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CONSTRUCTION DETAILS
40 CFR 146.82(a) & 146.86

Sugarberry CCS Hub

Facility Information

Facility Name: Sugarberry CCS Hub

Facility Contact: Sugarberry CCS, LLC
14302 FNB Parkway
Omaha, NE 68154

RRC Organization Report Number: 102245

Well locations: Projection WGS84

Well	County/State	Latitude	Longitude
SB-01	Hopkins, TX	33.202707	-95.338539
SB-02	Hopkins, TX	33.189225	-95.375952
SB-03	Hopkins, TX	33.196028	-95.405035
SB-04	Hopkins, TX	33.219565	-95.434859
SB-05	Hopkins, TX	33.207361	-95.385666

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List of Acronyms/Abbreviations

22Cr-110	22% Chromium Alloy
AMPP	Association for Materials Protection and Performance
AoR	Area of Review
API	American Petroleum Institute
Bbl	Barrel
BGS	Below Ground Surface
BH	Baker Huges
BHP	Bottomhole Pressure
BOP	Blowout Preventer
Ca	Calcium
$CaCl_2$	Calcium Chloride
CBR	Corrosion Barrier Ring
CCS	Carbon Capture and Sequestration
CFR	Code of Federal Regulations
Cl	Chloride
CMD	Chromoly Downshift
CMU	Chromoly Upshift
CO	Carbon Monoxide
CO_2	Carbon Dioxide
CRA	Chromium Alloy
DAS	Distributed Acoustic Sensing
DSA	Double-Studded Adapter
DTS	Distributed Temperature Sensing
DV	Diverter Tool
EPA	Environmental Protection Agency
ERRP	Emergency and Remedial Response Plan
F	Fahrenheit
Fe	Iron
Ft	Feet
FTS	Feed-through System
HCM	Hydraulic Communication Mandrel
HCO_3	Bicarbonate
ID	Inner diameter
KCl	Potassium Chloride
lb/ft	Pounds per foot
lb/gal	Pounds per gallon
LCM	Loss Control Material
LLC	Limited Liability Company
LTC	Long Thread Coupling
MASP	Maximum Allowable Surface Pressure
Mg	Magnesium
Mg/L	Milligrams per Liter
MMt	Million Metric Tons
MWD	Measure While Drilling

List of Acronyms/Abbreviations (Con't)

Na	Sodium
OD	Outer Diameter
PPG	Pound per Gallon
PPMV	Parts per Million by Volume
PPMW	Parts per Million by Weight
PSIA	Pounds per Square Inch Absolute
P/T	Pressure/Temperature
RRC	Railroad Commission of Texas
SLB	Company Formerly Known as Schlumberger
SO_4	Sulfate
SOW	Slip-on Weld
STC	Short Thread Coupling
TDS	Total Dissolved Solids
USDW	Underground Source of Drinking Water
W/mK	Watts per Meter-Kelvin

A. Introduction

The construction details for the injection wells at Sugarberry CCS Hub in Hopkins County, Texas (the "project") are described in this document. Sugarberry CCS, LLC will construct five (5) new underground injection control (UIC) Class VI wells (SB-01, SB-02, SB-03, SB-04 and SB-05) that will be utilized for the permanent sequestration of supercritical carbon dioxide (CO_2). This document addresses the Class VI permit information requirements included in 40 CFR 146.82(a) (11 and 12) and the well construction and completion requirements included in 40 CFR 146.86 and 16 TAC 5.203(e). Fluid movement into Underground Sources of Drinking Water (USDWs) and/or unauthorized zones will be mitigated during drilling operations with balanced (i.e., high density) drilling fluid and post-drilling through cementation of the surface and long string casings. The surface and subsurface components will be designed to specifically allow for the deployment of testing equipment and/or workover rig tools into and around the well, and a permanent annulus monitoring system will be installed to track pressure variance within and around the injection tubing.

The injection well design and construction details described herein are based on the subsurface information at well locations SB-01 and SB-05 (see Section 1.1 of the **Application Narrative** for well location map). Wells SB-01 and SB-05 were selected as representative wells due to the following: a) the well design for SB-01 utilizes a hydraulic sliding sleeve whereas the remaining wells utilize a mechanical sliding sleeve and, b) SB-05 will be drilled to the deepest stratigraphic depth in the acreage block and provides important depth estimates for the Eagle Ford Shale (confining unit), the Woodbine Formation (upper injection zone), and the Paluxy Formation (lower injection zone). The well design for SB-05 will be applied to the remaining well locations (SB-02, SB-03, SB-04) and adjusted for local geology as needed. Confining zone and injection zone lithology, depth, and thickness are described in detail in Section 1.1 of the **Application Narrative**. The following subsections provide information on construction procedures, injection pressures and rates, operating conditions, formation conditions, casing and tubing specifications, cementing specifications, packer and sliding sleeve specifications, annulus fluid properties, and wellhead design. Injection well construction specifications and diagrams are provided in **Figures 4-1 and 4-2**.

