West Virginia Mine Drainage Task Force Symposium Workshop:

PHREEQ-N-AMDTreat Model to Evaluate Water-Quality Effects from Passive and Active Treatment of Mine Drainage

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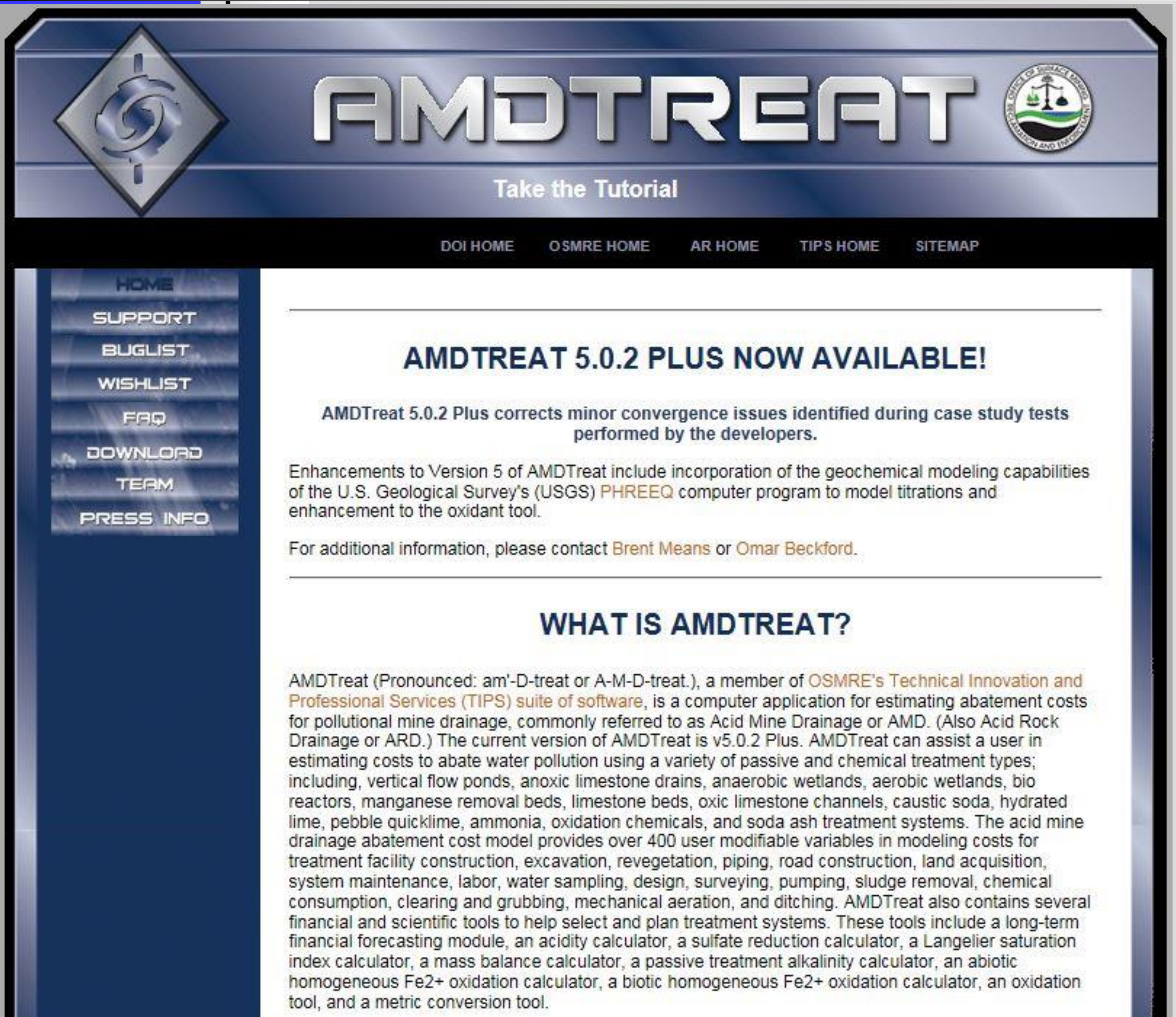
"PHREEQ-N-AMDTREAT"

http://amd.osmre.gov/


AMDTREAT

Take the Tutorial

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PRESS INFO

AMDTREAT 5.0.2 PLUS NOW AVAILABLE!

AMDTreat 5.0.2 Plus corrects minor convergence issues identified during case study tests performed by the developers.

Enhancements to Version 5 of AMDTreat include incorporation of the geochemical modeling capabilities of the U.S. Geological Survey's (USGS) PHREEQ computer program to model titrations and enhancement to the oxidant tool.

For additional information, please contact Brent Means or Omar Beckford.

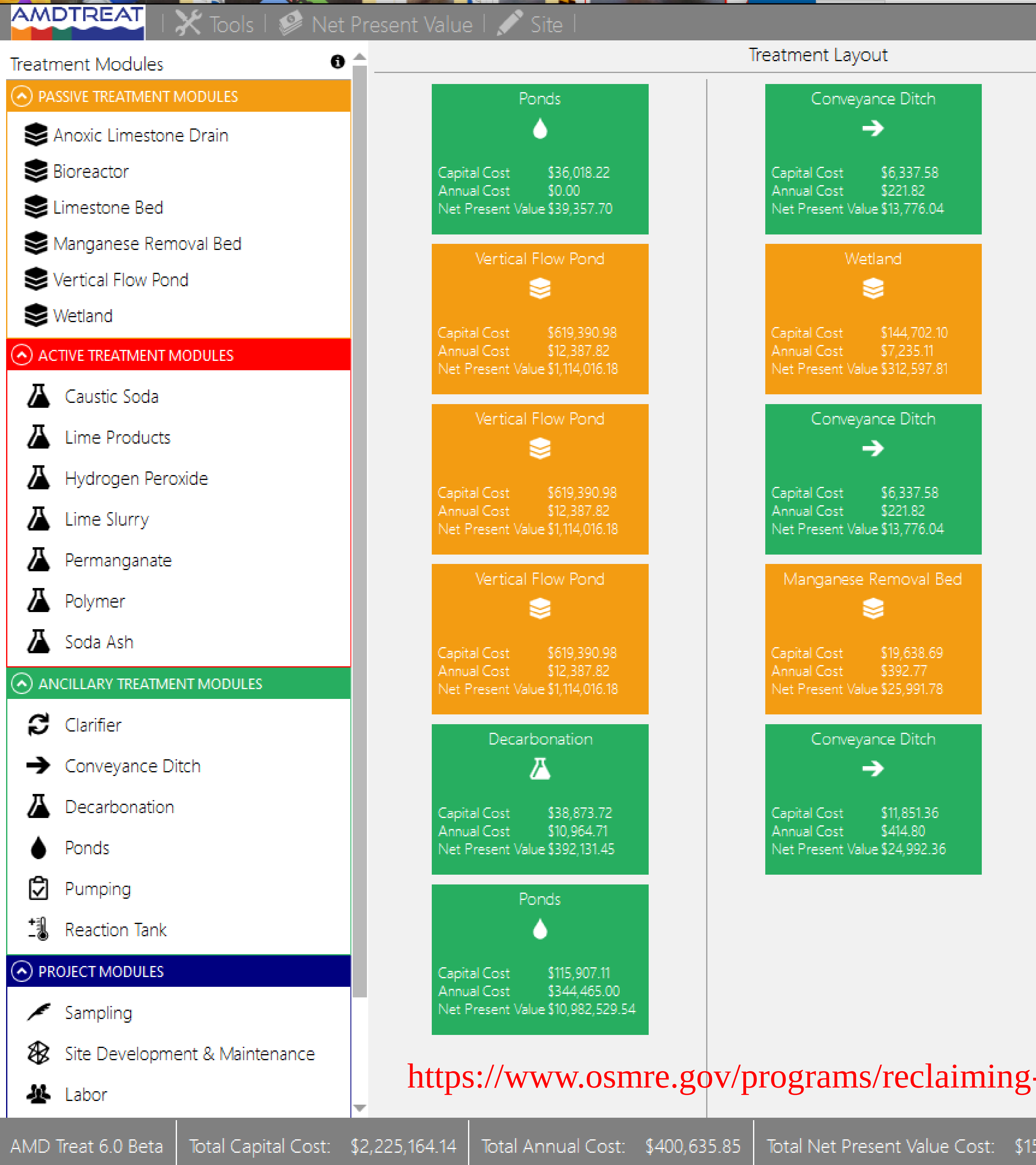
WHAT IS AMDTREAT?

AMDTreat (Pronounced: am'-D-treat or A-M-D-treat.), a member of OSMRE's Technical Innovation and Professional Services (TIPS) suite of software, is a computer application for estimating abatement costs for pollutional mine drainage, commonly referred to as Acid Mine Drainage or AMD. (Also Acid Rock Drainage or ARD.) The current version of AMDTreat is v5.0.2 Plus. AMDTreat can assist a user in estimating costs to abate water pollution using a variety of passive and chemical treatment types; including, vertical flow ponds, anoxic limestone drains, anaerobic wetlands, aerobic wetlands, bio reactors, manganese removal beds, limestone beds, oxic limestone channels, caustic soda, hydrated lime, pebble quicklime, ammonia, oxidation chemicals, and soda ash treatment systems. The acid mine drainage abatement cost model provides over 400 user modifiable variables in modeling costs for treatment facility construction, excavation, revegetation, piping, road construction, land acquisition, system maintenance, labor, water sampling, design, surveying, pumping, sludge removal, chemical consumption, clearing and grubbing, mechanical aeration, and ditching. AMDTreat also contains several financial and scientific tools to help select and plan treatment systems. These tools include a long-term financial forecasting module, an acidity calculator, a sulfate reduction calculator, a Langelier saturation index calculator, a mass balance calculator, a passive treatment alkalinity calculator, an abiotic homogeneous Fe2+ oxidation calculator, a biotic homogeneous Fe2+ oxidation calculator, an oxidation tool, and a metric conversion tool.

AMDTreat is a computer application for estimating abatement costs for AMD (acidic or alkaline mine drainage).

AMDTreat is maintained by OSMRE.

The *obsolete* version of AMDTreat 5.0+ has been recoded from FoxPro to C++ to facilitate its use on computer systems running Windows 10. ***One of three*** PHREEQC geochemical models described below has been incorporated to run with the recoded AMDTreat 6.0 program.

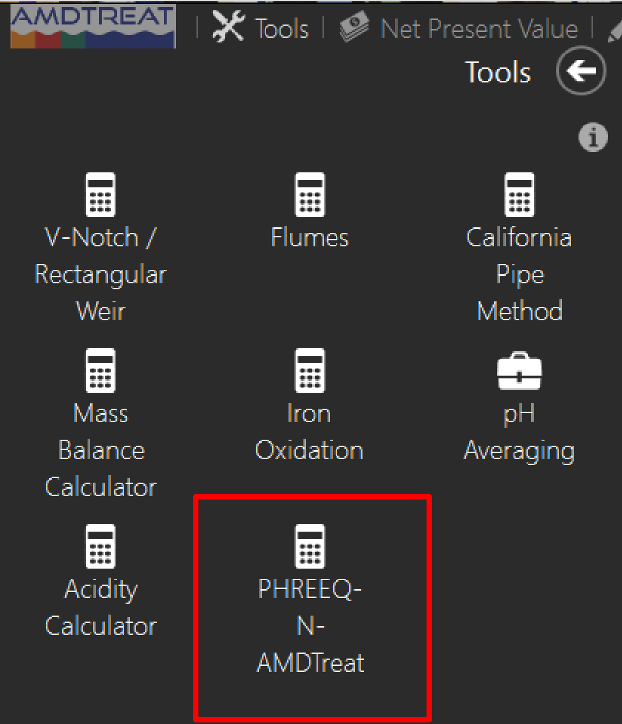


"AMDTreat 6.0"

AMDTreat 6.0 (2022) is a newly updated computer application for estimating costs and sizing of facilities to abate AMD (acidic or alkaline mine drainage) that is maintained by the Office of Surface Mining Reclamation and Enforcement (OSMRE).

The PHREEQ-N-AMDTreat water-quality modeling tool, developed by the USGS with support from OSMRE, was recently incorporated with AMDTreat 6.0 (beta version shown here).

https://www.osmre.gov/programs/reclaiming-abandoned-mine-lands/amdtreat



Cravotta, C.A. III, 2020. Interactive PHREEQ-N-AMDTreat water-quality modeling tools to evaluate performance and design of treatment systems for acid mine drainage (software download): U.S. Geological Survey Software Release. https://doi.org/10.5066/P9QEE3D5

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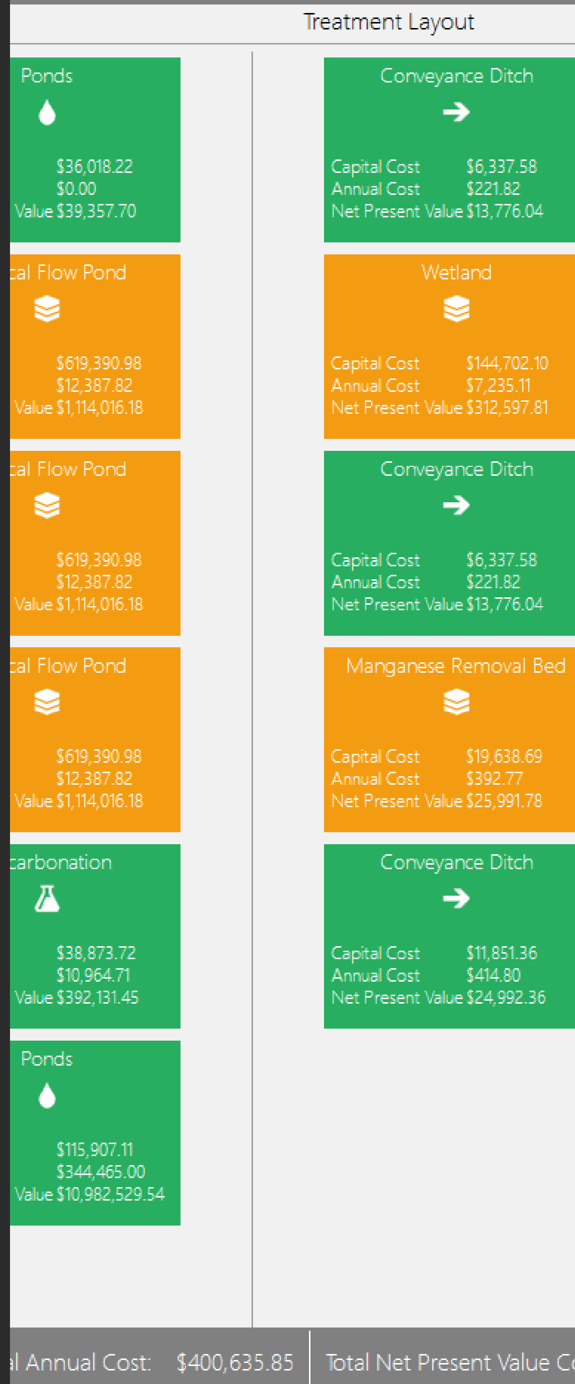


"PHREEQ-N-AMDTreat"

- **TreatTrainMix2 model simulates effects on water quality by treatment system components; useful for costs/benefits analysis.**
  - ✓ **CO_2 outgassing and O_2 ingassing;**
  - ✓ **Iron and manganese oxidation;**
  - ✓ **Limestone dissolution;**
  - ✓ **Oxidation of organic carbon coupled with reduction of Fe^{III}, sulfate, and nitrate.**
  - ✓ **Active treatment with H_2O_2 and/or caustic chemicals.**
  - ✓ **Mass and composition of solids formed, including Fe, Mn, and Al adsorbed by hydrous metal oxides (HMeO = HFO + HMO + HAO).**
- ***An expanded stand-alone model includes rare-earth elements attenuation by adsorption and precipitation.***

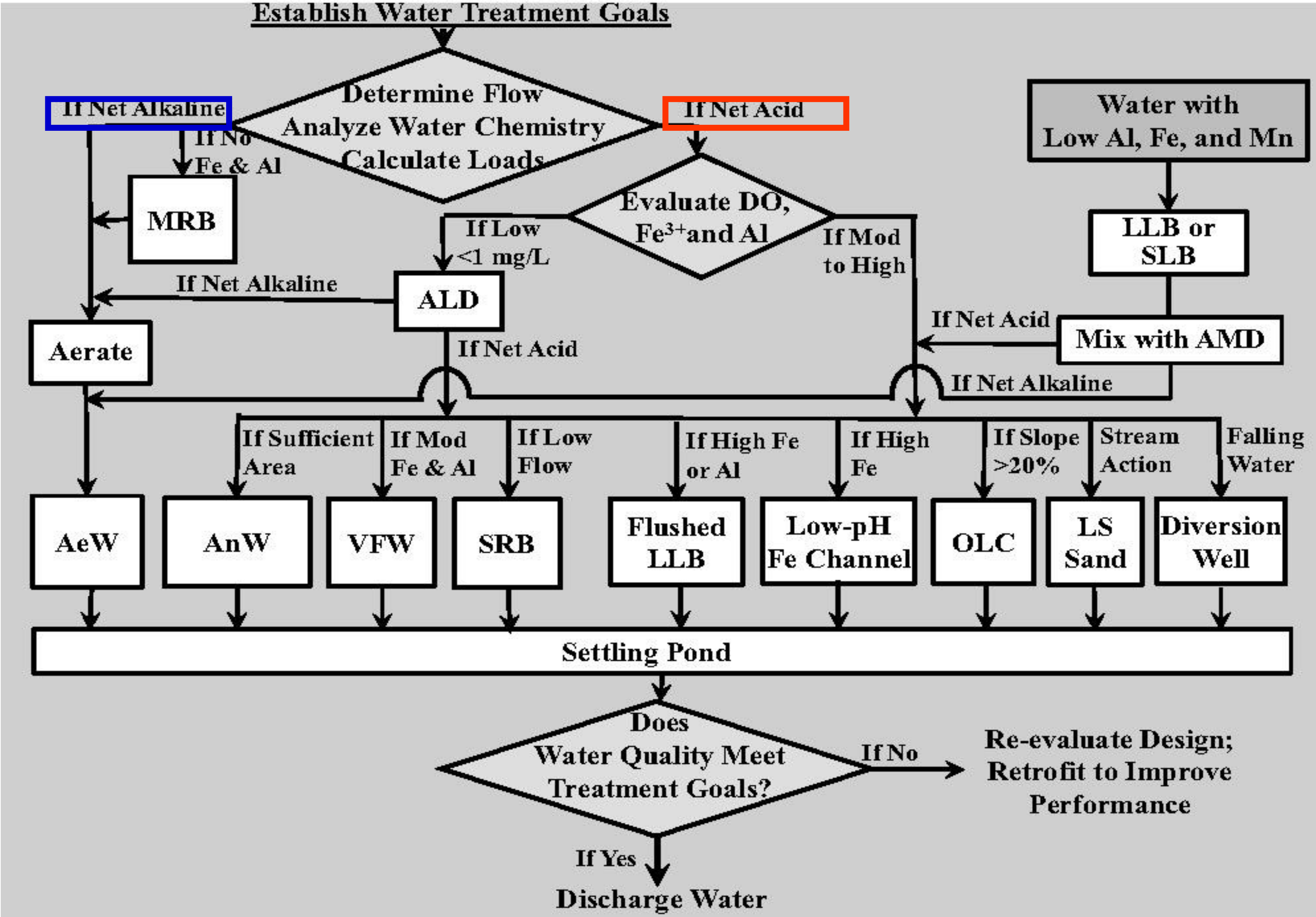
Treatment of AMD
(Acidic or Alkaline Mine Drainage)

Al^{3+}

Fe^{2+} / Fe^{3+}

Mn^{2+}

Passive ⟷	Active
Increase pH/oxidation with aeration, natural substrates & microbes	Increase pH/oxidation with aeration &/or industrial chemicals
Reactions slow	Reactions fast, efficient
Large area footprint	Moderate area footprint
Low maintenance	High maintenance



Skousen, J.G., Zipper, C.E., Rose, A.W., Ziemkiewicz, P.F., Nairn, R., McDonald, L.M., and Kleinmann, R.L., 2017. Review of passive systems for acid mine drainage treatment. Mine Water Environ. 36, 133-153.

PHREEQ-N-AMDTreat Models

Simulate water-quality changes during passive and active treatment.

Three complementary, user-friendly tools use same thermodynamic database and input water-quality data for a given AMD:

- ✓ "CausticTitration.exe"
- ✓ "ParallelTreatment.exe"
- ✓ "TreatTrainMix2.exe" *(→incorporated with AMDTreat 6.0)*

Graphical and tabular output indicates changes in pH, concentrations of metals, TDS, and SC plus the cumulative quantity of precipitated solids as a function of retention time or the amount of caustic added.

Evaluate design/performance and costs/benefits of alternatives.

