Kg/pH		
Base to raise starting pH	24,565	OH^- eq		

Initial GW and Soil Concentrations			
Average Conc.	GW	Soil	GW+Soil
Units	(mg/L)	(mg/Kg)	(Kg)
PCE	0.0	0.0	0
TCE	0.1	0.5	4
DCE	0.0	0.0	0
VC	0.0	0.0	0
Oxygen	2.0	NA	55
Nitrate	3.0	NA	83
Fe(III) --> Fe(II)	10.0	0.0	276
Sulfate	0.5	NA	14

	Amount Added		Amount Consumed
Reagents	Kg	lb	
Acetic Acid	0		100%
Lactic Acid	0		100%
Glucose	0		100%
Soybean Oil	14,482	31,860.5	40%
Caustic Soda	3,698	8,135.8	100%
Caustic Potash	0		100%
Soda Ash	0		100%
Baking Soda	15,228	33,500.9	100%
Hydrated Lime	0		100%
Magnesium Hydroxide	0		100%

Base Demand Summary	OH^- eq
Influent Acidity	17,821
Base to raise starting pH	24,565
Acidity from Dechlorination	85
Acidity from Added Substrate	304,621
Acidity from e^- accept / donors	-221,354
Total Base Demand	125,738
Total Base Added	125,738
Fraction of Base Demand Met	100%

Calculate Volume of NaHCO3/NaOH Buffer Solution Required per Injection Well

Number of Injection Wells: 15

Total Mass NaHCO3 Required (lb)	Total Mass NaOH Required (lb)	Wt% NaOH	Wt% NaHCO3	Total Mass Buffer Solution (lb)	lb Buffer Soln./Gal.	Gallons of Buffer/Well
33,501	8,136	1.7	7.0	478584	8.382	3806

Figure C-2. Results of Base-Add-Design-Tool Calculations for NaOH/$NaHCO_3$ Buffer Solution – Optimistic Case.

Site Information				
Facility Name:	SRS			
Site Name:	CAGW OU - Pessimistic Case			
Owner:	DOE			
Aquifer Characteristics				
Description:	Silty fine-Medium Grain Sand			
Hydraulic Gradient:	0.017	m/m	0	ft/ft
Hydraulic Conductivity:	3.96	m/d	13	ft/d
Sediment Specific Gravity:	2.15	g/cm^3		
Porosity:	0.25	mL/cm^3		
Bulk Density:	1.61	g/cm^3	100	lb/ft^3
Treatment Zone				
Design Period:	5.0	yr		
Width:	73.2	m	240	ft
Length:	4.9	m	16	ft
Vertical Thickness:	3.1	m	10	ft
Volume:	1,088	m^3	38,427	ft^3
Treated Soil:	1,754,626	Kg	3,860,170	lb
Pore Volume:	272,035	L	71,864	gal
GW Flux:	5,472,703	L/yr	1,445,740	gal/yr
Total GW Vol.:	27,635,550	L	7,300,563	gal
Hydraulic Retention Time:	0.05	yr		
Geochemistry				
Target pH:	7.0	SU	α =	0.18
Background pH:	5.0	SU	α =	0.96
Total Inorganic Carbon:	30	mg/L		
Background CO_2 Acidity:	1.9	meq/L		
Background CO_2 Alkalinity:	0.0	meq/L		
Mineral Acidity:	0.0	meq/L		
Total GW Acidity	2	meq/L		
Aquifer Buffering Capac.:	15.0	meq/Kg/pH		
Base to raise starting pH	52,639	OH^- eq		

Initial GW and Soil Concentrations			
Average Conc.	GW	Soil	GW+Soil
Units	(mg/L)	(mg/Kg)	(Kg)
PCE	0.0	0.0	0
TCE	0.1	0.5	4
DCE	0.0	0.0	0
VC	0.0	0.0	0
Oxygen	6.0	NA	166
Nitrate	1.0	NA	28
Fe(III) --> Fe(II)	2.0	0.0	55
Sulfate	2.0	NA	55

	Amount Added		Amount Consumed
Reagents	Kg	lb	
Acetic Acid	0		100%
Lactic Acid	0		100%
Glucose	0		100%
Soybean Oil	14,482	31,860.5	60%
Caustic Soda	7,218	15,878.7	100%
Caustic Potash	0		100%
Soda Ash	0		100%
Baking Soda	29,720	65,383.9	100%
Hydrated Lime	0		100%
Magnesium Hydroxide	0		100%

Base Demand Summary	OH^- eq
Influent Acidity	53,462
Base to raise starting pH	52,639
Acidity from Dechlorination	85
Acidity from Added Substrate	456,932
Acidity from e^- accept / donors	-317,715
Total Base Demand	245,403
Total Base Added	245,403
Fraction of Base Demand Met	100%

Calculate Volume of NaHCO3/NaOH Buffer Solution Required per Injection Well

Number of Injection Wells: 15

Total Mass NaHCO3 Required (lb)	Total Mass NaOH Required (lb)	Wt% NaOH	Wt% NaHCO3	Total Mass Buffer Solution (lb)	lb Buffer Soln./Gal.	Gallons of Buffer/Well
65,384	15,879	1.7	7.0	934056	8.382	7429

Figure C-3. Results of Base-Add-Design-Tool Calculations for NaOH/$NaHCO_3$ Buffer Solution – Pessimistic Case.

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D. A. Crowley, 773-42A
T. L. Danielson, 773-42A
J. A. Dyer, 773-42A
N. V. Halverson, 773-42A
C. C. Herman, 773-A
T. P. Killeen, 730-4B
J. J. Mayer, 999-W
L. T. Reid, 773-A
J. A. Ross, 730-4B
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