B. Wellhead Injection Pressure

GEOS (V.0.2.0, Livermore, CA) was used as the primary computational model for delineating the Area of Review (AoR) for the project (see **Area of Review and Corrective Action Plan, Section 2.B**). In addition to the reservoir governing equations, injection wells are explicitly modeled in GEOS using a nodal analysis to ensure that the well operational details are directly coupled to reservoir conditions. GEOS contains a multiphase compositional well model in which wells have their own set of governing equations discretized along the wellbore trajectory that are coupled to the reservoir governing equations. Mass conservation for fluids entering and leaving the well is enforced, while equations-of-state are used to compute the fluid density in the well at current pressure and temperature conditions. The connection of each perforation to reservoir grid cells is computed using a Peaceman well index. The fluid pressure in the well is assumed to remain hydrostatic, based on the density of fluids present in the well. Wells may be operated with both maximum mass injection rates and maximum pressure controls.

The project's five (5) injection wells were modeled with GEOS (see **Area of Review and Corrective Action Plan, Section B.8**). These injection wells have dual completions in the Woodbine Formation and Paluxy Formation injection intervals. The wells are modeled with targeted rates of 17.5 lbs/second in the Woodbine and 45.42 lbs/second in the Paluxy (**Area of Review and Corrective Action Plan, Section B.8**, **Table 2-8**). Bottomhole constraints are applied to each well using the fracture gradient and a 90% safety factor (**Area of Review and Corrective Action Plan, Section B.8**, **Table 2-9**). With a pressure of 1,250 psi at the wellhead, the nodal analysis showed that the bottomhole pressure (BHP) constraints were not exceeded throughout the simulations, and that there is an ample safety factor at the specified flow rates (**Area of Review and Corrective Action Plan, Section B.8, Figures 2-26 and 2-27**).

C. Injection Well Construction Details

Drilling and construction operations will be conducted in compliance with 40 CFR 146.86 and 16 TAC 5.203(e). All phases of well construction will be supervised by licensed personnel with knowledge and experience related to drilling engineering and operations.

Prior to the drilling of the deep vertical wellbores, the conductor casing will be set to the specified depth (the conductor will either be driven into the ground or drilled, set, and cemented in place) and a cellar box will be constructed. Next, the surface and long string sections of the well will be drilled, cased, and cemented in place. The surface casing will be cemented with standard cement, and the long string casing will be cemented with CO_2-resistant cement, from total depth through the top of the confining zone, and Class A cement or equivalent from the confining zone to surface. The surface casing will be set in the Taylor Formation, below the lowermost USDW. The long string casing will be set within the top of the Glen Rose Formation, which lies directly below the Paluxy Formation and is identified as the lower confining unit. Perforations will be shot through the casing at specified intervals in both the Woodbine and Paluxy Formations to allow for injection zone stimulation (see **Stimulation Plan, Section 4.1**) and the eventual injection of CO_2. (see **Application Narrative, Section 1.1, Figure 1-4** for the stratigraphic column for the project). Approximately 150 feet of the Glen Rose Formation will be drilled to allow for wireline logging of the entire Paluxy Formation. The drilled section of the Glen Rose Formation will be cemented back to the Paluxy/Glen Rose contact (or higher) and will not be utilized for injection purposes.

D. Downhole Risks and Contingency Considerations While Drilling

Unexpected subsurface events may occur during the drilling of a well. Some common drilling problems include drill pipe failure, lost circulation, hole deviation, pressure kicks, and borehole instability. Drilling related risks and remedial actions are discussed in further detail in the **Emergency and Remedial Response Plan (Section 10)**. The following list addresses potential downhole risks and provides contingency plans, mitigation techniques, or response information if encountered:

- **Borehole Stability.** Balanced drilling fluids will be maintained during all drilling stages to control BHPs, support the wellbore and maintain hole stability, prevent formation fluid influx and seal permeable formations, circulate cuttings away from the drill bit to the surface, mitigate drilling damage to the targeted reservoir, and cool the drilling bit and

work string. Maintaining properly balanced drilling fluids and creating a proper "mudcake" on the borehole wall will prevent the movement of fluids into or between USDWs during drilling operations. Drilling fluid and formation gas samples will be analyzed throughout drilling operations to ensure proper mud weight and adequate downhole pressure control.

- **Pressure Control.** Well control will be maintained through the use and frequent testing of a blowout preventer (BOP) and care will be taken to prevent or minimize the discharge or spillage of drilling-related fluids and debris at the surface. If fluid and debris are discharged from the well and move beyond the confines of the cellar box, the appropriate mitigation response will be initiated and the site cleaned. The BOP will be tested as set forth in 16 TAC 3.13(a)(6).

- **Borehole Deviation.** A Measure While Drilling (MWD) system will be incorporated into the drill string to monitor real time inclination and azimuth during drilling of the surface and long string boreholes. If borehole deviations approach or exceed the accepted threshold, the driller will be alerted, and corrective action will be taken to reduce the deviation. See the **Pre-Operational Testing Program (Section 5)** for additional information on borehole deviation requirements and limits.

- **Drill Pipe Failure.** In the event of a drill pipe failure, the broken or severed piece of drill string will be fished and removed from the borehole or casing by a certified fishing vendor. After the debris or obstruction has been remediated, the casing or borehole will be inspected for damage or washouts and mitigated as needed prior to returning to drilling operations.