PHREEQ-N-AMDTreat: Modeled Variables

Variable description	Variable on User Interface
Solutions A and B*	
Design flow	Design flow (gpm)*
Mix fraction	Mix Fraction
Water temperature	Temp (C)
Specific conductance at 25C	SC (uS/cm)
Dissolved oxygen	DO (mg/L)
pH	pH
Acidity	Acidity (mg/L)
Net acidity, calculated	Estimate NetAcidity
Alkalinity	Alk (mg/L)
Total inorganic carbon	TIC (mg/L as C)
Total inorganic carbon, calculated	Estimate TIC
Total iron	Fe (mg/L)
Ferrous iron	Fe2 (mg/L)
Ferrous iron, calculated	Estimate Fe2
Aluminum	Al (mg/L)
Manganese	Mn (mg/L)
Sulfate	SO4 (mg/L)
Chloride	Cl (mg/L)
Calcium	Ca (mg/L)
Magnesium	Mg (mg/L)
Sodium	Na (mg/L)
Potassium	K (mg/L)
Silicon	Si (mg/L)
Nitrate	NO3N (mg/L)
Total dissolved solids	TDS (mg/L)
Dissolved organic carbon	DOC (mg/L as C)
Humate	Humate (mg/L as C)
Hydrogen peroxide, calculated (after conservative mixing of A and B)	Estimate H2O2.mol/L
Kinetic adjustment factor (multiplied by rate constant) applied equally to all steps of ParallelTreatment or TreatTrainMix2 tools	
Factor kCO2, multiplied by CO2 outgassing rate constant (kLaCO2)	factr.kCO2
Factor kO2, multiplied by CO2 outgassing rate constant to estimate O2 ingassing rate constant	factr.kO2
Factor kFeHOM, multiplied by homogeneous Fe2 oxidation rate constant	factr.kFeHOM
Factor kFeHET, multiplied by heterogeneous Fe2 oxidation rate constant	factr.kFeHET
Factor kFeIIMnOx, multiplied by heterogeneous Fe2 oxidation rate constant	factr.kFeIIMnOx
Factor kbact, multiplied by microbial rate constant (assumes Fe oxidizing bacteria MPN = 5.3e11 cells/L)	factr.kbact
Factor kFeNO3, multiplied by homogeneous Fe2 oxidation rate constant	factr.kFeNO3
Factor kMnHOM, multiplied by homogeneous Mn2 oxidation rate constant	factr.kMnHOM
Factor kMnHFO, multiplied by heterogeneous Mn2_HFO oxidation rate constant	factr.kMnHFO
Factor kMnHMO, multiplied by heterogeneous Mn2_HMO oxidation rate constant	factr.kMnHMO
Factor kSHFO, multiplied by FeIII reduction-sulfide oxidation rate constant	factr.kSHFO
Factor kSOC, multiplied by sedimentary organic carbon oxidation rate constant	factr.kSOC
Factor kDOC, multiplied by dissolved organic carbon oxidation rate constant	factr.kDOC
Factor kH2O2, peroxide Fe2 oxidation rate constant	factr.kFeH2O2
Exponential factor for calcite dissolution rate model	EXPcc

Input water-quality, one or two solutions (A+B)

Adjustment factors for rate constants

PHREEQ-N-AMDTreat: Modeled Variables

Variable description	Variable on User Interface
Kinetic adjustment and equilibrium variables used in CausticTitration tool	
Time, in seconds, for pre-aeration step	Time0
kCO2, CO2 mass-transfer rate for pre-aeration step; see Table S6	kLaCO2.1/s
Steady-state log PCO2, used with kCO2 in CO2 mass-transfer rate expression	Steady-state logPCO2
Concentration of caustic soda (NaOH) solution in weight percent	NaOH wt%soln
Equilibrium value (solid-phase precipitation limit) for all steps in CausticTitration, ParallelTreatment, or TreatTrainMix2 tools	
Saturation index for calcite precipitation as equilibrium phase	SI_CaCO3
Saturation index for siderite precipitation as equilibrium phase	SI_FeCO3
Saturation index for Fe(OH)3 precipitation as equilibrium phase; see Table S2	SI_Fe(OH)3
Saturation index for schwertmannite precipitation as equilibrium phase; see Table S2	SI_Schwertmannite
Saturation index for Al(OH)3 precipitation as equilibrium phase; see Table S2	SI_Al(OH)3
Saturation index for basaluminite precipitation as equilibrium phase; see Table S2	SI_Basaluminite
Kinetic adjustment factor applied differently to each step of ParallelTreatment or TreatTrainMix2 tools, i = (1:11)	
Target pH specified for caustic addition at steps 1-5	-->pH
Hours total for step (1:11)	Time.hrs
Water temperature at end of step (1:11)	Temp2.C
Hydrogen peroxide at beginning of step (1:11)	H2O2.mol
kCO2, CO2 mass-transfer rate at beginning of step (1:11); see Table S6	kLaCO2.1/s
Steady-state log PCO2, used with kCO2 in CO2 mass-transfer rate expression for each step (1:11)	Lg(PCO2.atm)
Calcite unit surface area at beginning of step (1:11); see Table S7	SAcc.cm2/mol
Calcite mass fraction in limestone at beginning of step (1:11)	M/M0cc
Sedimentary organic carbon mass at beginning of step (1:11)	SOC.mol
Sorbent mass at beginning of step (1:11)	HMeO.mg
Sorbent content as percent iron at beginning of step (1:11)	Fe%
Sorbent content as percent manganese at beginning of step (1:11)	Mn%
Sorbent content as percent aluminum at beginning of step (1:11)	Al%
Description of step (1:11)	Description

*Input values for two different solutions, A and B, may be entered. Suffix "B" applies to variable names for solution B.

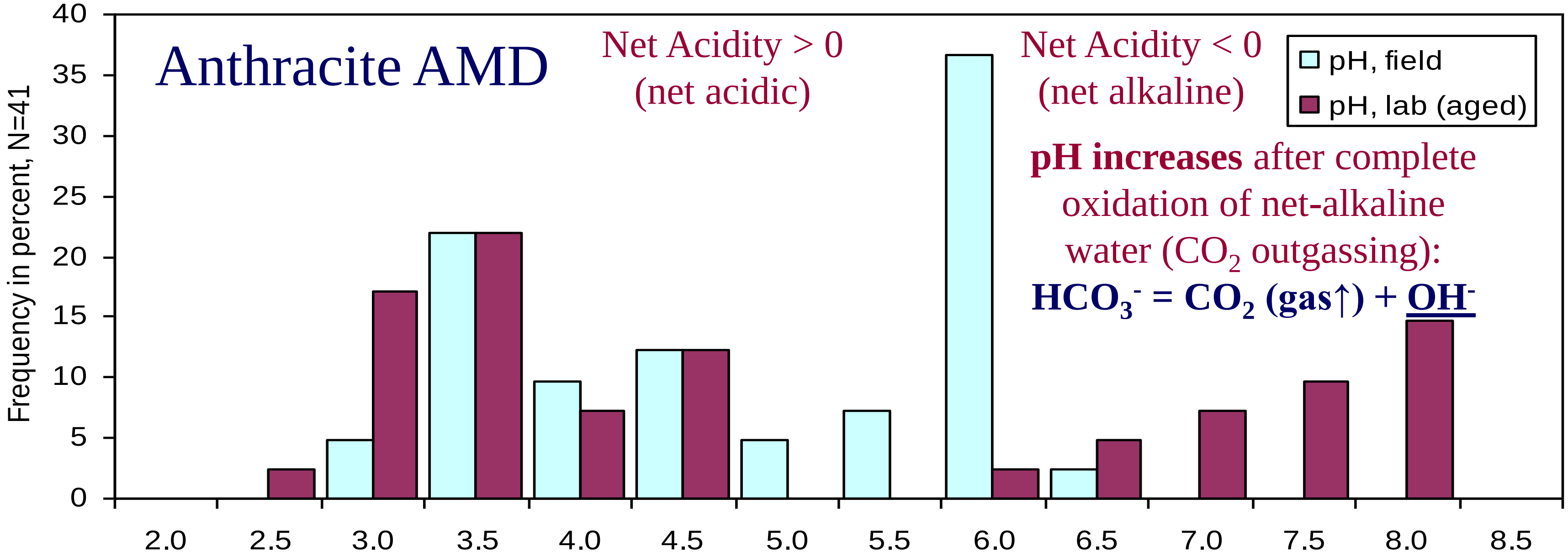
Variables applied in CausticTitration tool

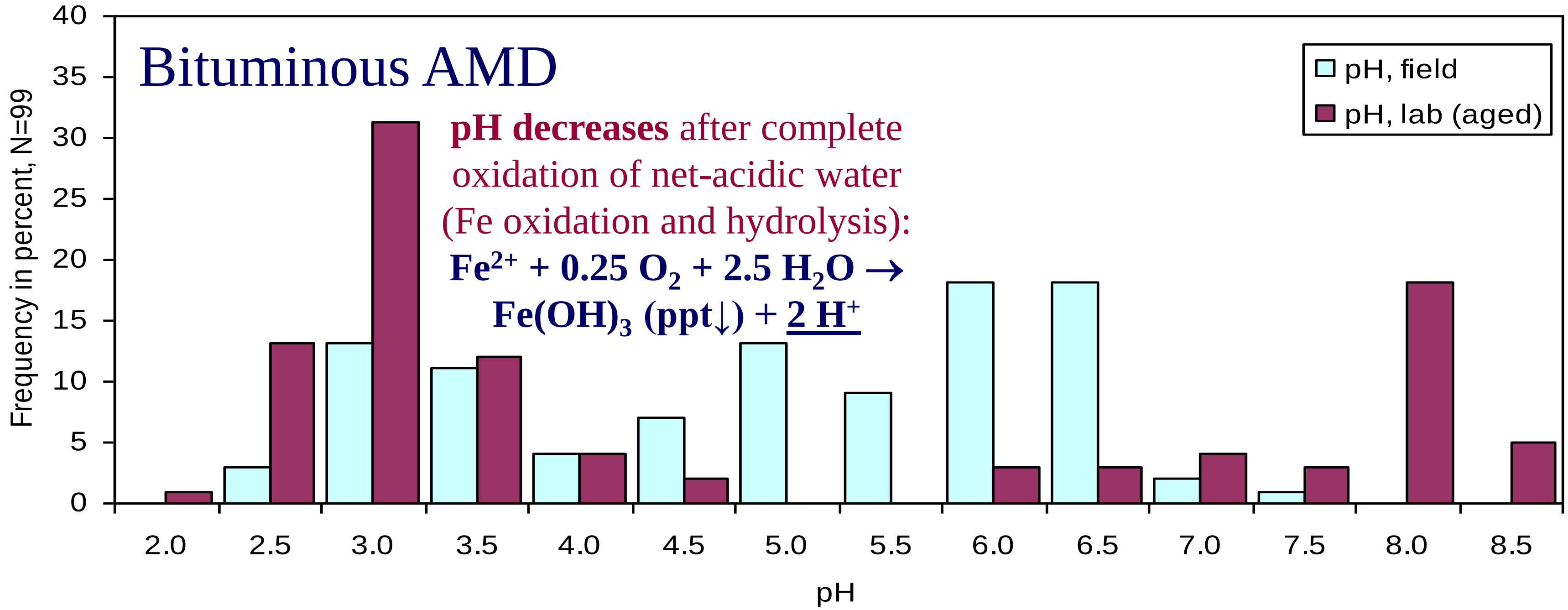
Solid-phase precipitation control

System variables for up to 11 treatment steps

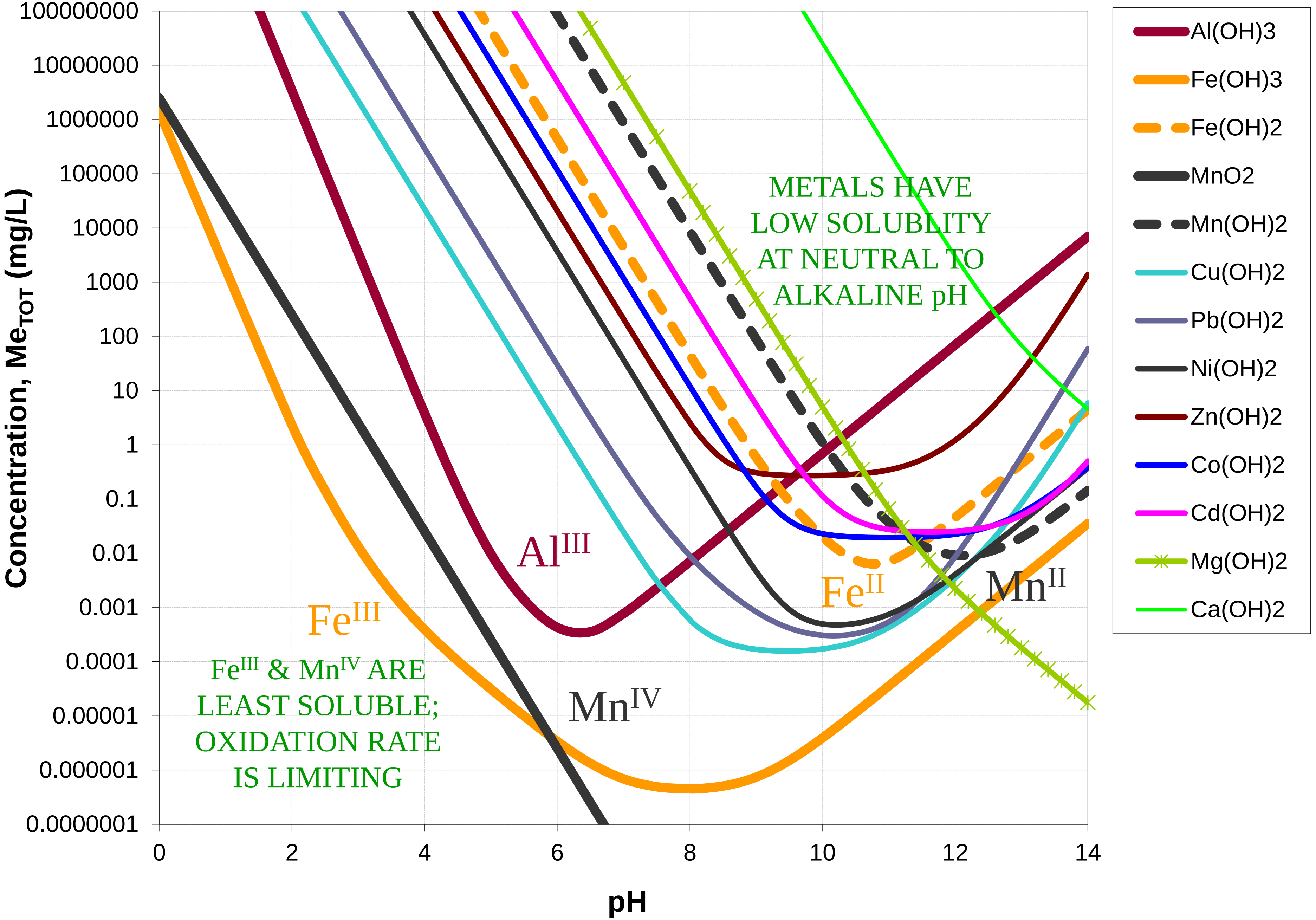
pH, Oxidation State, and Speciation Affect Attenuation of Metals