- **Lost Circulation.** Drilling fluid losses encountered while drilling are the result of overbalanced drilling fluids penetrating a formation, under-pressured zones accepting drilling fluid, or an unexpected increase in the permeability of a formation due to naturally occurring fractures or conduits within the rock. A pre-drill subsurface evaluation and review of local drilling reports can help identify potential loss zones and provide requisite drilling fluid densities to be incorporated into the drilling fluid program. In addition, loss control material (LCM) will be kept onsite during drilling operations and a certified mud engineer will be present to design and introduce LCM to the borehole as needed to mitigate these losses. If drilling fluid losses cannot be controlled by LCM, cement plugs will be pumped into the loss zone. If mitigation is still required post-cement, the zone will be isolated with an intermediate casing string, or the borehole will be abandoned.

E. Well Construction Procedures

The following general construction procedures will be used for drilling and completion of the injection wells. These procedures are based on currently available subsurface information and best practices for Class VI well construction as required in 40 CFR 146.86. A detailed, site-specific drilling prognosis will be developed for each well prior to the commencement of drilling operations. All site personnel will be trained in proper emergency responses, and a site-specific health and safety plan will be maintained onsite. Additionally, drilling and completion activities

will be annotated and tracked in daily drilling reports. All open and cased hole logging suites are provided in the **Pre-Operational Testing Plan (Section 5)** and contain information on deviation surveys, formation samples, and tests to be conducted during well drilling and well completion, prior to operation of the injection well. The following is the general well drilling procedure:

- **Prepare the location.** Survey the well pads; provide notification of subsurface work to local underground utility location authority; conduct earthwork grading to level the location and add construction well pad mats as needed; set conductor casing; excavate and board cellar; lay down containment for the drilling rig substructure.
- **Safety Meeting.** Conduct safety meeting with all parties involved in the drilling of the well. Document the date, time, attendees and content of the meeting.
- **Mobilize in and rig up.** Set rig substructure and rig appurtenances; raise derrick and install remaining equipment; mix spud fluids; prepare to drill surface hole.
- **Drill and complete surface hole.** Commence drilling of surface hole from surface to casing set depth; conduct deviation (1 degree or less) surveys while drilling; conduct logging; run casing with centralizers; cement casing and circulate 30% excess cement to surface wait on cement to set; pressure test casing; run cement bond log.
- **Drill and complete production hole.** Drill out float shoe; make up directional bottomhole assembly (BHA), run in hole, and drill to confining zone core point; conduct straight hole surveys; run core barrels and bit to core confining interval; drill to upper injection zone core point; conduct straight hole surveys; run core barrels and bit to core upper injection interval; drill to lower injection zone core point; conduct straight hole surveys; run core barrels and bit to core lower injection interval; drill to total depth; condition hole; conduct open hole logging; run casing with centralizers and strapped fiber optic monitoring system; cement casing with approximately 30% excess cement to surface; wait on cement to set; pressure test casing; run cased hole logs; perforate production casing at specified intervals; stimulate injection zones as needed; perform clean-out.
- **Run tubing, sliding sleeves, packers, and gauges.** Run tubing with sliding sleeves, packers, and pressure gauges; set hydraulic packers; displace annular fluids with treated fresh water containing biocide and corrosion inhibitor; pack off tubing in the surface head; top off annulus with treated fresh water; secure wellhead and shut-in well; pressure test annulus.
- **Rig down and demobilize.** Rig down; off-rent equipment; demobilize; restore location.
- **Pre-operational testing.** Set tree; pressure test tree and annulus; conduct reservoir testing; test fiber optic monitoring system, sliding sleeves, and downhole pressure gauges.

F. Demonstration of Well Material Compatibility

Well construction material compatibility with the injectate, formation brines (Woodbine and Paluxy Formations), and interactions thereof were evaluated using the corrosion modeling capabilities within the OLI Systems software (V.12.0.0.11, Parsippany, NJ). Corrosion rates and localized pitting potential were calculated for the indicated alloy selections specified in **Subsection G. Casing Summary** below. As corrosion worsens at higher pressure and temperature, the models were parameterized using the worst-case scenarios of downhole temperature and pressure, which are listed in **Tables 4-1** and **4-2** below. Calculation summaries, including model set-up and parameterization, are included in **Appendix A** of this plan. Corrosion calculations were generally

run as isothermal calculations under a complete agitation flow regime and inclusive of scales and passivating films.

The injectate composition used for the corrosion model is considered a worst-case scenario, comprised of the maximum component concentrations of the CO_2 stream tariff shown in **Table 6-1** of the **Summary of Requirements**. The anticipated water content of the stream of <20 lbs/MMscf is below the water saturation limit, and acid dropout phases from the CO_2 stream are not a concern for corrosion at wellhead and unwetted conditions. The formation brine compositions for the Woodbine and Paluxy Formations are represented in **Table 1-13** of the **Application Narrative (Section 1)**. Maximum bottomhole temperatures and pressures were modeled at 108.6 °F and 2,641 psi for the Woodbine Formation and 121.7 °F and 3,398 psi for the Paluxy Formation, as specified in **Table 6-1** of the **Summary of Requirements**. Bottomhole temperatures were estimated using the Geothermal Gradient Map of the Conterminous United States (Kron and Heiken, 1980). The practical upper temperature limit is 750 ºF for typical casing steel and 400 ºF for 22Cr-110, therefore heat-related degradation of casing is not expected.

The following four scenarios at the downhole conditions were evaluated in the corrosion models:

1. Installation – compatibility with formation brine

2. Injection – compatibility with a mixture of mostly CO_2 injectate combined with a small amount of formation brine (90% injectate/10% brine by volume)

3. Flowback – compatibility with a 50% injectate/50% brine mixture by volume

4. Plume Arrival to In-zone Observation (IOB) wells – compatibility with a 10% injectate/90% brine mixture by volume

Corrosiveness of the CO_2 stream and formation fluid mixture for each modeling scenario are indicated by the value for pH in **Tables 4-1** and **4-2**.

The general assessment of alloy compatibility under the scenarios was evaluated based on the maximal material loss expected during different stages of the project duration (10, 30, and 50 years). As stated in **Subsection G**, 9.625-in 47 lb/ft casing is specified for the long-string casing, and 5.5-in 17 lb/ft tubing is specified for the injection tubing. These materials have listed wall thicknesses of 0.472 inches and 0.304 inches, respectively. A conservative value of <10% of material loss based on the specified wall thickness and no localized pitting potential was used as a baseline for material compatibility. This value was chosen as a conservative estimate to ensure the strength integrity of the pipe. The general corrosion rates and pitting results are shown in **Tables 4-1 and 4-2**.

The corrosion modeling analyses indicate that material loss for the chromium alloys proposed for the injection and IOB wells falls below the conservative benchmark of <10% loss. Localized pitting corrosion was identified under simulated injection scenarios. In the case of Sugarberry CCS, LLC, 22Cr or better CRA is shown to be suitable for corrosion resistance throughout the life of the project for injection and IOB well sections that will encounter formation brines containing CO_2.

The OLI model does not have the ability to model interior coated pipe, but this type of tubing and piping, for instance Tuboscope TK-99 or equivalent, is designed for CO_2 and related injection fluids and presents an alternative to the use of high-grade chromium alloys. Tuboscope TK-99 has been laboratory- and field-tested and has shown viable corrosion resistance in CO_2, water, and hydrocarbon environments (Tuboscope TK-99 Specification Sheet, 2019).

Well locations utilizing J-55 or L-80 steel are not expected to encounter CO_2 or a corrosive environment.

Based on the information presented above, the proposed materials for project well construction are compatible with the fluids with which the materials are expected to come into contact, meeting the requirement of 40 CFR 146.86(b).

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Table 4-1. Corrosion Modeling Results – Woodbine Formation

Scenario	Injectate:Brine Ratio	pH	Alloy	Corrosion Rate	Pitting	Corrosion Loss (in)			Pipe Material Loss					
									9.625" 47 lb/ft			5.5" 17 lb/ft		
				in/yr	(Y/N)	10 year	30 year	50 year	10 year	30 year	50 year	10 year	30 year	50 year
Installation	0:10	5.84	Super13Cr	0.00005	N	0.0005	0.0015	0.0026	0%	0%	1%	0%	1%	1%
			22Cr	0.00001	N	0.0001	0.0002	0.0004	0%	0%	0%	0%	0%	0%
			25Cr	0.00001	N	0.0001	0.0002	0.0004	0%	0%	0%	0%	0%	0%
Injection	9:01	3.79	Super13Cr	0.00003	Y	0.0003	0.0008	0.0014	0%	0%	0%	0%	0%	0%
			22Cr	0.00001	N	0.0001	0.0003	0.0006	0%	0%	0%	0%	0%	0%
			25Cr	0.00001	N	0.0001	0.0003	0.0006	0%	0%	0%	0%	0%	0%
Flowback	5:05	4.19	Super13Cr	0.00005	N	0.0005	0.0015	0.0026	0%	0%	1%	0%	1%	1%
			22Cr	0.00001	N	0.0001	0.0002	0.0004	0%	0%	0%	0%	0%	0%
			25Cr	0.00001	N	0.0001	0.0002	0.0004	0%	0%	0%	0%	0%	0%
IOB Plume Arrival	1:09	4.26	Super13Cr	0.00005	N	0.0005	0.0015	0.0026	0%	0%	1%	0%	1%	1%
			22Cr	0.00001	N	0.0001	0.0002	0.0004	0%	0%	0%	0%	0%	0%
			25Cr	0.00001	N	0.0001	0.0002	0.0004	0%	0%	0%	0%	0%	0%