Bimodal pH, Net Acidic, and Net Alkaline AMD

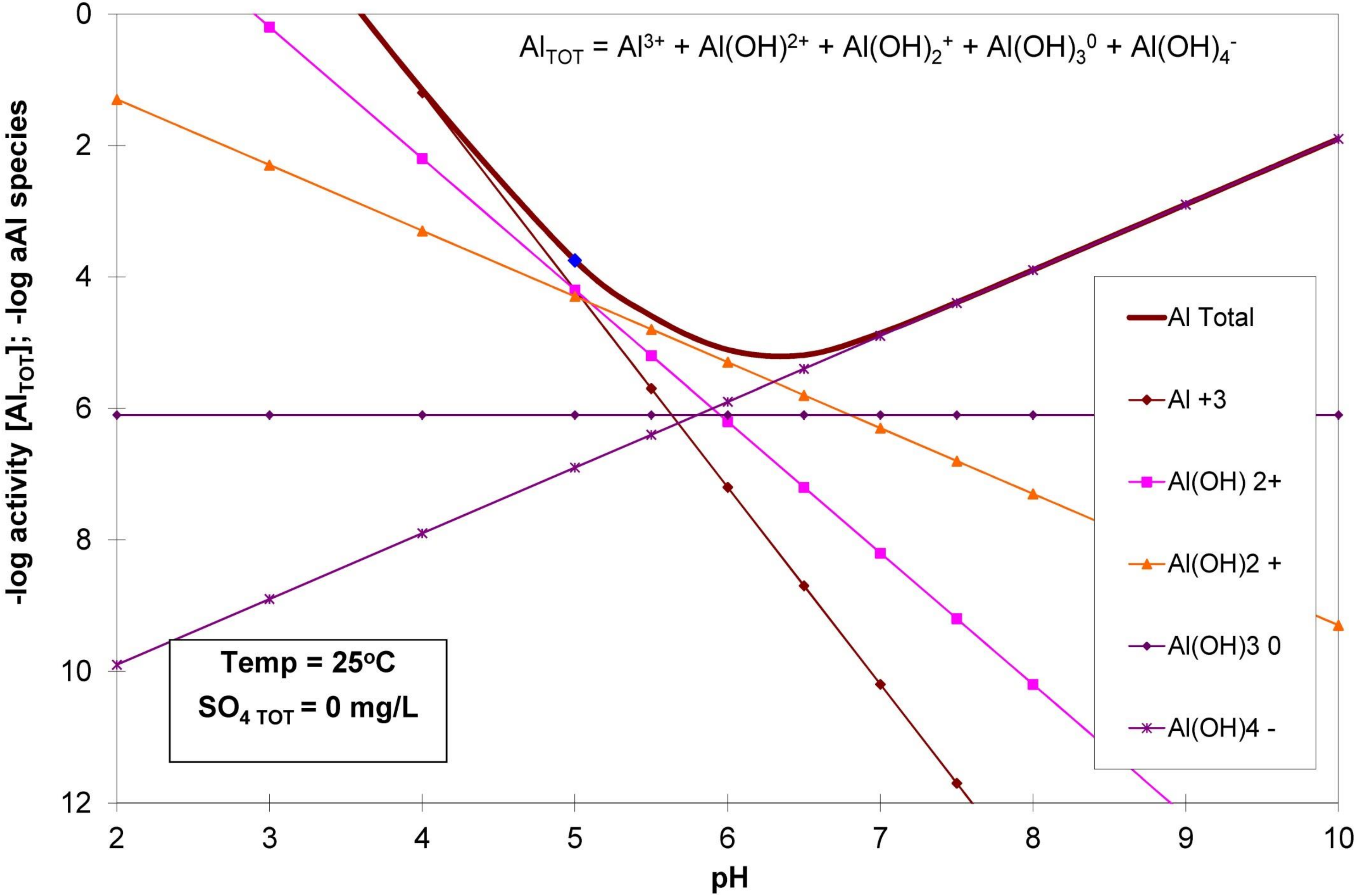




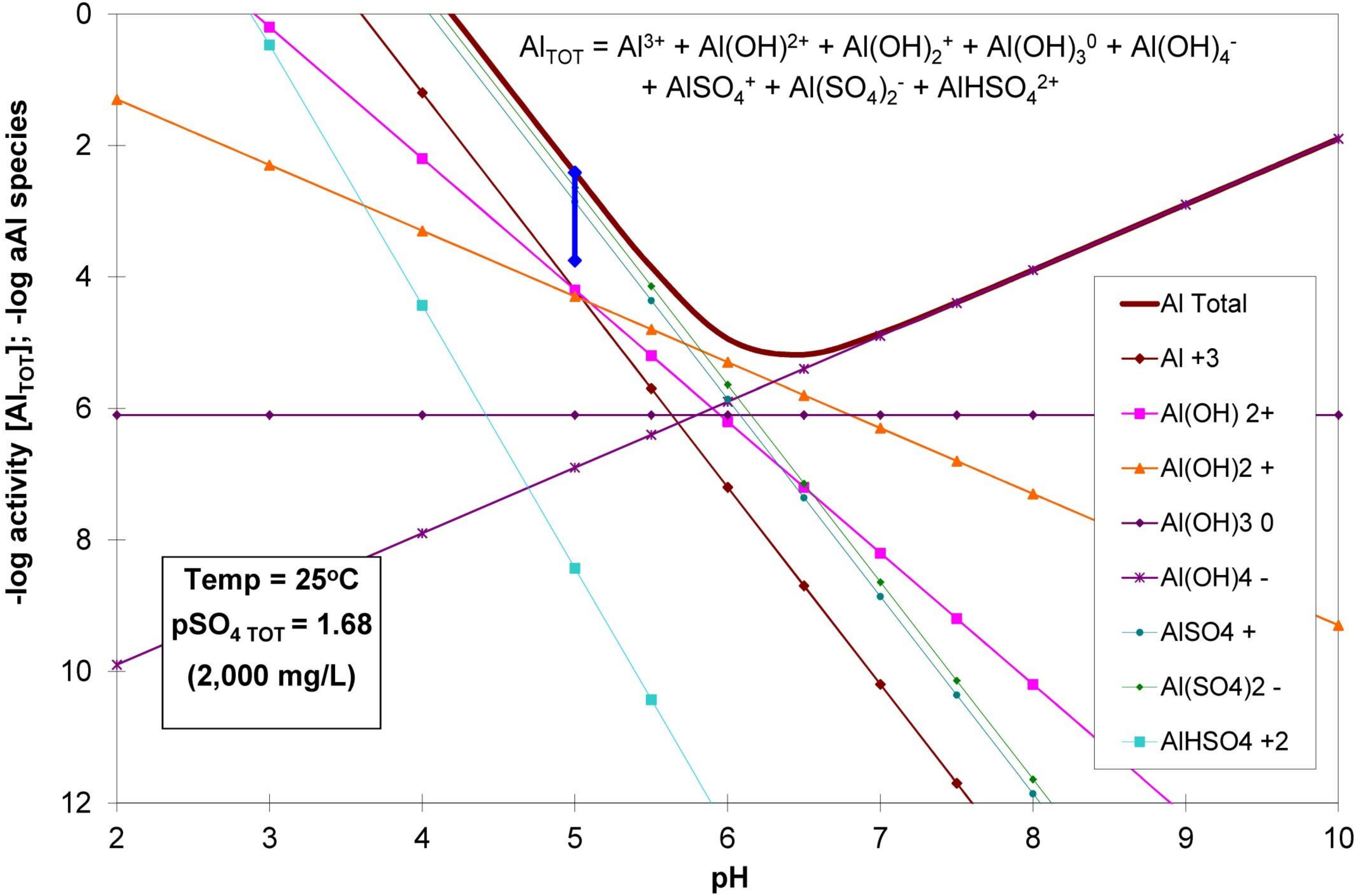
Solubilities of Metal Hydroxides



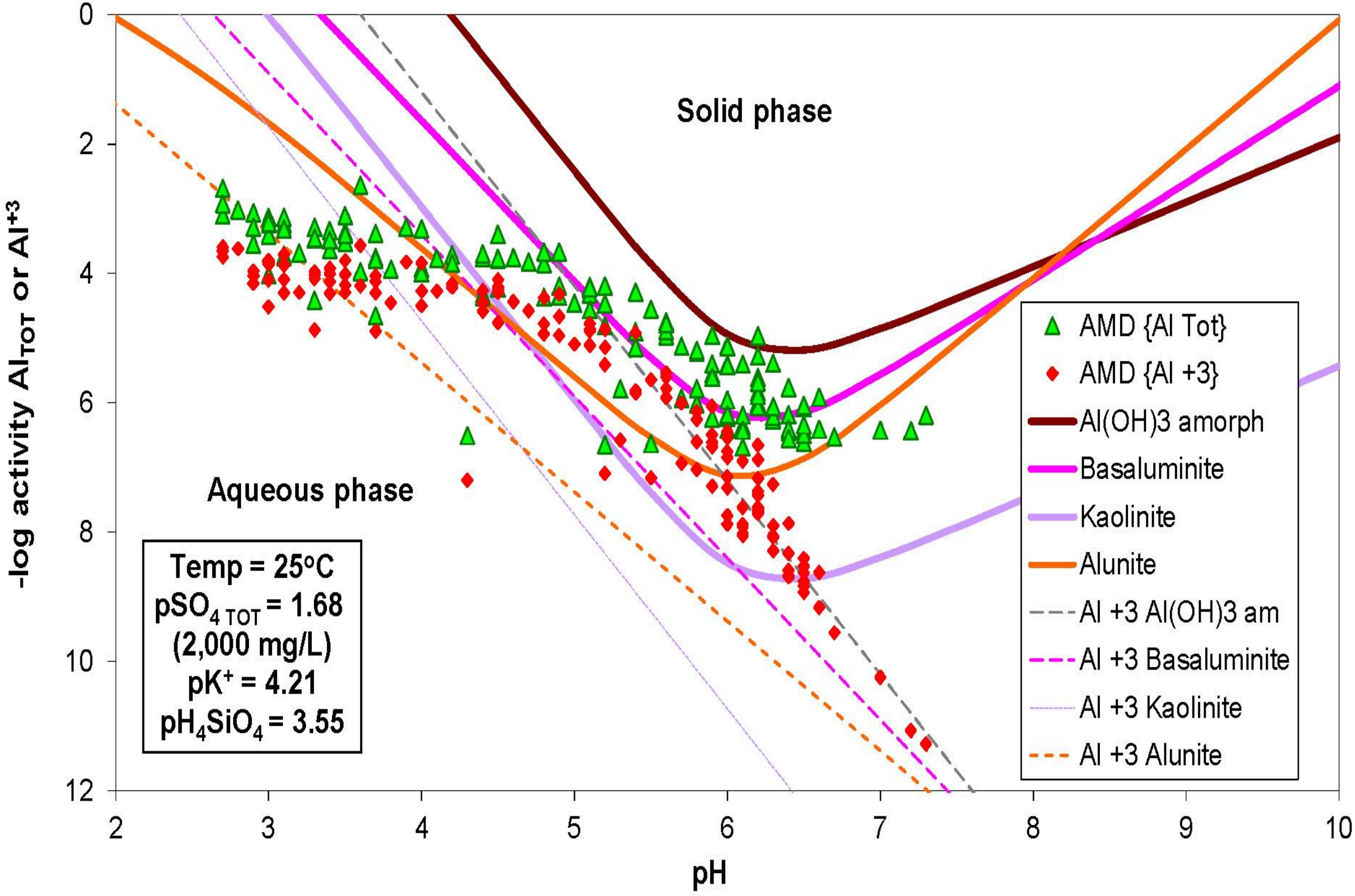
Al Solubility



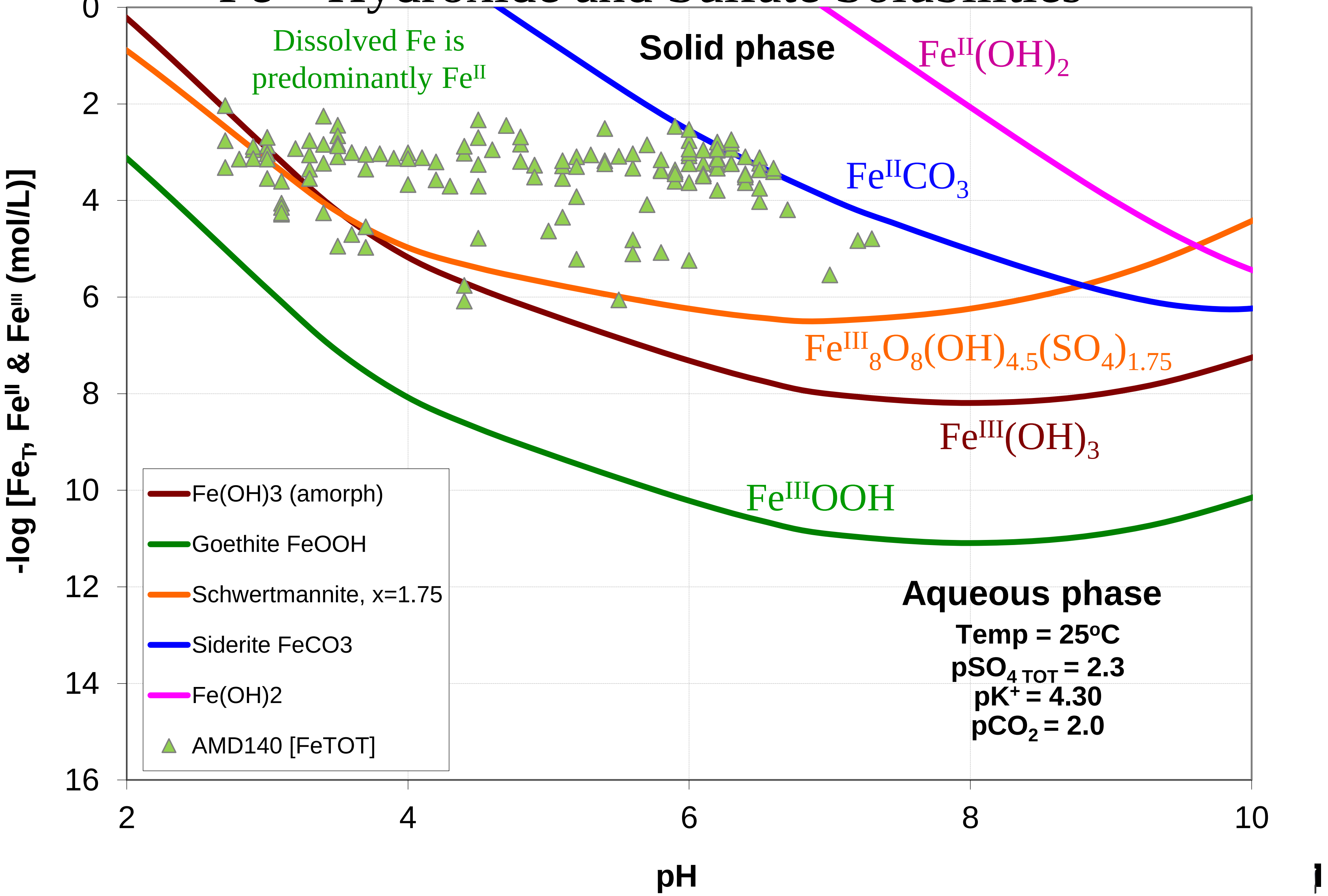
Al Solubility Considering Aqueous Sulfate Species



Al Solubility Considering Aqueous Sulfate Species



Fe Limited by Fe^{II}-Carbonate and Fe^{III}-Hydroxide and Sulfate Solubilities



Iron Oxidation Kinetics are pH Dependent
(pH is affected by gas exchange, hydrolysis, neutralization; abiotic and microbial processes can be involved)

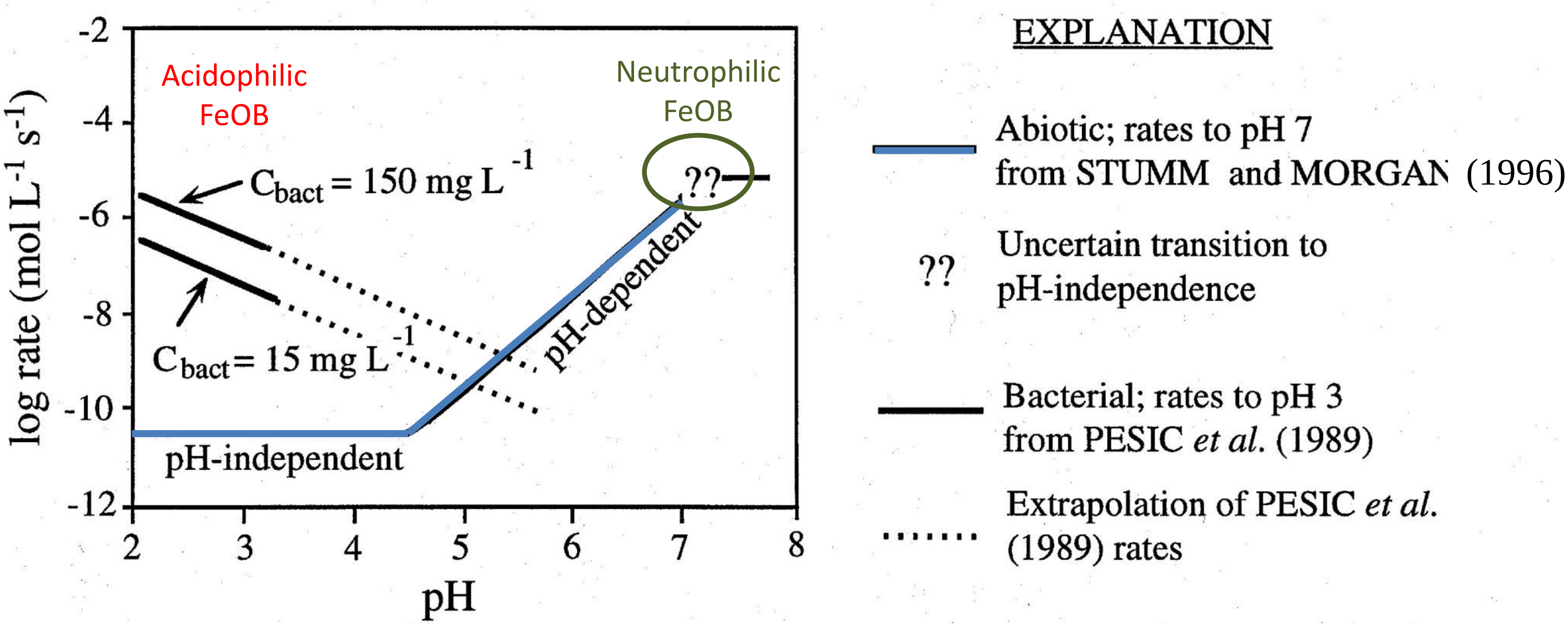


Fig. 3. Rate of Fe(II) oxidation versus pH based on abiotic and biological rate laws (Kirby et al., 1999)

** C_{bact} is concentration of iron-oxidizing bacteria (FeOB), in mg/L, as dry weight of bacteria (2.8E-13 g/cell or 2.8E-10 mg/cell).

The AMDTreat FeII oxidation kinetic model uses most probable number of iron-oxidizing bacteria per liter (MPNbact).

C_{bact} = 150 mg/L is equivalent to MPNbact = 5.3E11, where Cbact = MPNbact ·(2.8E-10).

Neutrophilic rate is adjusted for optimum conditions of pH (6.5-7.5) and low DO (1.9-2.2 mg/L) (Eggerichs et al., 2014).

Additionally, catalysis by adsorption to solids (heterogeneous oxidation) depends on pH (>5).

PHREEQ-N-AMDTreat Examples
Gas Exchange, pH, and Metals Attenuation

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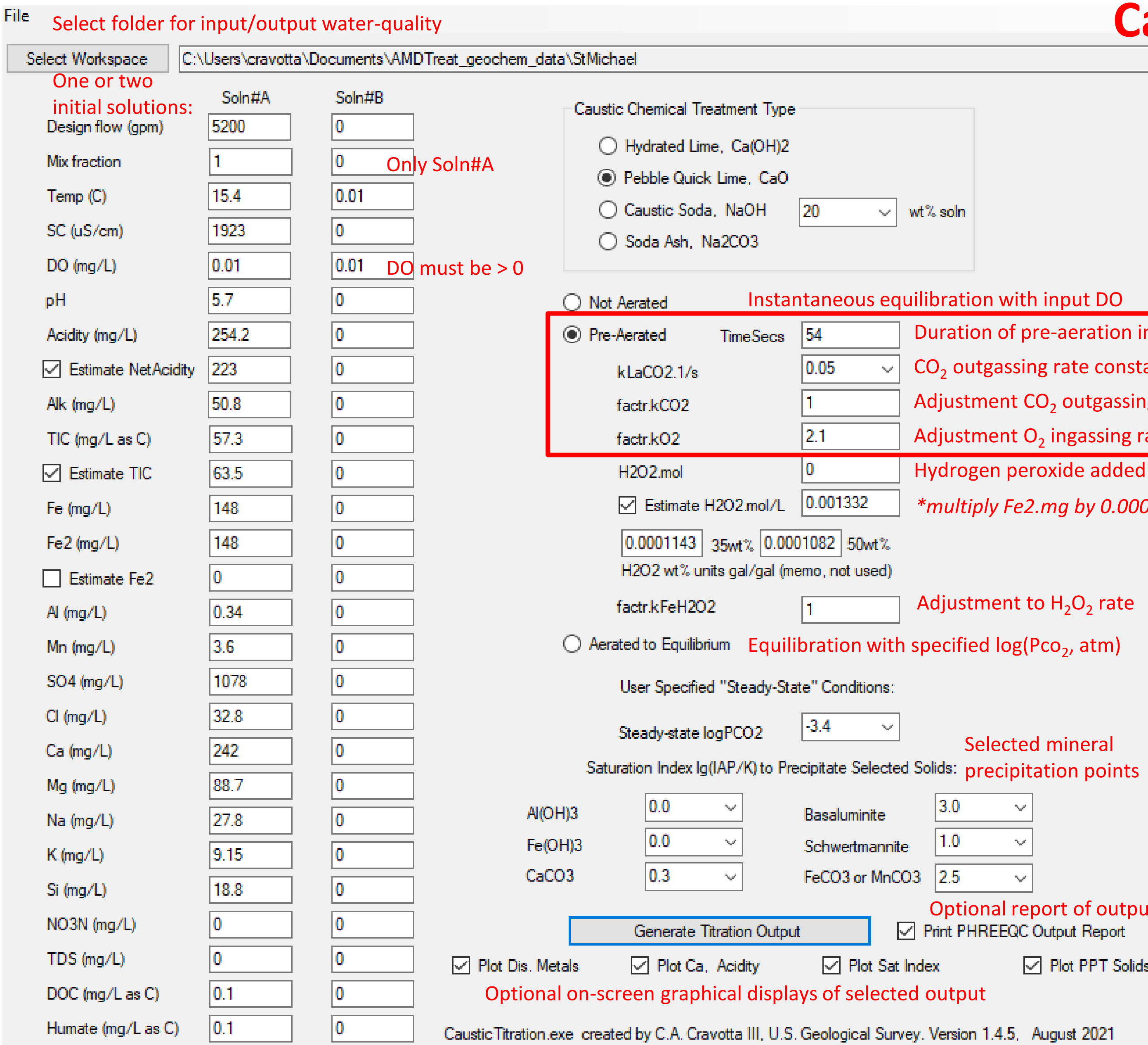
Caustic Titration with Pre-Aeration (Decarbonation)

St. Michael: pre-aeration decreases CO_2 acidity, caustic usage, and sludge

CausticTitration.exe



Options: **no aeration**, **kinetic pre-aeration** (w/wo H_2O_2), and equilibrium aeration.

Allows selection and evaluation of key variables that affect chemical usage efficiency.

Cravotta, C.A. III, 2021. Interactive PHREEQ-N-AMDTreat water-quality modeling tools to evaluate performance and design of treatment systems for acid mine drainage: Applied Geochemistry, 126, 10845. https://doi.org/10.1016/j.apgeochem.2020.104845

Caustic Titration with Pre-Aeration (Decarbonation)

St. Michael: pre-aeration decreases CO_2 acidity, caustic usage, and sludge

A. CausticTitration.exe: Not aerated (**CaO** reacted to achieve pH 8.5 is **675** mg/L as $CaCO_3$)

pH	Caustic asCaCO3mg	Fe_mg	Fe2_mg	Al_mg	Mn_mg	TDS_mg	NetAcidity_mg	SolidsPPT_mg	CO2_mg	O2_mg
5.699391	0.000000	148.253946	148.184017	0.340583	3.606177	1,844.993285	219.160655	0.000000	184.696702	0.000000
5.698863	0.000000	148.192824	148.184017	0.340589	3.606188	1,844.843522	219.051235	0.116997	184.743198	0.000000
6.000000	36.694286	148.189513	148.184989	0.340591	3.606212	1,881.558706	182.288486	0.125192	152.974763	0.000000
6.500000	112.570987	148.188619	148.186989	0.125352	3.606260	1,956.151328	106.359043	0.753005	87.623936	0.000000
7.000000	171.880310	148.189212	148.188493	0.204352	3.606297	2,016.003903	47.027779	0.526362	37.108986	0.000000
7.500000	304.913856	148.187159	148.186724	0.340595	3.606254	1,955.324734	108.502893	194.644240	8.208932	0.000000
8.000000	420.943189	148.184464	148.184105	0.340589	3.606190	1,859.127523	204.623649	406.792768	0.939037	0.000000
8.500000	674.529768	31.972639	31.972263	0.340599	3.606297	1,671.810545	44.644131	687.418049	0.074199	0.000000
9.000000	737.552245	3.319670	3.319157	0.340602	3.606323	1,629.448665	1.378623	753.285879	0.007021	0.000000
9.500000	752.060641	0.379644	0.378671	0.340601	3.606321	1,629.762183	-7.720410	763.426508	0.000694	0.000000
10.000000	767.704290	0.055916	0.053479	0.340601	2.441687	1,639.455711	-21.535525	767.660752	0.000068	0.000000
10.500000	1,067.563230	0.018483	0.011410	0.340618	0.266277	1,695.835449	-39.623063	935.930409	0.000005	0.000000
11.000000	1,171.884112	0.027497	0.005748	0.055888	0.034796	1,729.690739	-65.761207	987.130878	0.000000	0.000000

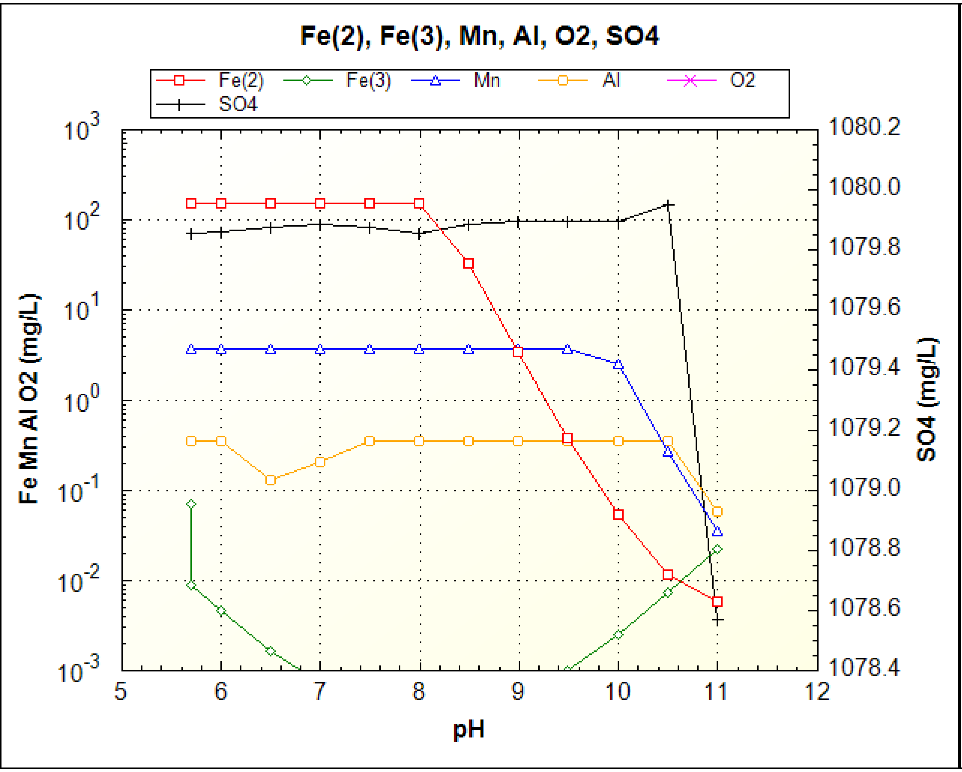
B. CausticTitration.exe: Pre-aerated, CO_2 decreased almost 90% (**CaO** reacted to achieve pH 8.5 is **290** mg/L as $CaCO_3$)

pH	Caustic asCaCO3mg	Fe_mg	Fe2_mg	Al_mg	Mn_mg	TDS_mg	NetAcidity_mg	SolidsPPT_mg	CO2_mg	O2_mg
5.700000	0.000000	148.253944	148.253944	0.340583	3.606177	1,796.954955	218.906769	0.000000	184.683994	0.010018
6.697709	0.000000	148.153294	148.152157	0.131429	3.606182	1,795.523678	218.803412	0.797321	17.796470	10.215814
6.000000	-28.616060	148.152569	148.151421	0.131434	3.606169	1,766.883972	247.467641	0.000009	42.257085	10.215762
6.500000	-7.568373	148.153121	148.151973	0.122499	3.606183	1,787.899450	226.379052	0.025841	24.223205	10.215800
7.000000	9.055535	148.153108	148.152391	0.131435	3.606193	1,804.585382	209.741323	0.000836	10.263163	10.215829
7.500000	18.349692	148.152996	148.152562	0.131435	3.606197	1,813.885563	200.442332	0.001376	3.580427	10.215841
8.000000	35.672893	148.152651	148.152292	0.131435	3.606191	1,810.601897	203.719540	20.603783	0.958068	10.215822
8.500000	289.472888	32.288226	32.287850	0.131439	3.606297	1,660.197303	45.284262	302.427612	0.075796	10.216122
9.000000	352.483745	3.743785	3.743272	0.131440	3.606322	1,626.972166	2.424687	368.515322	0.007173	10.216195
9.500000	367.272893	0.673854	0.672881	0.131440	3.606321	1,628.061164	-6.846925	378.974003	0.000709	10.216191
10.000000	383.349079	0.123433	0.122284	0.131440	2.431956	1,637.645626	-21.058240	383.628171	0.000070	10.216184
10.500000	683.966927	0.020465	0.019316	0.131446	0.264708	1,694.073381	-39.188404	552.424752	0.000005	10.216705
11.000000	786.717176	0.007691	0.006542	0.060071	0.034620	1,730.957523	-65.661659	598.666335	0.000000	10.216884