Table 4-2. Corrosion Modeling Results – Paluxy Formation

Scenario	Injectate:Brine Ratio	pH	Alloy	Corrosion Rate	Pitting	Corrosion Loss (in)			Pipe Material Loss					
									9.625" 47 lb/ft			5.5" 17 lb/ft		
				in/yr	(Y/N)	10 year	30 year	50 year	10 year	30 year	50 year	10 year	30 year	50 year
Installation	0:10	6.56	Super13Cr	0.00007	N	0.0007	0.0021	0.0035	0%	0%	1%	0%	1%	1%
			22Cr	0.00001	N	0.0001	0.0003	0.0005	0%	0%	0%	0%	0%	0%
			25Cr	0.00001	N	0.0001	0.0003	0.0005	0%	0%	0%	0%	0%	0%
Injection	9:01	2.54	Super13Cr	0.00003	Y	0.0003	0.0009	0.0014	0%	0%	0%	0%	0%	0%
			22Cr	0.00001	N	0.0001	0.0002	0.0004	0%	0%	0%	0%	0%	0%
			25Cr	0.00001	N	0.0001	0.0002	0.0004	0%	0%	0%	0%	0%	0%
Flowback	5:05	3.47	Super13Cr	0.00007	N	0.0007	0.0021	0.0035	0%	0%	1%	0%	1%	1%
			22Cr	0.00001	N	0.0001	0.0003	0.0006	0%	0%	0%	0%	0%	0%
			25Cr	0.00001	N	0.0001	0.0003	0.0005	0%	0%	0%	0%	0%	0%
IOB Plume Arrival	1:09	3.59	Super13Cr	0.00007	N	0.0007	0.0021	0.0035	0%	0%	1%	0%	1%	1%
			22Cr	0.00001	N	0.0001	0.0003	0.0005	0%	0%	0%	0%	0%	0%
			25Cr	0.00001	N	0.0001	0.0003	0.0005	0%	0%	0%	0%	0%	0%

G. Casing Summary

The following injection well casing design is based on the subsurface interpretation at well locations SB-01 (hydraulic sliding sleeve) and SB-05 (mechanical sliding sleeves). Subsurface formation depths are similar at both well locations, and all depth references mentioned herein are considered representative for both wells. The SB-05 casing design will also be utilized for wells SB-02, SB-03, and SB-04 (all mechanical sliding sleeves), and adjusted for local geology as needed.

The well design includes the following borehole dimensions and casing strings: a 20-inch-diameter conductor casing string set at a depth of approximately 80 feet below ground surface (BGS) inside a 26-inch borehole; a 13.375-inch diameter surface casing string set at a depth of approximately 2,150 feet BGS inside a 17.5-inch borehole; a 9.625-inch diameter long casing string set at the base of the Paluxy or the top of the upper Glen Rose Formation, at a depth of approximately 5,350 feet BGS inside a 12.25-inch borehole; and a 5.5-inch diameter injection tubing string set on a packer at approximately 4,150 feet BGS and hung inside the long string casing (see **Figures 4-1** and **4-2** for a conceptual casing schematic). The borehole diameters are considered conventional for the sizes of casing that will be used and should allow ample clearance between the outside of the casing and the borehole wall to ensure that a continuous cement seal will be emplaced along the entire length of the casing string. The long string borehole will be drilled approximately 150 feet into the upper section of the Glen Rose Formation to allow wireline logging tools to log the entirety of the Paluxy Formation. As mentioned in **Section B**, the drilled section of the Glen Rose Formation will be cemented back to the Paluxy/Glenn Rose contact (or higher) during cementation of the long string casing.

Casing material was selected based on modeled injectate fluid/formation fluid interactions and worst-case downhole temperatures and pressures (See **Section F**, above). Sections of the well expected to encounter injected CO_2, or a combination of injected CO_2 and formation brine, will be constructed of 22Cr-110 or better, which will help prevent and/or decrease rates of alloy pitting and corrosion over the life of the well. The structural specifications of the proposed casing strings meet or exceed the expected in-situ stresses and there are no indications that structural strength or integrity will decrease significantly over the life of the project.

Specific alloy compositions, grades, weights, and connection types listed herein may differ at the time of procurement due to changes in regulatory requirements, availability, and/or current materials testing results from institutions such as API, AMPP, EPA, or other entities with a focus on CCS. **Table 4-3** summarizes the open hole diameters and depth intervals and **Table 4-4** summarizes the casing program and casing specifications. Casing sections are discussed in further detail below. Cementing related information is provided in **Section I**.

G.1. Conductor Casing

The conductor casing will be composed of 20-inch diameter, 94-lb/ft, J-55 carbon steel with short thread couplings (STCs). The conductor casing will be set at 80 ft BGS and will be drilled or driven directly into the ground. If drilled, the conductor will be cemented in place. The conductor casing provides shallow wellbore stability for drilling of the surface and long string boreholes and protects the shallow subsurface from drilling contaminants.

G.2. Surface Casing

The surface casing will be composed of 13.375-inch diameter, 61-lb/ft, J-55 carbon steel with STCs. The surface casing will be set at 2,150 ft BGS, which is 350 ft below the base of the lowermost USDW. The surface casing will be cemented in place, and cement will be circulated from the casing shoe to surface. The surface casing will prohibit communication between the well and surrounding USDWs and/or unauthorized depths.

G.3. Long-String Casing

The long-string casing is 9.625-inch diameter pipe that is composed of three alloys: 1) L-80, 47-lb/ft carbon-steel installed from surface to 3,300 ft BGS; 2) corrosion-resistant 47lb/ft 22Cr-110 or better installed from 3,300 ft to 3,600 ft BGS (within the confining zone and across the upper packer); 4,100 ft to 4,220 ft BGS (across the lower packer), and 5,350 ft to 5,500 ft BGS (below the lower injection zone to TD); and 3) corrosion-resistant Super 13Cr-110 or better installed from 3,600 ft to 4,100 ft BGS and 4,220 ft to 5,350 ft BGS. 22Cr is proposed in the injection zone where pitting may be an issue due to contact with formation brine and injectate fluids. Super 13Cr is proposed in the injection zone where pitting is not a concern.

The long string casing will be set at the base of the Paluxy Formation or in the upper Glen Rose Formation. A Distributed Temperature Sensor (DTS)/Distributed Acoustic Sensor (DAS) Baker Hughes SureVIEW fiber optic cable, or equivalent, will be run on the exterior of the long string casing from surface to set point and cemented in place with the casing.

Table 4-3. Open Hole Diameters and Intervals

Borehole Section	Depth Interval (Feet BGS)	Open Hole Diameter (Inches)
Conductor	0 – 80	26
Surface	80 – 2,150	17.5
Long string	2,150 – 5,500	12.25

Table 4-4. Casing Specifications

Casing String	Depth Interval (Feet BGS)	Casing Dimensions (Inches)				Weight (lb/ft)	Grade (API)	Design Coupling	Thermal Conductivity (W/mK)	Burst Strength (psia)	Collapse Strength (psia)	Joint Yield Strength (1,000 lbs/ft)	Body Yield Strength (1,000 lbs/ft)
		OD	ID	Drift	Wall Thickness								
Conductor	0 – 80	20.0	19.124	18.936	0.438	94	J-55	STC	30 – 60	2,110	520	907	1,480
Surface	0 – 2,150	13.375	12.515	12.359	0.43	61	J-55	STC	30 – 60	3,090	1,540	595	962
Long String	0 – 3,300	9.625	8.681	8.525	0.472	47	L-80	LTC	30 – 60	6,870	4,760	1,122	1,086
	3,300 – 3,600	9.625	8.681	8.525	0.472	47	22Cr or better	Premium	15 - 20	6,870	4,760	1,122	1,086
	3,600 – 4,100’	9.625	8.681	8.525	0.472	47	Super 13Cr or better	Premium	14 - 17	6,870	4,760	1,122	1,086
	4,100 – 4,220	9.625	8.681	8.525	0.472	47	22Cr or better	Premium	15 - 20	6,870	4,760	1,122	1,086
	4,220 – 5,350	9.625	8.681	8.525	0.472	47	Super 13Cr or better	Premium	14 - 17	6,870	4,760	1,122	1,086
	5,350 – 5,500	9.625	8.681	8.525	0.472	47	22Cr or better	Premium	15 - 20	6,870	4,760	1,122	1,086

H. Tubing, Packer, & Sliding Sleeve Summary

Supercritical CO_2 will be injected into the injection zones through tubing, packers, and sliding sleeves that are comprised of corrosion resistant materials. The injection tubing will be fitted with two retrievable isolation packers, two hydraulic (SB-01) or mechanical (SB-02, SB-03, SB-04 and SB-05) sliding sleeve, two selective landing nipples, and one inline pressure gauge. The packers will be placed at the top and base of the upper injection zone (Woodbine Formation). The sliding sleeves will be placed directly above and directly below the lower packer and will enable injection into the Woodbine and/or Paluxy Formations and will accommodate CO_2 injection rate fluctuations and/or CO_2 injection rate design changes at the surface. The selective landing nipples, or "no-go" tools, will be placed directly above each packer. The selective landing nipples will allow for plugs, gauges, or other tools to be utilized within each injection zone. An inline pressure gauge will be incorporated into the tubing string, with a gauge placed within the upper packer. The pressure gauge will collect real-time pressure data within the injection tubing to assess injection rates and injection efficiency in the downhole environment.

The injection tubing will be 5.5-inch, 17-lb/ft, 22Cr-110 or better, or lined carbon steel tubing, with gas tight premium threads. If lined carbon steel tubing is used, corrosion barrier rings (CBRs) will be placed at all connections. Tubing specifications are provided in **Table 4-5.** The packers, sliding sleeves, and downhole gauges will be components from Baker Hughes CCS Completions and Monitoring Technology, or equivalent.

The packers will be 9.625-in x 5.5-in 22Cr or better Feed Through Premier Packers, or equivalent. A feed-through packer allows for control lines to pass through the packer(s) from one zone to another, which will be required for the hydraulic sliding sleeve actuator line and the pressure data cables. Packer specifications are provided in **Table 4-6**.

Directly below the upper packer and in line with the tubing string will be a Dual SureSENS Electronic Pressure Gauge (upper packer only), or equivalent, followed by a hydraulically activated InFORCE HCM-A Sliding Sleeve, or equivalent (well SB-01), or a Chrome-Moly Downshift (CMD)/Chrome-Moly Upshift (CMU) mechanically actuated sliding sleeve, or equivalent (wells SB-02 through SB-05). The hydraulic sliding sleeve will be operated from the surface via a hydraulic control line, which is run on the exterior of the tubing string and ported through both the wellhead and upper packer. Mechanical sliding sleeves will be opened or closed via wireline. The real-time data acquired from the pressure gauge will be transmitted in a tubing encapsulated cable, which is also run on the exterior of the tubing string and ported through the upper packer and wellhead.