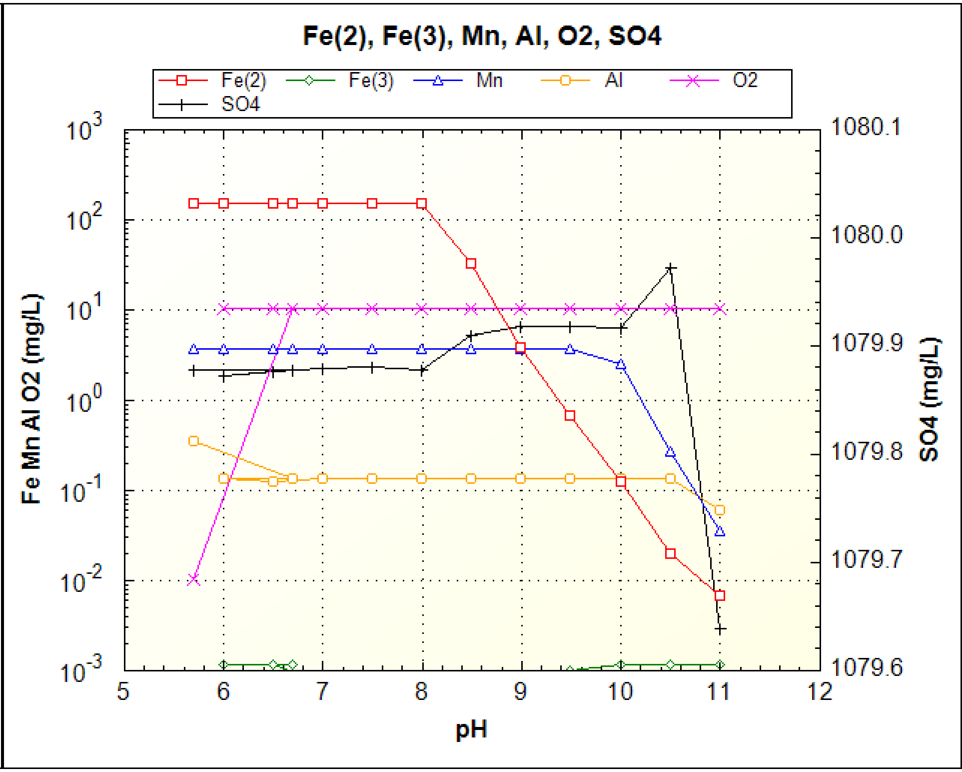
Caustic Titration with Pre-Aeration (Decarbonation)

St. Michael: pre-aeration decreases CO_2 acidity, caustic usage, and sludge

CausticTitration.exe: **Not aerated** (Graph1)



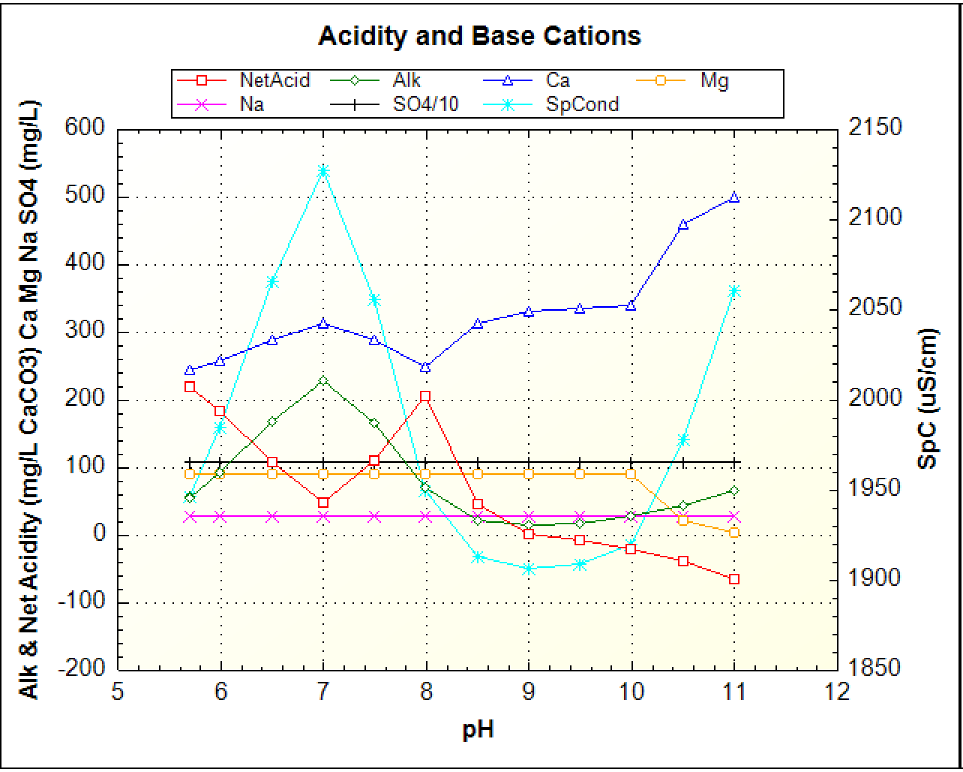
CausticTitration.exe: **Pre-aerated** (Graph1)



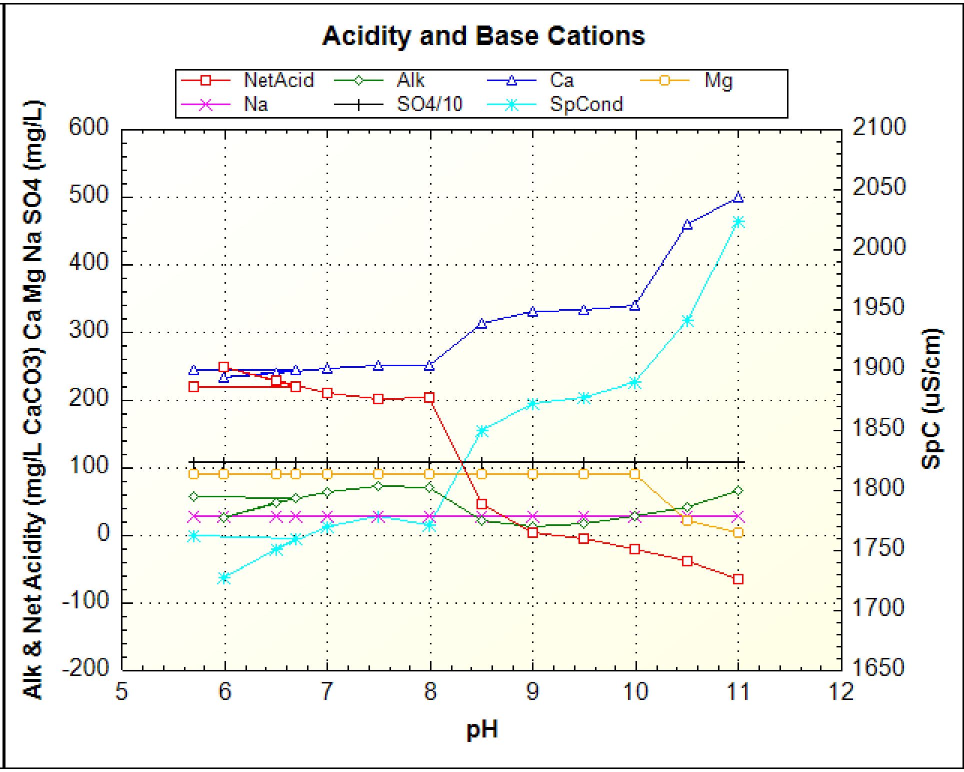
Caustic Titration with Pre-Aeration (Decarbonation)

St. Michael: pre-aeration decreases CO_2 acidity, caustic usage, and sludge

CausticTitration.exe: **Not aerated** (Graph2)



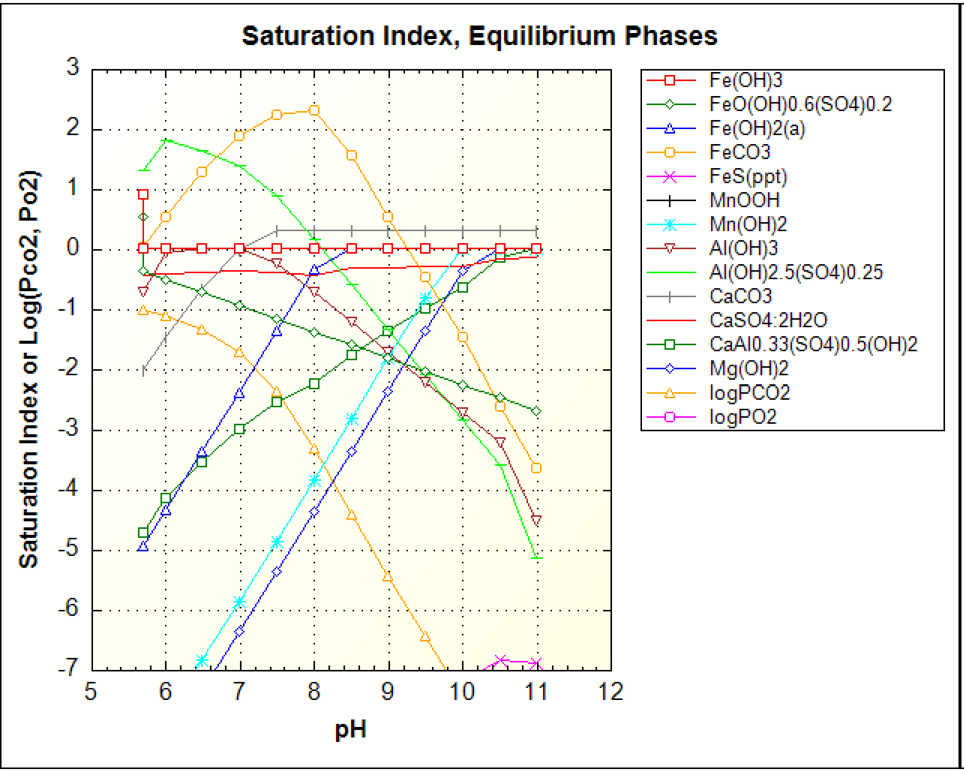
CausticTitration.exe: **Pre-aerated** (Graph2)



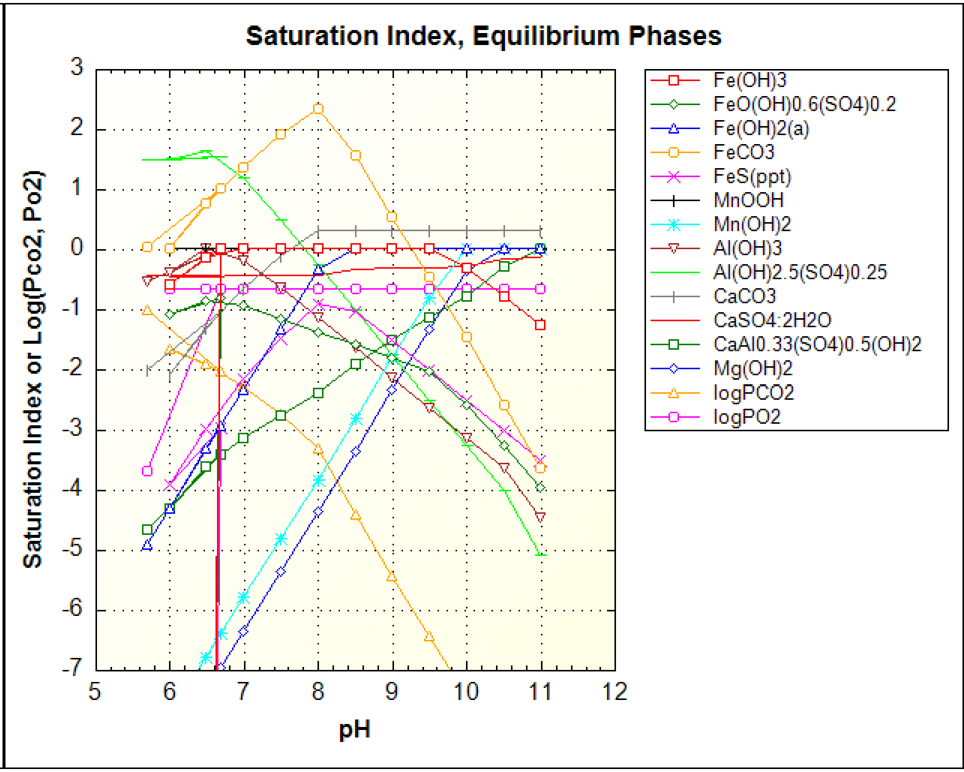
Caustic Titration with Pre-Aeration (Decarbonation)

St. Michael: pre-aeration decreases CO_2 acidity, caustic usage, and sludge

CausticTitration.exe: **Not aerated** (Graph3)



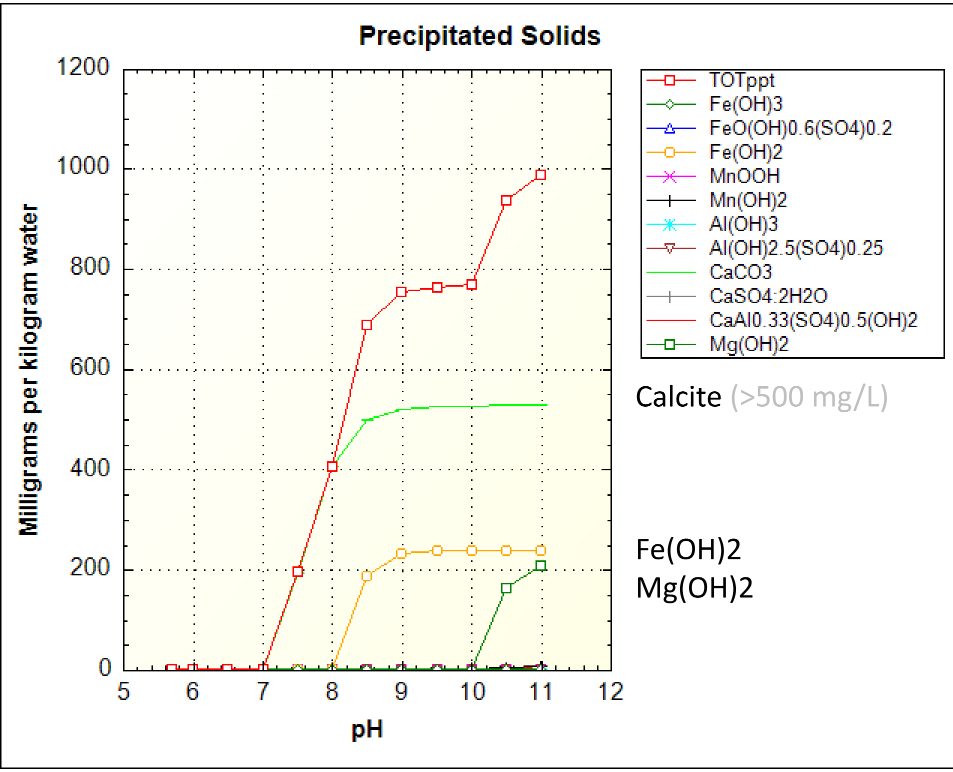
CausticTitration.exe: **Pre-aerated** (Graph3)



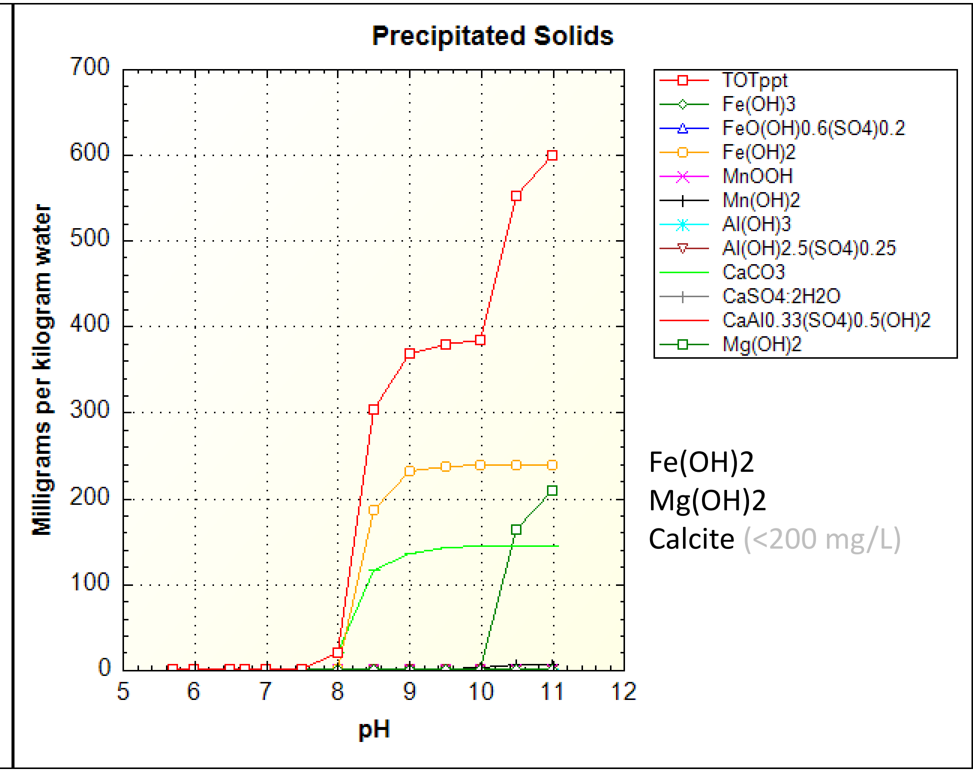
Caustic Titration with Pre-Aeration (Decarbonation)

St. Michael: pre-aeration decreases CO_2 acidity, caustic usage, and sludge

CausticTitration.exe: **Not aerated** (Graph4)



CausticTitration.exe: **Pre-aerated** (Graph4)



pH $\geq$ 8.5: Calcite > 500 mg/L
pH $\geq$ 10.5: Mg(OH)2 > 100 mg/L

pH $\geq$ 8.5: Calcite < 200 mg/L
pH $\geq$ 10.5: Mg(OH)2 > 100 mg/L

Automatic scale change for Y axis

PHREEQ-N-AMDTreat: Parallel & Sequential Models

Kinetics Constants, Adjustment Factors

Kinetics (adjustment factor applied to all steps)

factr.kCO2	1	factr.kO2	2.1	EXPcc	0.67	Outgassing/Ingassing (CO_2/O_2)
factr.kFeHOM	1	factr.kFeHET	1	factr.kFeNO3	0.25	Iron Oxidation (homogenous+heterogeneous abiotic + microbial)
factr.kFeH2O2	1	factr.kbact	1	factr.kFeIIMnOx	1	
factr.kMnHOM	1	factr.kMnHFO	1	factr.kMnHMO	0.5	Manganese Oxidation
factr.kSHFO	1	factr.kSOC	100	factr.kDOC	1	Organic Carbon Oxidation
SI_CaCO3	0.3	SI_Al(OH)3	0.0	SI_Fe(OH)3	0.0	Solids Precipitation (saturation index/equilibrium)
SI_FeCO3,MnCO3	2.5	SI_Basaluminite	3.0	SI_Schwertmannite	1.0	

Caustic can be added at steps 1 - 5

If adding caustic at step 1, 2, 3, 4, and/or 5: choose caustic agent, activate relevant +Caustic checkbox(es) and enter target pH value for the step(s)

○ CaO ◉ Ca(OH)2 ○ Na2CO3 ○ NaOH [20] wt% soln

H_2O_2 estimate, stoichiometric FeII oxidation

☑ Estimate H2O2.mol/L [0.000177]

[1.52E-05] 35wt% [1.44E-05] 50wt%

System variables: Duration Temp Peroxide Aeration Limestone/Compost Sorbent Mass/Composition (for each step)