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Table 4-5. Tubing Specifications

Tubing String	Depth Interval (Feet BGS)	Tubing Dimensions (Inches)				Weight (lb/ft)	Grade (API)	Design Coupling	Thermal Conductivity (W/mK)	Burst Strength (psia)	Collapse Strength (psia)	Joint Yield Strength (1,000 lbs/ft)	Body Yield Strength (1,000 lbs/ft)
		OD	ID	Drift	Wall Thickness								
Injection tubing	0 – 4,150	5.5	4.892	4.767	0.304	17	22 Cr or better	Premium	14 - 17	7,740	6,390	428	397

Table 4-6. Packer Specifications

Packer Type and Material	Packer Setting Depth Feet (BGS)	Length Feet	Nominal Casing Weight lbs/ft	Packer Main Body Outer Diameter Inches	Packer Inner Diameter Inches
Upper Packer – Baker Hughes Removable CRA Feed Through Premier (Chromium Alloy), or equivalent	3,550	7.5	47 – 53.5	8.310	4.685
Lower Packer – Baker Hughes Removable CRA Feed Through Premier (Chromium Alloy), or equivalent	4,150	7.5	47 – 53.5	8.310	4.685

Packer Type and Material	Tensile Rating psi	Burst Rating psi	Collapse Rating psi	Max. Casing Inner Diameter Inches	Min. Casing Inner Diameter Inches
Upper Packer – Baker Hughes Removable CRA Feed Through Premier (Chromium Alloy), or equivalent	300,000	7,500	7,500	8.681	8.525
Lower Packer – Baker Hughes Removable CRA Feed Through Premier (Chromium Alloy), or equivalent	300,000	7,500	7,500	8.681	8.525

I. Cementing Program

The following section discusses the type, quantity, and grade of cement to be used for each casing string. The placement of cement and the use of specialty casing, float, or cementing equipment is also provided. The cementing of the conductor casing (if needed), surface casing, and long string casing will be in accordance with the requirements of 40 CFR 146.86(b). All cement volume calculations include 30% excess cement to account for borehole variation and to provide sufficient cement volumes to surface.

Casing centralizers will be run as needed to ensure sufficient bond to pipe and borehole. Centralizers will be placed at casing connections or at mid-joint intervals using stop rings. Float shoes and float collars will be run on the lowermost joint of the surface and long string casings. A two-stage cement diverter tool (DV) will be run on the long string casing and placed at 3,000 ft BGS, which is 200 ft above the confining zone. All casing strings run above 3,000 ft BGS will be cemented with a Class A or greater cement and all casing strings run below this depth will be cemented with SLB's EverCRETE CO_2 resistant cement (or equivalent). Cement and cement additives will be compatible with the CO_2 stream and formation fluids from total depth through the confining zone and of sufficient quality and quantity to maintain integrity over the design life of the CO_2 sequestration project. The location and integrity of the cement will be verified with cement bond logs and/or casing inspection logs. Proposed cement types and volumes for each casing string are summarized in **Table 4-7.**

I.1. Conductor Casing Cement

The 20-inch conductor casing will be set at approximately 80 ft BGS and will be driven in place or drilled and cemented. The total depth will be determined at the time of drilling and be sufficient to penetrate any loose or unconsolidated material to ensure the casing is set in competent rock. If drilled, the conductor casing will be cemented with 133 sacks of 15.6 ppg Class A cement. The cement will be pumped through the casing and displaced with fresh water until the required excess cement has reached the surface. The conductor casing cement will be allowed to dry a minimum of 48 hours before commencing further operations.

I.2. Surface Casing Cement

The 13.375-inch surface casing will be set at approximately 2,150 ft BGS. The total depth will be determined at the time of drilling and be sufficient to protect the lowermost USDW. The surface casing will be equipped with a float shoe and a float collar. Centralizers will be placed at the midpoint of the first five (5) casing joints and will be placed at every other surface casing collar thereafter until reaching the base of the conductor casing. The surface casing will be cemented in one stage with 1,753 sacks of 15.6 ppg Class A cement. The cement will be pumped through the casing and displaced with drilling fluid until the required excess cement has reached the surface. The surface casing cement will be allowed to dry a minimum of 24 hours before commencing further operations. A radial bond log will be run from total depth to surface to verify adequate placement of cement.