Step	+Caustic?-->pH?	Time.hrs	Temp2.C	H2O2.mol	kLaCO2.1/s	Lg(PCO2.atm)	SAcc.cm2/mol	M/M0cc	SOC.mol	HMeO.mg	Fe%	Mn%	Al%	Description
☑ 1:	☐ 7.5	6	15.1	0	0.00066	-3.4	0	1	0	0	100	0	0	Aer3
☑ 2:														Aer2
☑ 3:														Aer1
☑ 4:														Aer0
☑ 5:														H2O2
☐ 6:														NULL
☐ 7:														NULL
☐ 8:														NULL
☐ 9:														NULL
☐ 10:														NULL
☐ 11:		0	15.1	0	0	-3.4	0	1	0	0	0	0	0	NULL

Caustic Addition:

Steps 1 - 5

Choose caustic agent

Specify target pH

H_2O_2:

factr.kFeH2O2

Outgassing & Ingassing:

Rate (kLaCO2.1/s)

factr.kCO2

factr.kO2

steady-state logPCO2

Limestone / Organic Carbon:

Surface area (SAcc.cm2/mol)

Mass available (M/M0cc)

equilibrium approach (EXPcc)

calcite saturation limit (SI_CaCO3)

Organic carbon mass available (SOC.mol)

factr.kSHFO (reduction of FeIII)

factr.kSOC (solid organic carbon)

factr.kDOC (dissolved organic carbon)

Sorbent (recirculated solids):

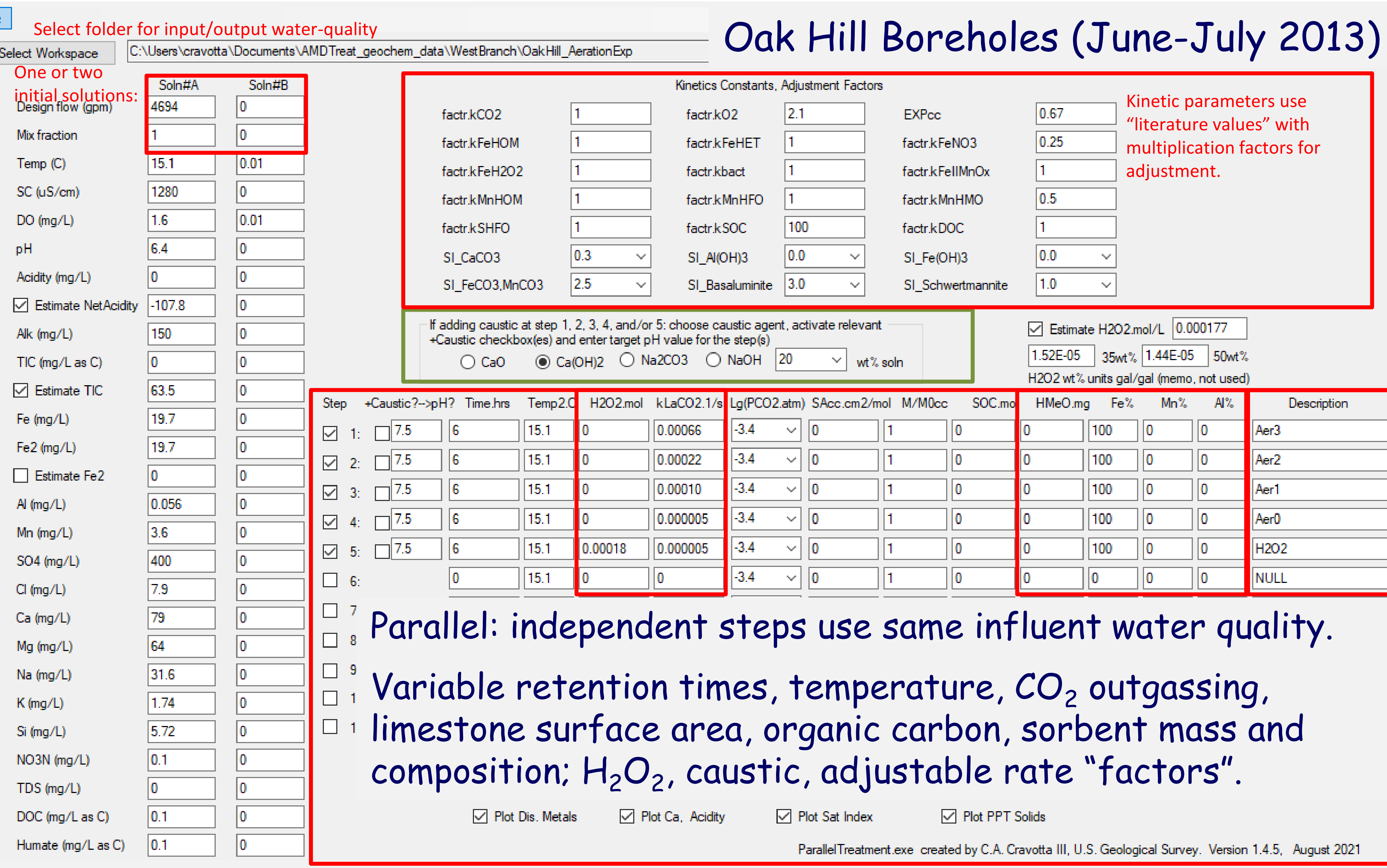
Mass total Fe+Mn+Al (HMeO.mg)

Composition (%) Fe, Mn, and Al

[Generate Kinetics Output]

☑ Print PHREEQC Output Report

PHREEQ-N-AMDTreat: “ParallelTreatment.exe”



Cravotta, C.A. III, 2021. Interactive PHREEQ-N-AMDTreat water-quality modeling tools to evaluate performance and design of treatment systems for acid mine drainage: Applied Geochemistry, 126, 10845. https://doi.org/10.1016/j.apgeochem.2020.104845

PHREEQ-N-AMDTreat: Parallel Model

Effects of O_2 Ingassing and CO_2 Outgassing on pH and Fe^{II} Oxidation Rates

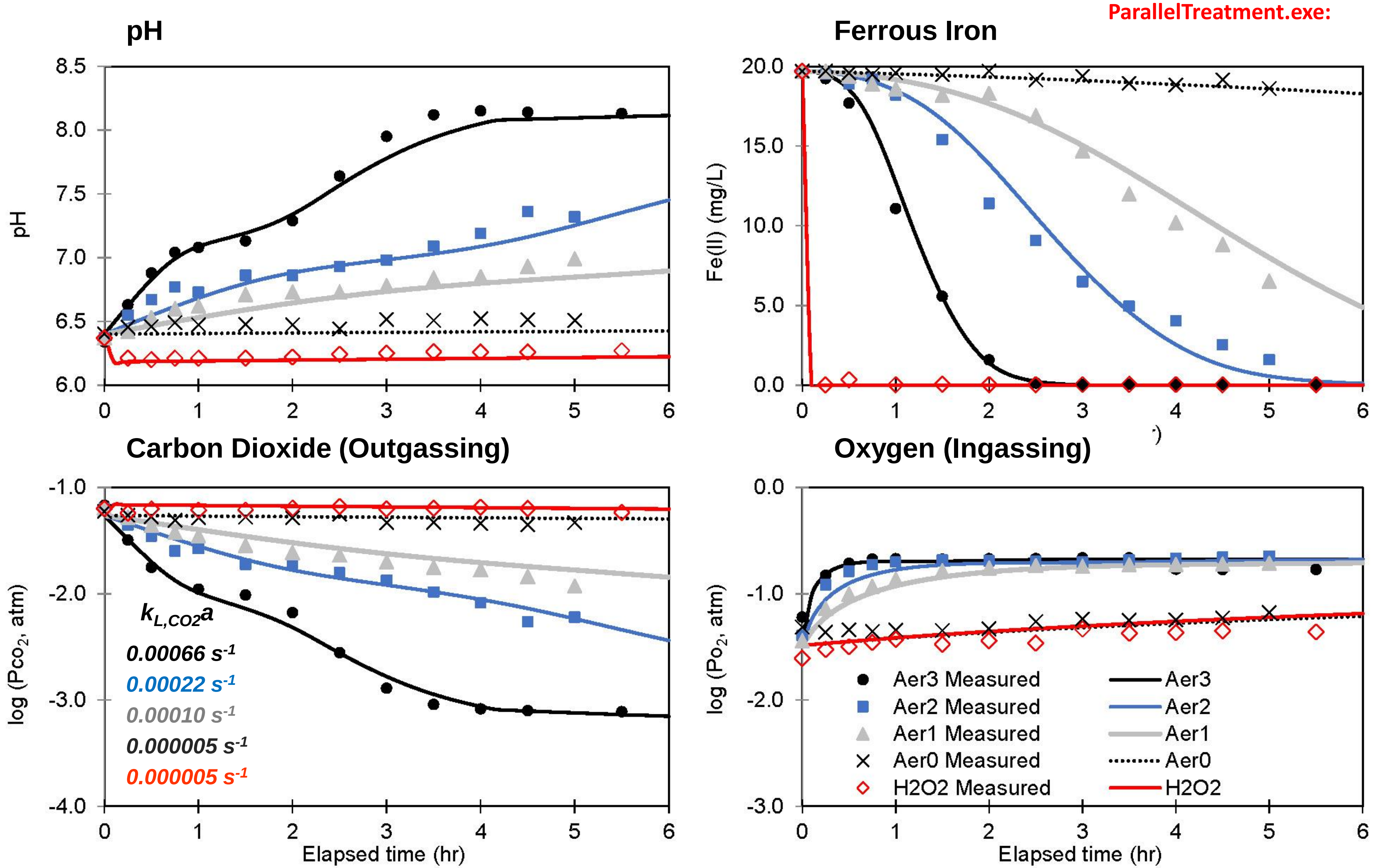
Batch Aeration Tests at Oak Hill Boreholes (summer 2013, 6-hour duration)

Control Not Aerated

Aerated

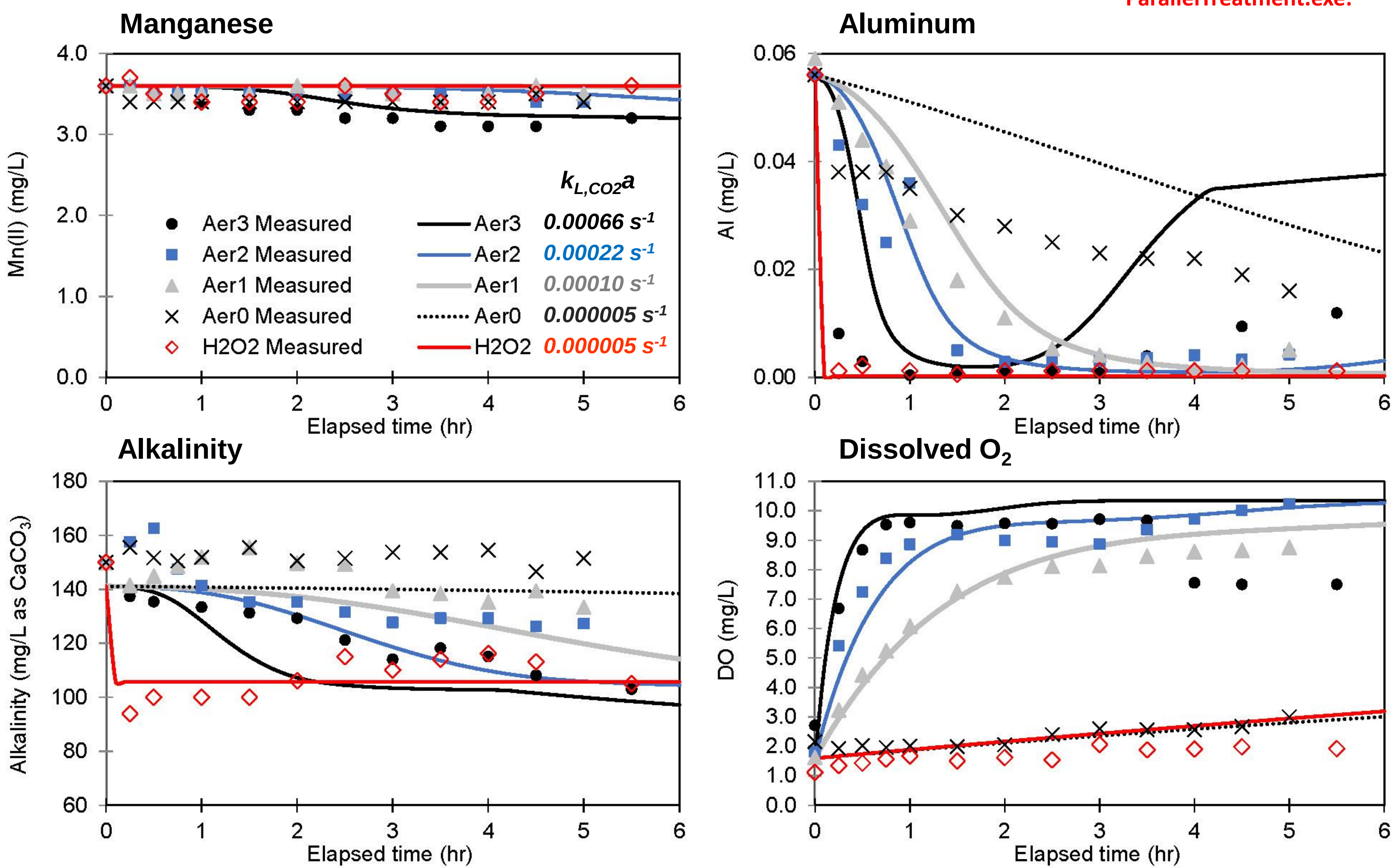
H_2O_2 Addition

PHREEQ-N-AMDTreat: Parallel Model
Batch Aeration Tests at Oak Hill Boreholes



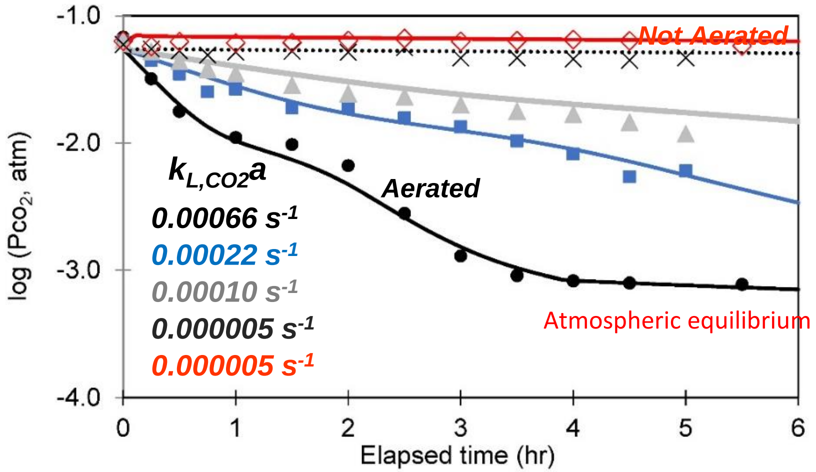
PHREEQ-N-AMDTreat: Parallel Model
Batch Aeration Tests at Oak Hill Boreholes

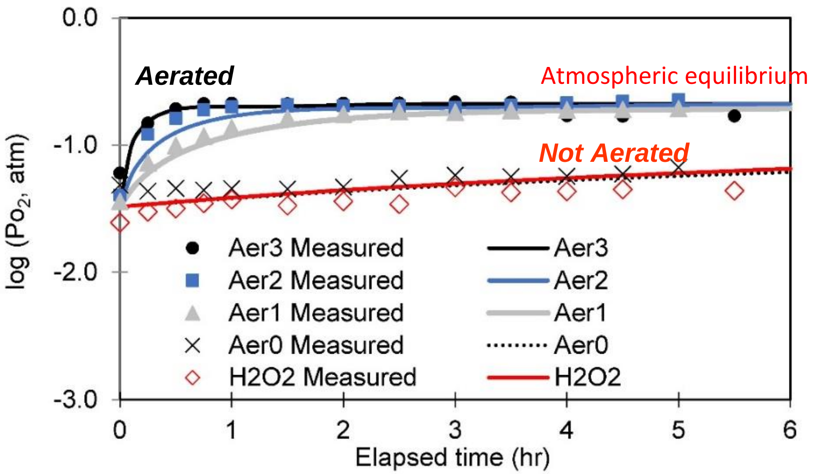
ParallelTreatment.exe:

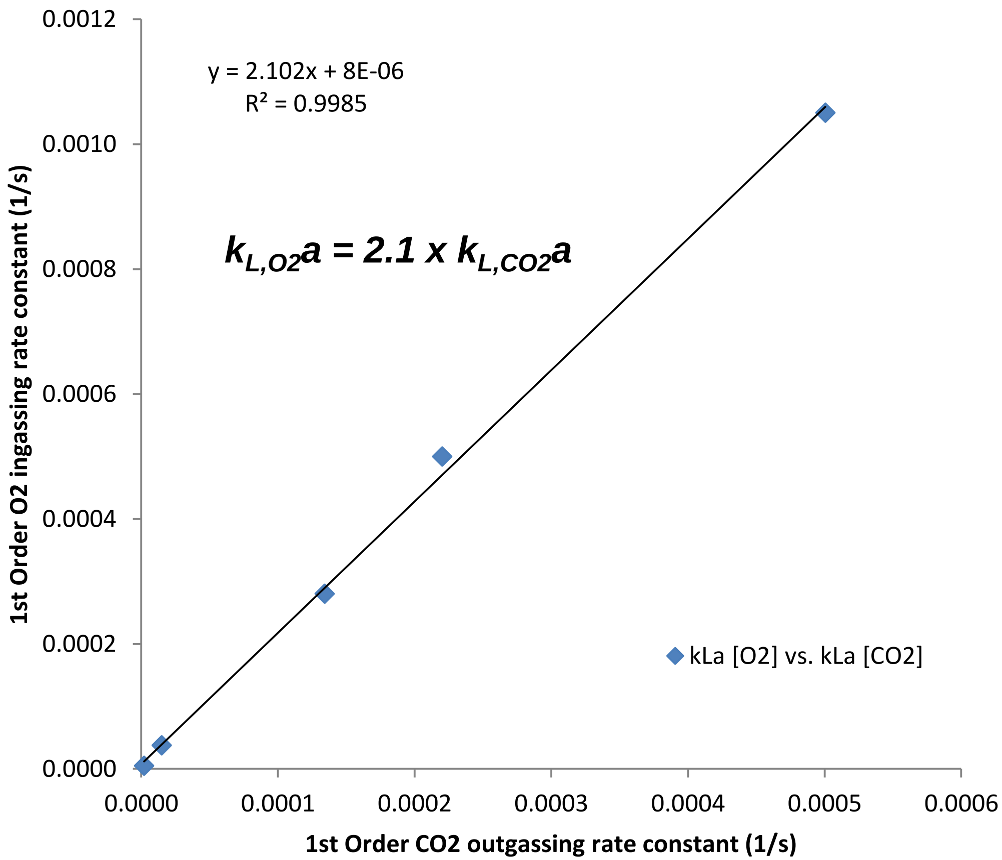


CO_2 Outgassing is Proportional to O_2 Ingassing
(model specifies first-order rates for out/in gassing)

$-d[C]/dt = k_{L,C}a\cdot([C] - [C]_S)$ exponential, asymptotic approach to steady state







CO_2 Outgassing & O_2 Ingassing Rate Constants Estimated for Various Treatment Technologies

Table S2. *Typical empirical values of rate constants for CO_2 outgassing and O_2 ingassing*

Site	Temper-ature (°C)		CO_2 Outgas $k_{L,CO2}a$ (s^{-1})	log(s^{-1})	O_2 Ingas $k_{L,O2}a$ (s^{-1})	log(s^{-1})
Treatment Systems						
Maelstrom (Sykesville, Trent, St.Michaels)	20	Fast	0.03	-1.52	0.063	-1.20
Surface Aerator (Renton, other)	20		0.001	-3.00	0.0021	-2.68
Mechanical Aerator (Lancashire)	20		0.0006	-3.22	0.00126	-2.90
Aeration Cascade/Level Spreader (Silver Cr)	20		0.01	-2.00	0.021	-1.68
Rip-rap Spillway/Ditch (Silver Cr, Pine Forest,	20		0.005	-2.30	0.0105	-1.98
Pond (Silver Cr, Pine Forest, Lion Mining, Flight93)	20		0.00001	-5.00	0.000021	-4.68
Wetland (Silver Cr, Pine Forest, Lion Mining)	20		0.00001	-5.00	0.000021	-4.68
Anoxic limestone drain (Pine Forest)	20	Slow	0.000001	-6.00	0.0000021	-5.68
Oak Hill Aeration Expts.						
Aer3	20	Fast	0.00066	-3.18	0.00139	-2.86
Aer2	20		0.00022	-3.66	0.00046	-3.34
Aer1	20		0.00010	-4.00	0.00021	-3.68
Aer0	20	Slow	0.000005	-5.30	0.000011	-4.98

*Gas mass-transfer rate corrected to 20°C per Rathbun (1998, Eq. 56) using the expression:

kL,a_20 = kL,a_TC /(1.0241^(TC-20)).

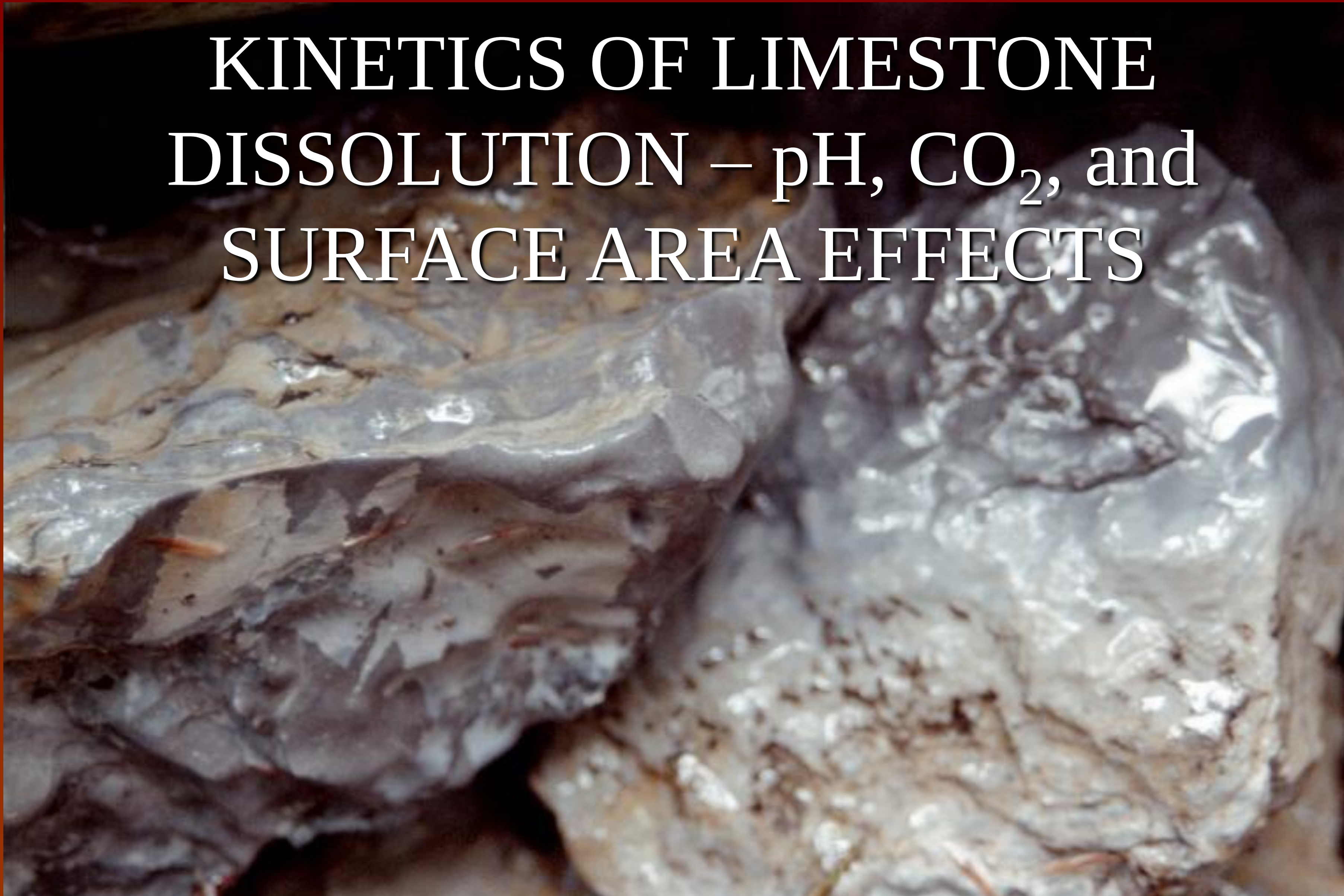
kL,a_TC = kL,a_20 * (1.0241^(TC-20)).

$kL,a\_20 = (LN((C_1-C_S)/(C_2-C_S))/t) / (1.0241^{(TEMPC - 20)})$, where C is CO_2 or O_2.

Dissolved O_2, temperature, and pH were measured using submersible electrodes.

Dissolved CO_2 was computed from alkalinity, pH, and temperature data.

KINETICS OF LIMESTONE DISSOLUTION – pH, CO_2, and SURFACE AREA EFFECTS



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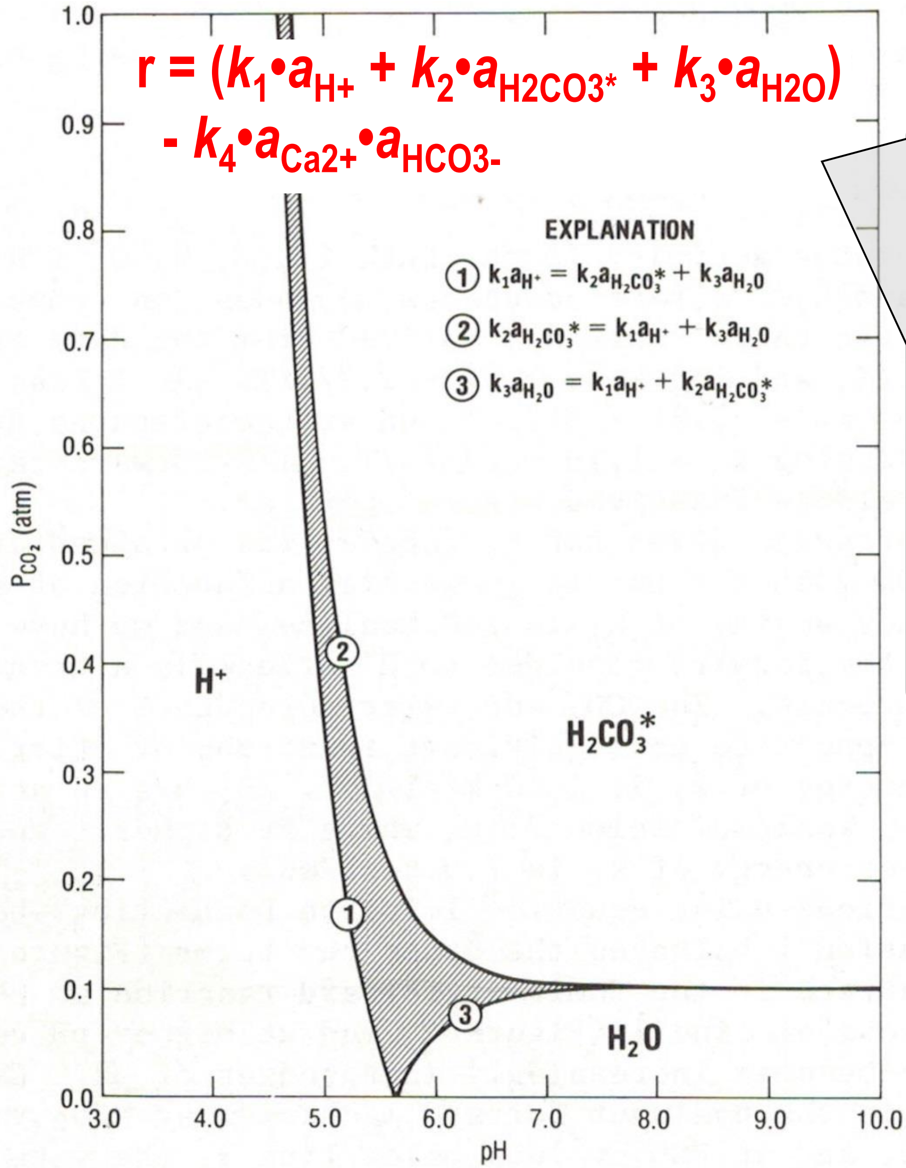
science for a changing world

Limestone Dissolution Rate Model for AMDTreat
("PWP" model emphasizes pH and CO_2)

$$r = (k_1 \cdot a_{H+} + k_2 \cdot a_{H2CO3*} + k_3 \cdot a_{H2O}) - k_4 \cdot a_{Ca2+} \cdot a_{HCO3-}$$



According to Plummer, Wigley, and Parkhurst (1978), the rate of $CaCO_3$ dissolution is a function of three forward (dissolution) reactions:

$CaCO_3 + H^+ \rightarrow Ca^{2+} + HCO_3^-$ — k_1

$CaCO_3 + H_2CO_3^* \rightarrow Ca^{2+} + 2\,HCO_3^-$ — k_2

$CaCO_3 + H_2O \rightarrow Ca^{2+} + HCO_3^- + OH^-$ — k_3

and the backward (precipitation) reaction:

$Ca^{2+} + HCO_3^- \rightarrow CaCO_3 + H^+$ — k_4

Although H^+, $H_2CO_3^*$, and H_2O reaction with calcite occur simultaneously, the forward rate is dominated by a single species in the fields shown. More than one species contributes significantly to the forward rate in the gray stippled area. Along the lines labeled 1, 2, and 3, the forward rate attributable to one species balances that of the other two.

Limestone Dissolution Rate Model for AMDTreat
(surface area correction for coarse aggregate)

Surface area for various coarse aggregates (bold indicates sizes commonly used in limestone beds; 2NS used in cubitainers).

Gradation Number		Weight (g)	Particle Dimensions (cm)				Particle Surface Area (cm^2)			Unit Surface Area (cm^2/g)		
AASHTO	PA	Average Particle	Long Axis	Inter-mediate	Short Axis	Average Axis	Rectan-gular Prism	Sphere	Ellipsoid	Rectan-gular Prism	Sphere	Ellipsoid
R-5		**22160.145**	**45.72**	**22.86**	**13.34**	**27.31**	**3919.35**	**2342.26**	**2862.08**	**0.18**	**0.11**	**0.13**
R-4		**7113.133**	**30.48**	**16.51**	**8.89**	**18.63**	**1841.93**	**1089.98**	**1319.11**	**0.26**	**0.15**	**0.19**
R-3		**1185.522**	**16.51**	**8.89**	**5.08**	**10.16**	**551.61**	**324.29**	**395.61**	**0.47**	**0.27**	**0.33**
1	**4**	**341.978**	**8.89**	**6.35**	**3.81**	**6.35**	**229.03**	**126.68**	**155.24**	**0.67**	**0.37**	**0.45**
3	**3A**	**78.166**	**5.08**	**3.81**	**2.54**	**3.81**	**83.87**	**45.60**	**56.39**	**1.07**	**0.58**	**0.72**
5		**9.771**	**2.54**	**1.91**	**1.27**	**1.91**	**20.97**	**11.40**	**14.10**	**2.15**	**1.17**	**1.44**
57	**2B**	**3.257**	**2.54**	**1.27**	**0.635**	**1.48**	**11.29**	**6.90**	**8.25**	**3.47**	**2.12**	**2.53**
	2NS	**9.771**	**2.54**	**1.91**	**1.27**	**1.91**	**20.97**	**11.40**	**14.10**	**2.15**	**1.17**	**1.44**
67	2	1.832	1.91	0.95	0.635	1.16	7.26	4.26	5.28	3.96	2.32	2.88
	1NS	1.221	1.27	0.95	0.635	0.95	5.24	2.85	3.52	4.29	2.33	2.89
7		1.221	1.27	0.95	0.635	0.95	5.24	2.85	3.52	4.29	2.33	2.89
8		0.382	0.95	0.79	0.3175	0.69	2.62	1.49	1.70	6.87	3.90	4.44
	1B	0.382	0.95	0.79	0.3175	0.69	2.62	1.49	1.70	6.87	3.90	4.44

Particle dimensions were estimated on the basis of ranges for graded materials reported in Pennsylvania Department of Environmental Protection, 2000, Erosion and sediment pollution control program manual: Harrisburg, Pennsylvania Dept. Environmental Protection Bureau of Watershed Management, Document No. 363-2134-008, 180 p. (tables 9 and 10A).

Plummer, Wigley, and Parkhurst (1978) reported unit surface area (SA) of 44.5 and 96.5 cm^2/g for "coarse" and "fine" particles, respectively, used for empirical testing and development of PWP rate model. These SA values are 100 times larger than those for typical limestone aggregate. ***Multiply cm^2/g by 100 g/mol to get surface area (A) units of cm^2/mol used in AMDTreat rate model.***

Surface area computed for various geometric forms:
- Sphere: 4pi*(Average of Axes/2)^2
- Rectangular Prism: 2*(Long Axis*Short Axis)+2*(Long Axis*Intermediate Axis)+2*(Short Axis*Intermediate Axis)
- Ellipsoid: (pi*D^2)/S, where D=2*(vol/(4/3pi))^(1/3) S=1.15-0.25E E=Long Axis/D

Volume computed for same geometric forms:
- Sphere: 4/3*pi*(Average Axis/2)^3
- Rectangular Prism: (Long Axis*Short Axis*Intermediate Axis)
- Ellipsoid: 4/3*pi* (Long Axis/2*Short Axis/2*Intermediate Axis/2)
  - For ellipsoid sphere, this reduces to 0.5236*Long Axis*Short Axis*Intermediate Axis
  - Santomartino and Webb (2007, AG, 22:2344–2361) estimated volume of ellipsoid as 0.6*volume of rectangular prism of same dimensions.

PHREEQ-N-AMDTreat “TreatTrainMix2.exe”:

Select folder for input/output water-quality

Select Workspace | C:\Users\cravotta\Documents\AMDTreat_geochem_data\WestBranch\OAK+PKN

TreatTrainMix2.exe Sequential Model of Successive Treatment Steps (1-11)

One or two initial solutions:

	Soln#A	Soln#B
Design flow (gpm)	2830	8976
Mix fraction	0.24	0.76
Temp (C)	14.7	10.9
SC (uS/cm)	1000	570
DO (mg/L)	2	9.9
pH	6.3	6.4
Acidity (mg/L)	-111	-20
☑ Estimate NetAcidity	-110.6	-19.9
Alk (mg/L)	150	34
TIC (mg/L as C)	0	0
☑ Estimate TIC	73.3	15.7
Fe (mg/L)	18	5.15
Fe2 (mg/L)	18	5.15
☐ Estimate Fe2	0	0
Al (mg/L)	0.06	0.07
Mn (mg/L)	3.7	2.45
SO4 (mg/L)	390	240
Cl (mg/L)	8.8	17.5
Ca (mg/L)	99	40.5
Mg (mg/L)	55	42
Na (mg/L)	32	10
K (mg/L)	1.74	1.77
Si (mg/L)	5.72	5.72
NO3N (mg/L)	0.1	0.1
TDS (mg/L)	0	0
DOC (mg/L as C)	0.1	0
Humate (mg/L as C)	0.1	0

Kinetics Constants, Adjustment Factors

factr.kCO2	1	factr.kO2	2.1	EXPcc	0.67
factr.kFeHOM	1	factr.kFeHET	1	factr.kFeNO3	0.25
factr.kFeH2O2	1	factr.kbact	1	factr.kFeIIMnOx	1
factr.kMnHOM	1	factr.kMnHFO	1	factr.kMnHMO	0.5
factr.kSHFO	1	factr.kSOC	100	factr.kDOC	1
SI_Fe(OH)3	0.0	SI_Al(OH)3	0.0	SI_CaCO3	0.3
SI_Schwertmannite	1.0	SI_Basaluminite	3.0	SI_FeCO3,MnCO3	2.5

Kinetic parameters use “literature values” with multiplication factors for adjustment.

Solids Precipitation (SI=0 is equilibrium)

Option to add specified caustic agent to adjust pH at beginning of steps 1-5:

If adding caustic at step 1, 2, 3, 4, and/or 5: choose caustic agent, activate relevant +Caustic checkbox(es) and enter target pH value for the step(s)

○ CaO ◉ Ca(OH)2 ○ Na2CO3 ○ NaOH | 20 | wt% soln

☑ Estimate H2O2.mol/L 7.4E-05

6.4E-06 35wt% 6E-06 50wt%

H2O2 wt% units gal/gal (memo, not used)

Step	+Caustic?-->pH?	Time.hrs	Temp2.C	H2O2.mol	kLaCO2.1/s	Lg(PCO2.atm)	SAcc.cm2/mol	M/M0cc	SOC.mol	HMeO.mg	Fe%	Mn%	Al%	Description
☑ 1:	☐ 7.5	0.25	14.7	0	0.000005	-3.4	0	1	0	0	100	0	0	Sedimentation pond
☑ 2:	☐ 7.5	0.05	14.7	0.000074	0.005	-3.4	0	1	0	0	100	0	0	H2O2+Mixing
☑ 3:	☐ 7.5	4	15.1	0	0.000005	-3.4	0	1	0	3	99.8	0.1	0.1	Oxidation/settling pond
☑ 4:	☐ 7.5	0.01667	15.1	0	0.005	-3.4	33	1 R-3	0	2	99.8	0.1	0.1	Aeration riprap
☑ 5:	☐ 7.5	1	15.5	0	0.000005	-3.4	144	0.1 AASHTO#5		2	95	5	0	Aerobic wetland
☑ 6:		0.0333	15.5	0	0.005	-3.4	33	1 R-3	0	2	95	5	0	Aeration riprap
☑ 7:		0.5	16	0	0.0005	-3.4	72	1 AASHTO#3		20	10	90	0	Mn removal bed
☑ 8:		0.01667	17	0	0.005	-3.4	33	1 R-3	0	1	100	0	0	Ditch
☑ 9:														
☑ 10														
☑ 11														

Sequential. Variable retention times, temperature, H_2O_2, caustic, CO_2 outgassing, limestone surface area, organic carbon, sorbent, plus adjustable rates.

☑ Plot Dis. Metals ☐ Plot Ca, Acidity ☐ Plot Sat Index ☐ Plot PPT Solids

TreatTrainMix2.exe created by C.A. Cravotta III, U.S. Geological Survey. Version 1.4.5, August 2021

Cravotta, C.A. III, 2021. Interactive PHREEQ-N-AMDTreat water-quality modeling tools to evaluate performance and design of treatment systems for acid mine drainage: Applied Geochemistry, 126, 10845. https://doi.org/10.1016/j.apgeochem.2020.104845

PHREEQ-N-AMDTreat: TreatTrainMix2 Model
Pine Forest ALD* + Pond + Aerobic Wetlands

Step	Treatment
0	Untreated
1	ALD
2	Riprap
3	Pond
4	Riprap
5	Wetland
6	Cascade
7	Wetland
8	Cascade
9	Wetland
10	Riprap
11	NULL

*Flushable ALD, Biofouled

PHREEQ-N-AMDTreat: TreatTrainMix2 Model

TreatTrainMix2.exe: Passive treatment

Biofouled ALD+Aerobic Pond+Wetlands
Pine Forest (151212)

elect Workspace | C:\Users\cravotta\Documents\AMDTreat_geochem_data\MillCreek\PineForestLowerTreatment

	Soln#A	Soln#B
Design flow (gpm)	690	0
Mix fraction	1	0
Temp (C)	11.63	0.01
SC (uS/cm)	700	0
DO (mg/L)	0.4	0.01
pH	5.79	0
Acidity (mg/L)	0	0
☑ Estimate NetAcidity	-1.7	0
Alk (mg/L)	33	0
TIC (mg/L as C)	0	0
☑ Estimate TIC	39.2	0
Fe (mg/L)	14	0
Fe2 (mg/L)	14	0
☐ Estimate Fe2	0	0
Al (mg/L)	0.09	0
Mn (mg/L)	3.1	0
SO4 (mg/L)	330	0
Cl (mg/L)	4	0
Ca (mg/L)	56	0
Mg (mg/L)	51	0
Na (mg/L)	7.4	0
K (mg/L)	0.54	0
Si (mg/L)	5.4	0
NO3N (mg/L)	1.5	0
TDS (mg/L)	450	0
DOC (mg/L as C)	3.67	0
Humate (mg/L as C)	0.67	0

Kinetics Constants, Adjustment Factors

factr.kCO2	1	factr.kO2	2.1	EXPcc	0.67
factr.kFeHOM	1	factr.kFeHET	1	factr.kFeNO3	0.25
factr.kFeH2O2	1	factr.kbact	2	factr.kFeIIMnOx	1
factr.kMnHOM	1	factr.kMnHFO	1	factr.kMnHMO	0.5
factr.kSHFO	1	factr.kSOC	100	factr.kDOC	5
SI_Fe(OH)3	0.0	SI_Al(OH)3	0.0	SI_CaCO3	0.3
SI_Schwertmannite	1.0	SI_Basaluminite	3.0	SI_FeCO3,MnCO3	2.5

If adding caustic at step 1, 2, 3, 4, and/or 5: choose caustic agent, activate relevant +Caustic checkbox(es) and enter target pH value for the step(s)

○ CaO ◉ Ca(OH)2 ○ Na2CO3 ○ NaOH 20 wt% soln

☑ Estimate H2O2.mol/L 0.000126

1.08E-05 35wt% 1.02E-05 50wt%

H2O2 wt% units gal/gal (memo, not used)

Step		+Caustic?	->pH?	Time.hrs	Temp2.C	H2O2.mol	kLaCO2.1/s	Lg(PCO2.atm)	SAcc.cm2/mol	M/M0cc	SOC.mo	HMeO.mg	Fe%	Mn%	Al%	Description
☑	1:	☐	7.5	4	11.63	0	0.00001	-3.4	72	1	0	116	99	0.1	0.9	ALD
☑	2:	☐	7.5	0.0083	11.6	0	0.02	-3.4	33	1	0	1	95	5	0	Aeration riprap
☑	3:	☐	7.5	13	12.16	0	0.00002	-3.4	0	1	0	3	95	5	0	Oxidation/settling pond
☑	4:	☐	7.5	0.0028	12.16	0	0.005	-3.4	0	1	0	1	95	5	0	Aeration cascade
☑	5:	☐	7.5	8	12.15	0	0.00005	-3.4	0	1	0.1	3	60	40	0	Aerobic wetland
☑	6:			0.0028	12.15	0	0.005	-3.4	0	1	0	1	60	40	0	Aeration riprap
☑	7:			6.1	12.04	0	0.00005	-3.4	0	1	0.1	2	40	60	0	Aerobic wetland
☑	8:			0.0028	12.04	0	0.005	-3.4	0	1	0	1	40	60	0	Aeration riprap
☑	9:			1.1	11.88	0	0.00001	-3.4	0	1	0.1	2	20	80	0	Aerobic wetland
☑	10:			0.0042	11.88	0	0.005	-3.4	0	1	0	1	20	80	0	Aeration riprap
☑	11:			0	11.88	0	0	-3.4	0	1	0	0	100	0	0	NULL

Generate Kinetics Output

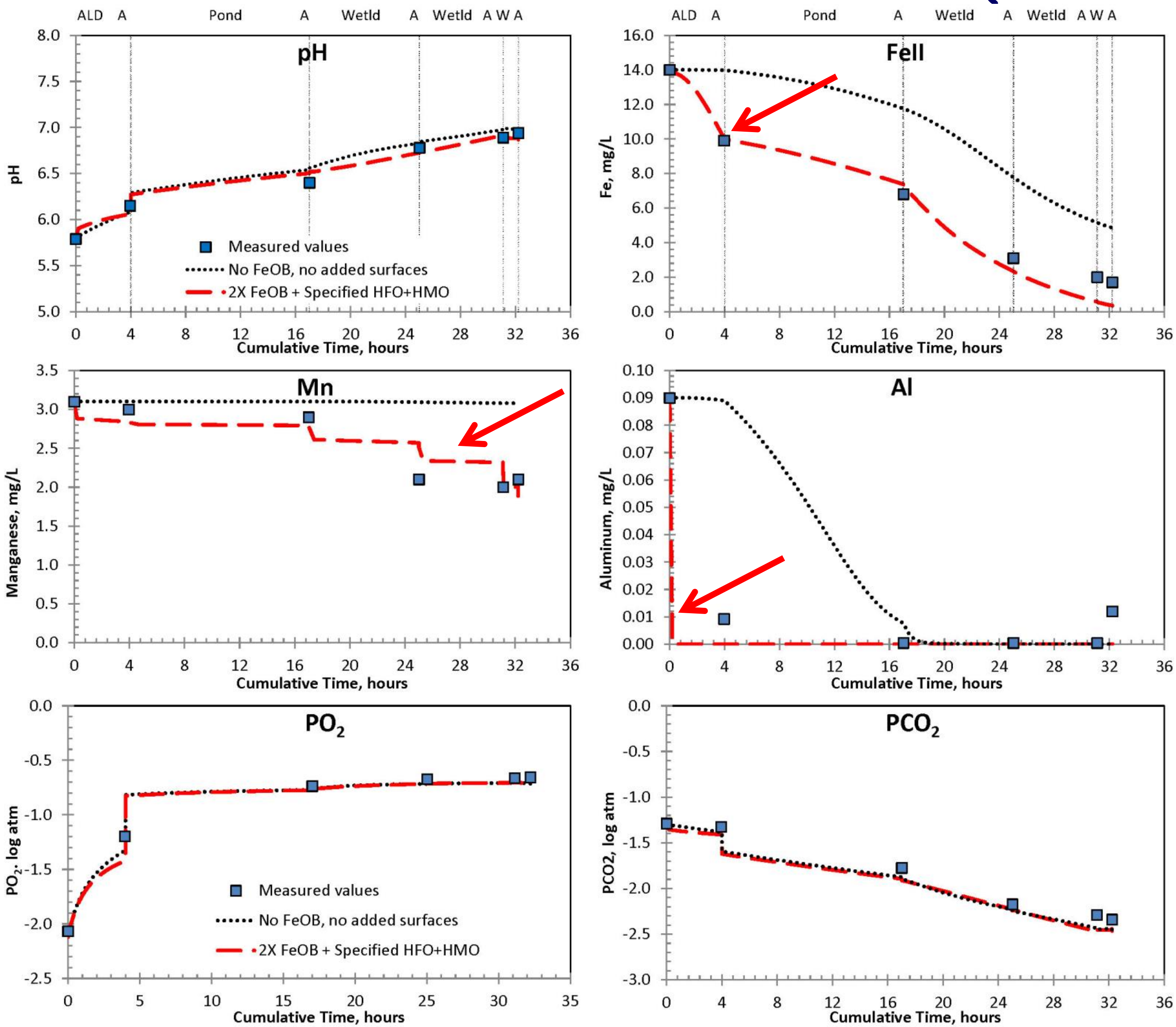
☐ Print PHREEQC Output Report

☑ Plot Dis. Metals ☐ Plot Ca, Acidity ☐ Plot Sat Index ☐ Plot PPT Solids

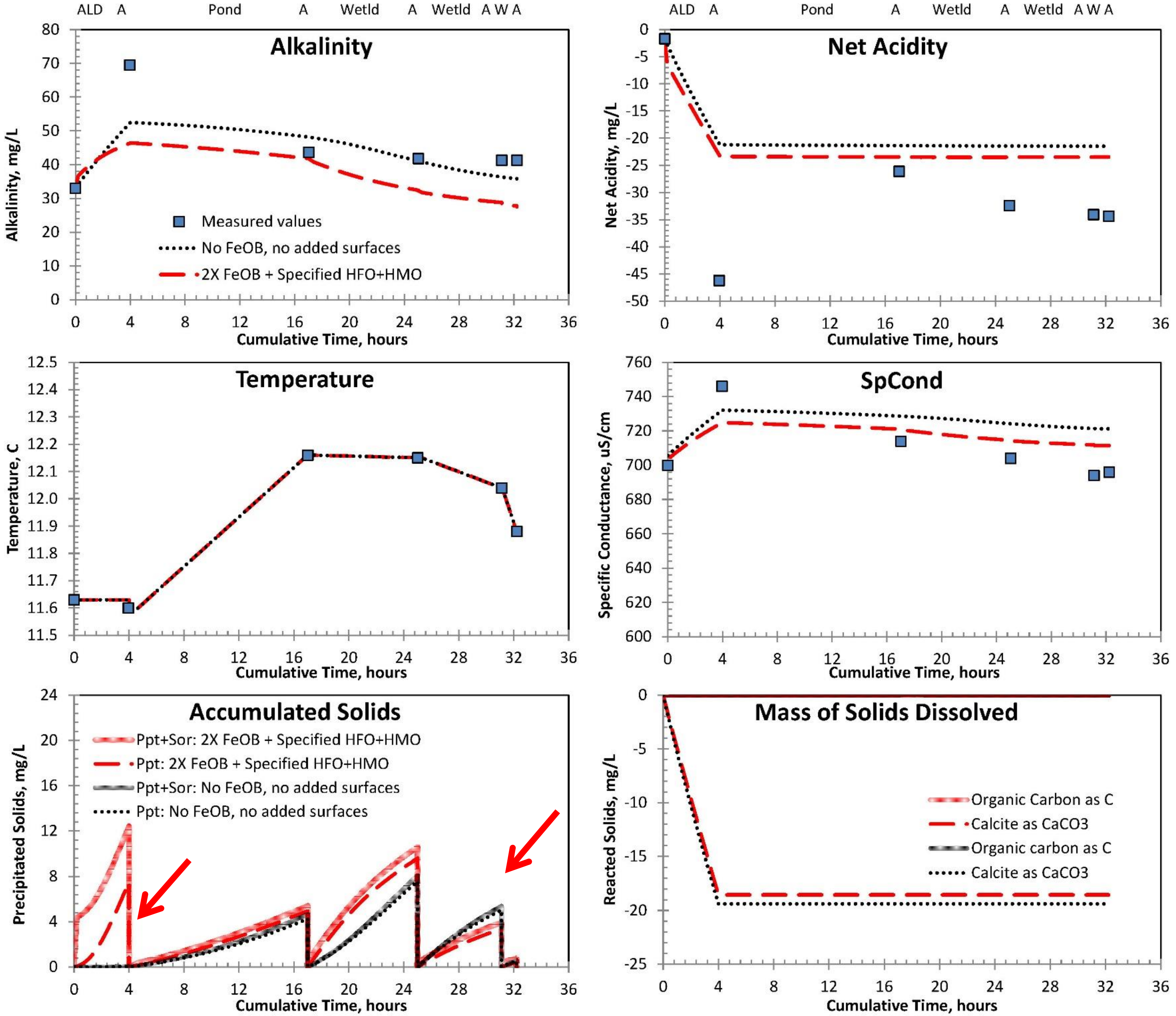
TreatTrainMix2.exe created by C.A. Cravotta III, U.S. Geological Survey. Version 1.4.5, August 2021

Variable retention times, temperature, (caustic, H_2O_2,) CO_2 outgassing/ingassing, limestone surface area, organic carbon, sorbent, plus adjustable rates.

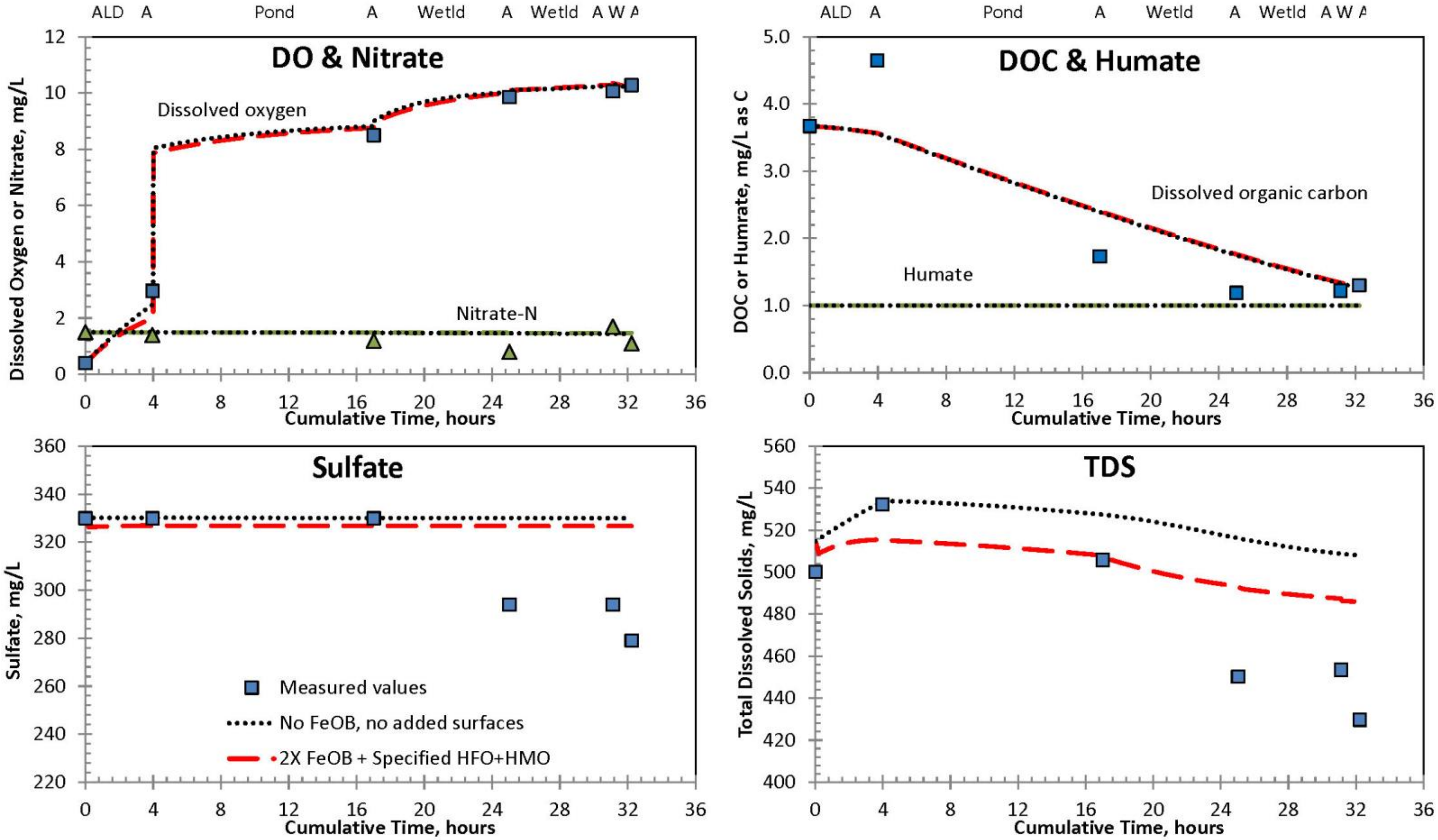
Pine Forest ALD + Aerobic Wetlands (151212)



Pine Forest ALD + Aerobic Wetlands (151212)



Pine Forest ALD + Aerobic Wetlands (151212)



Pre-Aeration, Lime Dosing, Solids Recirculation

TreatTrainMix2.exe: Active treatment

St. Michael AMD: net acidic with high Fe & CO_2 moderate Mn

Select Workspace: C:\Users\cravotta\Documents\AMDTreatTrainREYs_wateq\StMichael

	Soln#A	Soln#B
Design flow (gpm)	5200	0
Mix fraction	1	0
Temp (C)	15.4	0.01
SC (uS/cm)	1923	0
DO (mg/L)	2.2	0.01
pH	5.7	0
Acidity (mg/L)	254.2	0
☑ Estimate NetAcidity	223	0
Alk (mg/L)	50.8	0
TIC (mg/L as C)	57.3	0
☐ Estimate TIC	63.5	0
Fe (mg/L)	148	0
Fe2 (mg/L)	148	0
☐ Estimate Fe2	0	0
Al (mg/L)	0.34	0
Mn (mg/L)	3.6	0
SO4 (mg/L)	1078	0
Cl (mg/L)	32.8	0
Ca (mg/L)	242	0
Mg (mg/L)	88.7	0
Na (mg/L)	27.8	0
K (mg/L)	9.15	0
Si (mg/L)	18.8	0
NO3N (mg/L)	0	0
TDS (mg/L)	0	0
DOC (mg/L as C)	0.1	0
Humate (mg/L as C)	0.1	0

Kinetics Constants, Adjustment Factors

factr.kCO2	1	factr.kO2	2.1	EXPcc	0.67
factr.kFeHOM	1	factr.kFeHET	1	factr.kFeNO3	0.25
factr.kFeH2O2	1	factr.kbact	1	factr.kFeIIMnOx	1
factr.kMnHOM	1	factr.kMnHFO	1	factr.kMnHMO	0.5
factr.kSHFO	1	factr.kSOC	100	factr.kDOC	1
SI_Fe(OH)3	0.0	SI_Al(OH)3	0.0	SI_CaCO3	2.5
SI_Schwertmannite	1.0	SI_Basaluminite	3.0	SI_FeCO3,MnCO3	2.5

If adding caustic at step 1, 2, 3, 4, and/or 5: choose caustic agent, activate relevant +Caustic checkbox(es) and enter target pH value for the step(s)

◉ CaO ○ Ca(OH)2 ○ Na2CO3 ○ NaOH 20 wt% soln

☑ Estimate H2O2.mol/L 0.001332

0.0001143 35wt% 0.0001082 50wt%

H2O2 wt% units gal/gal (memo, not used)

Step	+Caustic?-->pH?	Time.hrs	Temp2.C	H2O2.mol	kLaCO2.1/s	Lg(PCO2.atm)	SAcc.cm2/mol	M/M0cc	SOC.mo	HMeO.mg	Fe%	Mn%	Al%	Description
☑ 1:	☐ 7.5	0.015	16.1	0	0.05	-3.4	0	1	0	0	100	0	0	Maelstrom (54 sec)
☑ 2:	☑ 8.5	0.015	16.1	0	0.0001	-3.4	0	1	0	0	100	0	0	Lime Fe(OH)2 ppt equil
☑ 3:	☑ 9.3	0.110	18.4	0	0.0001	-3.4	0	1	0	227.7	97.51	1.95	0.53	Lime+Solids Fe(OH)3 ppt
☑ 4:	☑ 8.5	0.110	18.4	0	0.0001	-3.4	0	1	0	0	97.51	1.95	0.53	Lime pH 8.4 effl to clarifier
☑ 5:	☐ 7.5	14.20	18.9	0	0.0000001	-3.4	0	1	0	1.7	100	0	0	Clarifier 4.43 Mgal
☑ 6:		0.03	19.5	0	0.0005	-3.4	0	1	0	0	100	0	0	Outflow ditch
☑ 7:		0	19.5	0	0	-3.4	0	1	0	0	100	0	0	NULL
☑ 8:		0	15.4	0	0	-3.4	0	1	0	0	0	0	0	NULL
☑ 9:		0	15.4	0	0	-3.4	0	1	0	0	0	0	0	NULL
☑ 10:		0	15.4	0	0	-3.4	0	1	0	0	0	0	0	NULL
☑ 11:		0	15.4	0	0	-3.4	0	1	0	0	0	0	0	NULL

Generate Kinetics Output

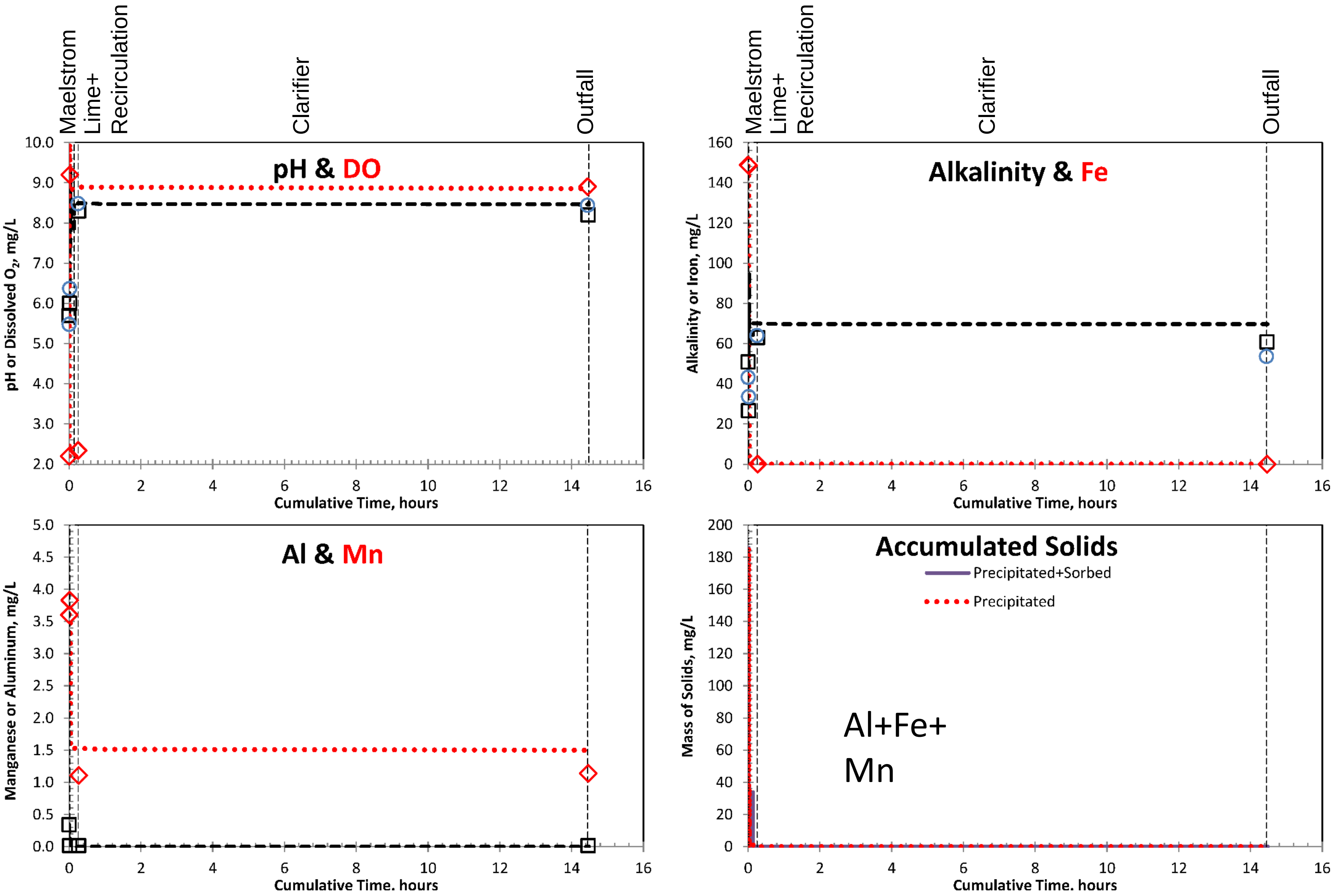
☐ Print PHREEQC Output Report

☑ Plot Dis. Metals ☐ Plot Ca, Acidity ☐ Plot Sat Index ☐ Plot PPT Solids

TreatTrainMix2.exe created by C.A. Cravotta III, U.S. Geological Survey. Version 1.4.5, August 2021

UI for active treatment of net-acidic AMD through (1) Maelstrom oxidizer; (2-4) lime dosing and sludge recirculation; (5) clarifier; and (6) outflow ditch.

Pre-Aeration, Lime Dosing, Solids Recirculation
St. Michael AMD, Cambria County, PA



PHREEQ-N-AMDTreat: TreatTrainMix2 Model Application

Hypothetical Passive Treatment Scenarios for Howe Bridge Mine Discharge

"ALD" + Aerobic Ponds + "OLD" + Mn-Removal Bed

TreatTrainMix2.exe: Passive treatment

Howe Bridge, high Fe & Mn

elect Workspace | C:\Users\cravotta\Documents\AMDTreatValidationSimulations\HOWBRALD

	Soln#A	Soln#B
Design flow (gpm)	16.1	0
Mix fraction	1	0
Temp (C)	11.3	0.01
SC (uS/cm)	1270	0
DO (mg/L)	1.12	0.01
pH	5.88	0
Acidity (mg/L)	180	0
☑ Estimate NetAcidity	210.5	0
Alk (mg/L)	60	0
TIC (mg/L as C)	32.4	0
☑ Estimate TIC	58.8	0
Fe (mg/L)	128	1E-08
Fe2 (mg/L)	129	0
☐ Estimate Fe2	128	0
Al (mg/L)	0.067	1E-08
Mn (mg/L)	22.3	1E-08
SO4 (mg/L)	684	1E-06
Cl (mg/L)	4.9	0
Ca (mg/L)	101	1E-06
Mg (mg/L)	63	1E-06
Na (mg/L)	12.2	1E-06
K (mg/L)	5.24	0
Si (mg/L)	7.05	0
NO3N (mg/L)	0	0
TDS (mg/L)	1150	0
DOC (mg/L as C)	0	0
Humate (mg/L as C)	0	0

Kinetics Constants, Adjustment Factors

factr.kCO2	1	factr.kO2	2.1	EXPcc	0.67
factr.kFeHOM	1	factr.kFeHET	1	factr.kFeNO3	0.25
factr.kFeH2O2	1	factr.kbact	1	factr.kFeIIMnOx	1
factr.kMnHOM	1	factr.kMnHFO	1	factr.kMnHMO	0.5
factr.kSHFO	1	factr.kSOC	100	factr.kDOC	1
SI_Fe(OH)3	0.0	SI_Al(OH)3	0.0	SI_CaCO3	0.3
SI_Schwertmannite	1.0	SI_Basaluminite	1.0	SI_FeCO3,MnCO3	2.5

If adding caustic at step 1, 2, 3, 4, and/or 5: choose caustic agent, activate relevant +Caustic checkbox(es) and enter target pH value for the step(s)

○ CaO ◉ Ca(OH)2 ○ Na2CO3 ○ NaOH 20 wt% soln

☑ Estimate H2O2 mol/L 0.001152

9.89E-05 35wt% 9.36E-05 50wt%

H2O2 wt% units gal/gal (memo, not used)

Step	+Caustic?-->pH?	Time.hrs	Temp2.C	H2O2.mol	kLaCO2.1/s	Lg(PCO2.atm)	SAcc.cm2/mol	M/M0cc	SOC.mo	HMeO.mg	Fe%	Mn%	Al%	Description
☑ 1:	☐	21.7	9.8	0	0.0000001	-3.4	72	1	0	19.8	84.0	16.0	0	ALD Howe Bridge 300
☑ 2:	☐	0.05	12	0	0.01	-3.4	45	1	0	0	100	0	0	Aeration cascade
☑ 3:	☐	20.0	12	0	0.00001	-3.4	0	1	0	0	100	0	0	Aerobic pond
☑ 4:	☐	0.05	12	0	0.01	-3.4	45	1	0	0	100	0	0	Aeration cascade
☑ 5:	☐	40.0	12	0	0.0000001	-3.4	45	1	0	20	84.0	16.0	0	Limestone bed
☑ 6:		0.05	12	0	0.005	-3.4	45	1	0	0	100	0	0	Aeration cascade
☑ 7:		8.0	12	0	0.00001	-3.4	0	1	0	0	100	0	0	Aerobic pond
☑ 8:		0.05	12	0	0.01	-3.4	45	1	0	0	100	0	0	Aeration cascade
☑ 9:		5.0	12	0	0.0000001	-3.4	144	1	0	50	0	100	0	Mn removal bed
☑ 10:		5.0	12	0	0.0000001	-3.4	144	1	0	50	0	100	0	Mn removal bed
☑ 11:		5.0	12	0	0.0000001	-3.4	144	1	0	50	0	100	0	Mn removal bed

Generate Kinetics Output

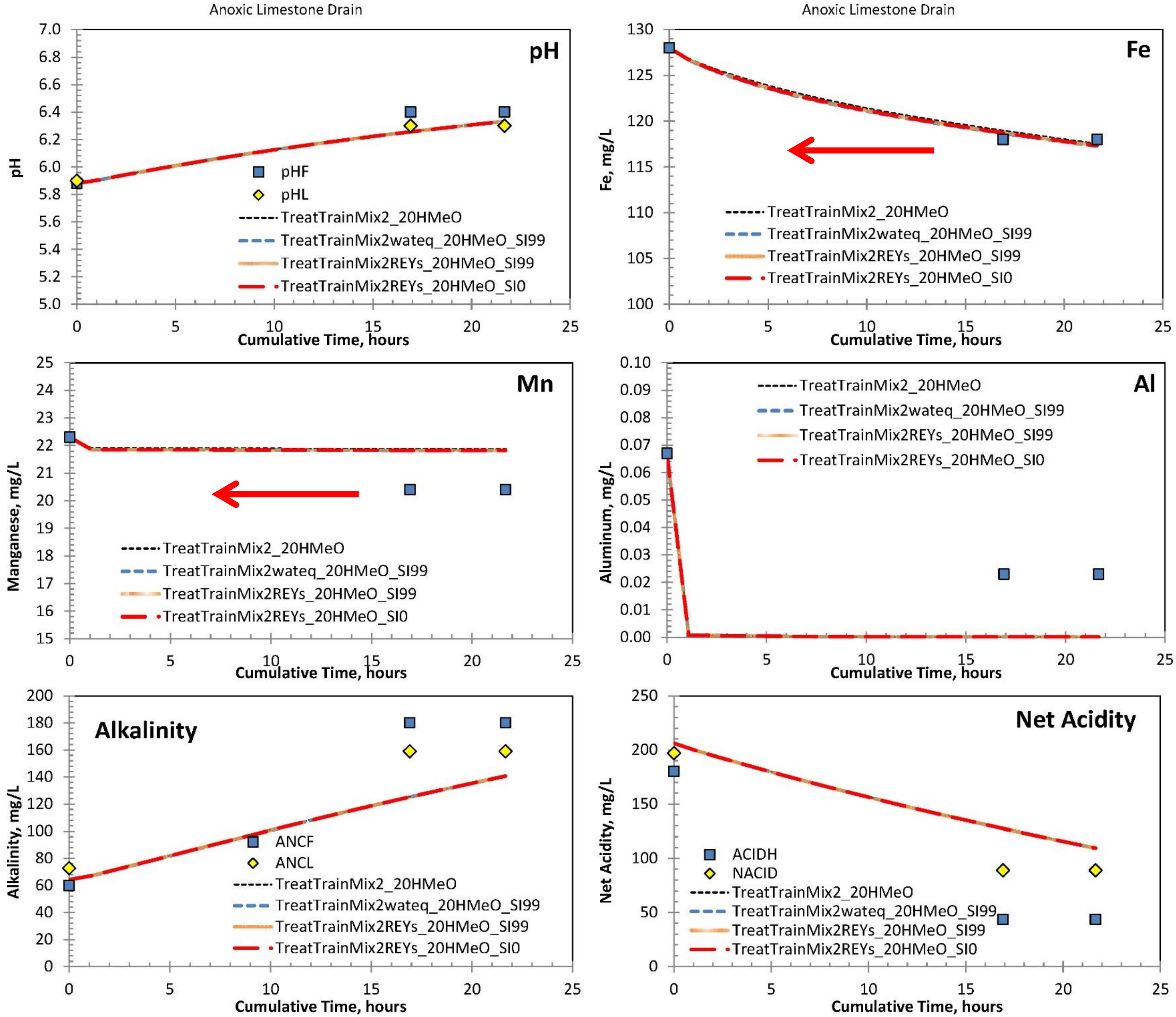
☐ Print PHREEQC Output Report

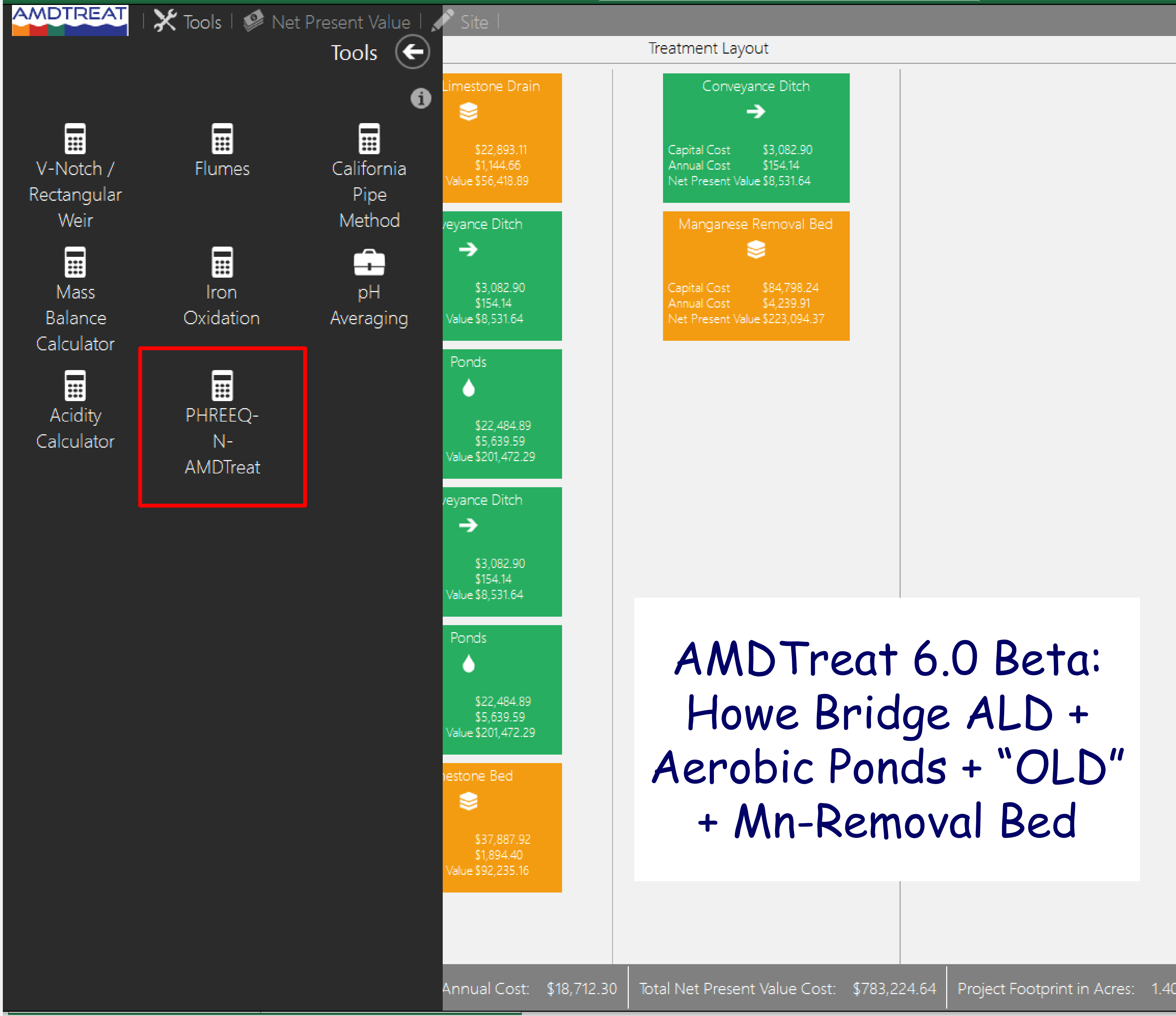
☑ Plot Dis. Metals ☐ Plot Ca, Acidity ☐ Plot Sat Index ☐ Plot PPT Solids

TreatTrainMix2.exe created by C.A. Cravotta III, U.S. Geological Survey. Version 1.4.5, August 2021

UI for passive treatment of net-acidic AMD through (1) anoxic limestone drain; *with added steps for (3) aerobic pond; (5) oxic limestone bed; (7) aerobic pond; and (9-11) manganese removal bed with intermediate aeration steps (2, 4, 6, 8)*

Howe Bridge ALD, only (210608)




AMDTREAT
Tools
Net Present Value
Site
Tools
Treatment Layout
V-Notch / Rectangular Weir
Flumes
California Pipe Method
Mass Balance Calculator
Iron Oxidation
pH Averaging
Acidity Calculator
PHREEQ-N-AMDTreat
Limestone Drain
$22,893.11
$1,144.66
Value $56,418.89
eyance Ditch
$3,082.90
$154.14
Value $8,531.64
Ponds
$22,484.89
$5,639.59
Value $201,472.29
eyance Ditch
$3,082.90
$154.14
Value $8,531.64
Ponds
$22,484.89
$5,639.59
Value $201,472.29
estone Bed
$37,887.92
$1,894.40
Value $92,235.16
Conveyance Ditch
Capital Cost $3,082.90
Annual Cost $154.14
Net Present Value $8,531.64
Manganese Removal Bed
Capital Cost $84,798.24
Annual Cost $4,239.91
Net Present Value $223,094.37
AMDTreat 6.0 Beta: Howe Bridge ALD + Aerobic Ponds + "OLD" + Mn-Removal Bed
Annual Cost: $18,712.30
Total Net Present Value Cost: $783,224.64
Project Footprint in Acres: 1.40

“ALD” + Aerobic Ponds + “OLD” + Mn-Removal Bed

AMDTreat 6.0 Beta PHREEQ-N-AMDTreat tool:

Howe Bridge, high Fe & Mn

PHREEQ-N-AMDTreat | Model Input | Errors

Treatment Modules To Be Modeled

Treatment Module	Step	Treatment Layer/ Technology	Treatment pH (s.u.)	Retention Time (hrs)	Temperature (°C)	Decarbonation Rate: kLaCO$_2$ (sec^{-1})	Limestone Surface Area (cm^2/mol)	Fraction of Limestone Available To React	Solid Organic Carbon	Sorbent Mass (Fe+Mn+Al) (mg/L)	Fe %	Mn %	Al %
ALD	1	Limestone Layer	6.88	21.700(	9.80	0.0000001	AASHTO #3 (72)	1.00	0.00	19.80	84.0(	16.0(	0.00
Conveyance Ditch	2	Water Layer	6.88	0.0500	12.00	0.0100000	AASHTO #1 (45)	1.00	0.00	0.00	100.(	0.00	0.00
Ponds	3	Water Layer	6.88	20.000(	12.00	0.0000100	0	1.00	0.00	10.00	100.(	0.00	0.00
Conveyance Ditch	4	Water Layer	6.88	0.0500	12.00	0.0100000	AASHTO #1 (45)	1.00	0.00	0.00	100.(	0.00	0.00
Limestone Bed	5	Water Layer	6.88	0.0000	12.00	0.0000100	0	1.00	0.00	0.00	100.(	0.00	0.00
	6	Limestone Layer	6.88	40.000(	12.00	0.0000001	AASHTO #1 (45)	1.00	0.00	20.00	84.0(	16.0(	0.00
Conveyance Ditch	7	Water Layer	6.88	0.0500	12.00	0.0050000	AASHTO #1 (45)	1.00	0.00	0.00	100.(	0.00	0.00
Ponds	8	Water Layer	6.88	8.0000	12.00	0.0000100	0	1.00	0.00	0.00	100.(	0.00	0.00
Conveyance Ditch	9	Water Layer	6.88	0.0500	12.00	0.0100000	AASHTO #1 (45)	1.00	0.00	0.00	100.(	0.00	0.00
Mn Removal Bed	10	Limestone Layer	6.88	5.0000	12.00	0.0000001	AASHTO #5 (144	1.00	0.00	50.00	0.00	100.(	0.00
Mn Removal Bed	11	Limestone Layer	6.88	5.0000	12.00	0.0000001	AASHTO #5 (144	1.00	0.00	50.00	0.00	100.(	0.00

Total Retention Time (hrs) **99.9**

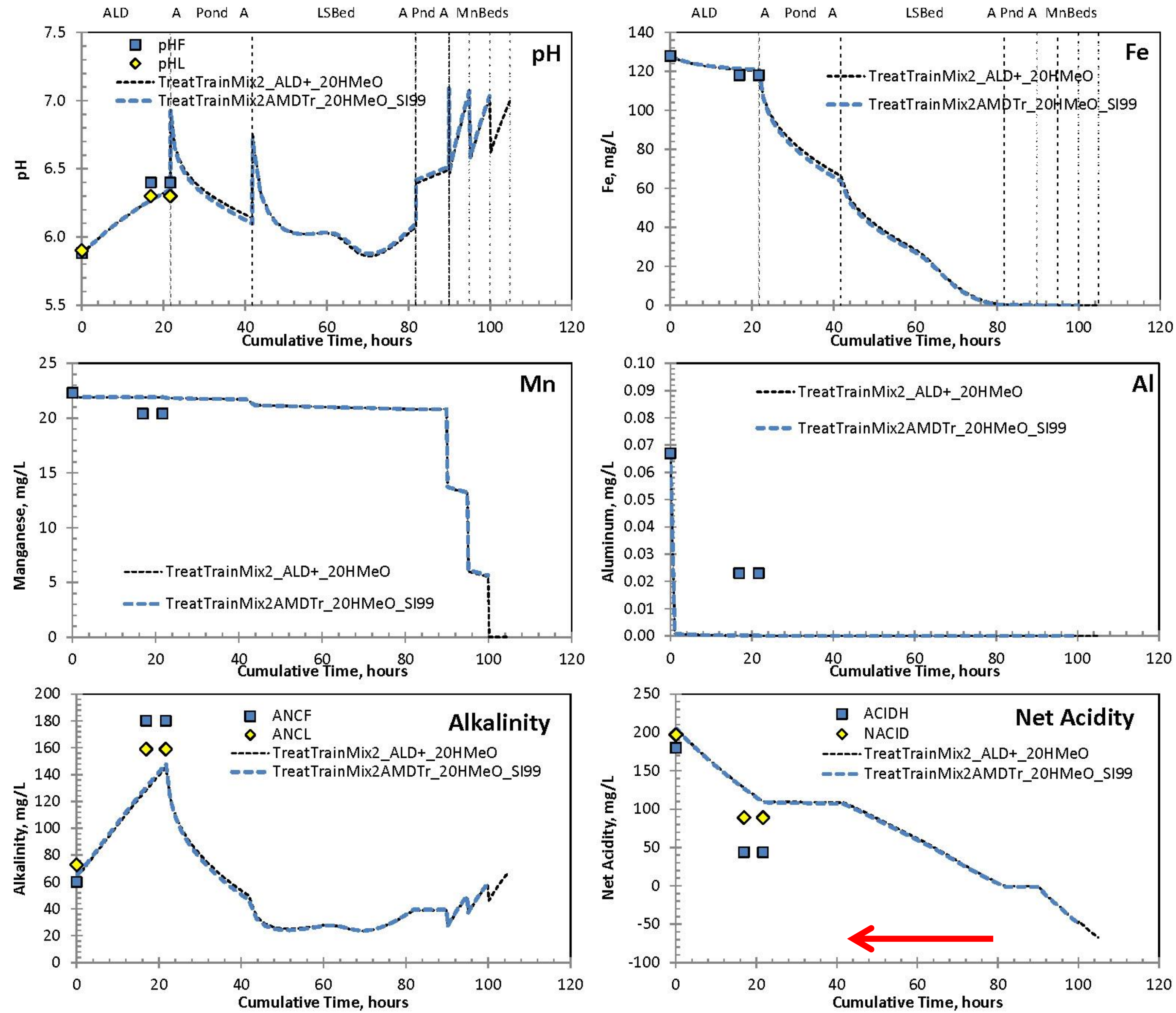
Model Output

☑ Print PHREEQC Output Report

Select Workspace: C:\Users\cravotta\Documents\AMDTreat_geochem_data\AMDTreatBeta\HoweBric

AMDTreat 6.0 Beta “PHREEQ-N-AMDTreat” tool (1) anoxic limestone drain; (3) aerobic pond; (5) oxic limestone bed; (7) aerobic pond; and (9-11) manganese removal bed with intermediate aeration steps (2, 4, 6, 8).

Howe Bridge ALD + Aerobic Ponds + OLD + Mn-Removal Bed



AMDTREAT | Tools | Net Present Value | Site |

Treatment Modules

- PASSIVE TREATMENT MODULES
- ACTIVE TREATMENT MODULES
- ANCILLARY TREATMENT MODULES
- PROJECT MODULES
- PLACEHOLDER MODULE
  - Placeholder

Treatment Layout

Anoxic Limestone Drain
Capital Cost $22,893.11
Annual Cost $1,144.66
Net Present Value $56,418.89

Conveyance Ditch
Capital Cost $3,082.90
Annual Cost $154.14
Net Present Value $8,531.64

Ponds
Capital Cost $22,484.89
Annual Cost $5,639.59
Net Present Value $201,472.29

Conveyance Ditch
Capital Cost $3,082.90
Annual Cost $154.14
Net Present Value $8,531.64

Ponds
Capital Cost $22,484.89
Annual Cost $5,639.59
Net Present Value $201,472.29

Limestone Bed
Capital Cost $37,887.92
Annual Cost $1,894.40
Net Present Value $92,235.16

Conveyance Ditch
Capital Cost $3,082.90
Annual Cost $154.14
Net Present Value $8,531.64

Manganese Removal Bed
Capital Cost $84,798.24
Annual Cost $4,239.91
Net Present Value $223,094.37

AMDTreat 6.0 Beta: Howe Bridge ALD + Aerobic Ponds + "OLD" + Mn-Removal Bed

Total capital cost: $193,632
Net present value cost: $783,225
Project footprint: 1.40 acres

AMD Treat 6.0 Beta | Total Capital Cost: $193,631.94 | Total Annual Cost: $18,712.30 | Total Net Present Value Cost: $783,224.64 | Project Footprint in Acres: 1.40

Conclusions

- ✓ PHREEQ-N-AMDTreat tools that include equilibrium and kinetics models are useful to evaluate AMD treatment performance and design.
- ✓ Graphical and tabular output indicates the pH and solute concentrations in effluent plus quantity of precipitated solids.
- ✓ By adjusting kinetic variables or chemical dosing, various passive and/or active treatment strategies can be simulated.
- ✓ AMDTreat cost-analysis software can be used to evaluate the feasibility for installation and operation of treatments that produce the desired effluent quality.

Disclaimer / Release Status

"Although this software program has been used by the U.S. Geological Survey (USGS), no warranty, expressed or implied, is made by the USGS or the U.S. Government as to the accuracy and functioning of the program and related program material nor shall the fact of distribution constitute any such warranty, and no responsibility is assumed by the USGS in connection therewith."

- ✓ FY2017-2020 Development, beta testing and review.
- ✓ FY2021 USGS software release, available for download: https://doi.org/10.5066/P9QEE3D5
- ✓ FY2021 Documentation, open-access Applied Geochemistry article: https://doi.org/10.1016/j.apgeochem.2020.104845
- ✓ FY2022 Incorporation with AMDTreat 6.0 for release by OSMRE: https://www.osmre.gov/programs/reclaiming-abandoned-mine-lands/amdtreat

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