I.3. Long String Casing Cement

The 9.625-inch-long string casing will be set approximately 15 feet below the Paluxy Formation and in the Glen Rose Formation at 5,350 ft BGS. The long string casing will be equipped with a float shoe and a float collar. Centralizers will be placed at the midpoint of the first two (2) casing joints and will be placed at every other casing collar thereafter until reaching the base of the surface casing. A DV tool will be installed in the long string casing at 3,000 ft BGS. This will allow for a two-stage cement operation, with a CO_2 resistant cement blend pumped below the DV tool and a Class A cement blend pumped above the DV tool. The long string casing below the DV tool will be cemented in one stage with 1,120 sacks of 15.82 ppg EverCRETE, or equivalent, cement (the rat hole in the Glenn Rose Formation will also be cemented in this stage). The cement will be pumped through the long string casing and displaced with drilling fluid until the cement reaches the depth of the DV tool. The long string casing above the DV tool will be cemented in one stage with 931 sacks of 15.6 ppg Class A cement. This cement will be pumped through the DV tool ports and displaced with drilling fluid until the required excess cement has reached the surface. The long string casing cement will be allowed to dry a minimum of 72 hours before commencing further operations. A radial bond log and/or ultrasonic imaging tool (USIT) will be run from total depth to surface to verify adequate placement of cement.

Table 4-7. Cementing Program

Casing String	Casing Depth Interval Feet	Borehole Diameter Inches	Casing Outside Diameter Inches	Cement Interval Feet	Cement
Conductor	0 – 80	26	20	0 – 80	Class A with 2% $CaCl_2$ (calcium chloride) and 0.25 lb/sack cell flake; 15.6 lb/gal; yield 1.18 ft^3/sack; 133 sacks
Surface	0 – 2,150	17.5	13.375	0 – 2,150	Class A with 2% $CaCl_2$ (Calcium Chloride) and 0.25 lbs/sack cell flake; cement weight 15.6 lb/gal; yield 1.18 ft^3/sack; quantity: 1,753 sacks
Stage 1 Long string Below DV Tool	0 – 5,350	12.25	9.625	3,000 – 5,350	EverCRETE CO_2-resistant cement (or similar); weight 15.82 lb/gal; yield 1.12 ft^3/sack; quantity 1,120 sacks
Stage 2 Long string Above DV Tool				0 – 3,000	Class A with 2% $CaCl_2$ (calcium chloride) and 0.25 lb/sack cell flake; weight 15.6 lb/gal; yield 1.18 ft^3/sack; quantity 931 sacks

J. Perforations

The long string casing will be perforated across the Woodbine and Paluxy Formations with deep-penetrating shaped charges. Due to the installation of fiber optics, a fiber optic identification tool will be run downhole prior to perforating and oriented perforations will be used to avoid damage to the fiber optic cable. The perforation intervals will be determined by post-drilling geologic analysis (well logs, core analyses, fluid testing, drill stem test, etc.). The estimated perforation intervals for the Woodbine Formation will be set between 3,570-4,100 feet BGS, and the estimated perforation intervals for the Paluxy Formation will be set between 5,070-5,283 feet BGS. Estimated perforation interval depths for SB-01 and SB-05 are listed in **Table 4-8**. Perforation interval depths for wells SB-02, SB-03, and SB-04 will be adjusted for local geology as needed.

Table 4-8. Injection Zone Perforation Intervals (SB-01 and SB-05)

Perforated Zones	Top of Perforation (BGS, ft)	Base of Perforation (BGS, ft)	Mid-point of Perforation (BGS, ft)	Perforation Interval (ft)
Upper Injection Zone (Upper Woodbine)	3,570	3,680	3,625	110
Upper Injection Zone (Lower Woodbine)	3,865	4,100	3,982	235
Lower Injection Zone (Paluxy)	5,070	5,283	5,177	213

K. Annulus Fluid

The annular space above the top packer and between the 9.625-inch-long string casing and the 5.5-inch injection tubing will be filled with a mixture of fresh water, corrosion inhibitor, biocide, and oxygen scavenger. This fluid will provide a positive pressure differential to stabilize the tubing and will inhibit corrosion of the casing and tubing. The additive hydrostatic pressure of the annulus fluid column will also ensure that the downhole annular pressure will be greater than injection pressure. Annular fluid pressure at the surface will be controlled to remain at or above 1,375 psia during injection operations (see **Section 7** of the **Testing and Monitoring Plan** for a full description of the injection well annulus monitoring system).

L. Wellhead and Tree

The wellhead will consist of the following components, from base to top:

- 13.625-inch 5,000 psia X 13.375-inch slip-on-weld (SOW) casing head assembly
- 13-inch x 9.625-inch slips with packoff
- 13.625-inch 5,000 psia x 13.625-inch 5,000 psia double-studded adapter (DSA) with control line port
- 13.625-inch 5,000 psia x 11-inch 5,000 psia tubing spool
- 11-inch x 5.5-inch tubing hanger
- 11-inch x 5.5-inch 5,000 psia seal flange
- 5-inch 5,000 psia Master valve

- 5-inch 5,000 psia Hydraulic Surface Safety Valve (SSV)
- 5-inch 5,000 psia x 5-inch 5,000 psia Studded Tee Joint
- 5-inch 5,000 psia Swab valve
- 5-inch 5,000 psia tree cap flange

The wellhead and tree will be composed of materials compatible with the injection fluid. Critical components that encounter the CO_2 injection fluid will be made of corrosion-resistant alloy, such as stainless steel or a chromium/steel mixture **(Table 4-9 and 4-10)**. Materials that do not contact the injection fluid, such as the surface casing and shallow section of the long-string casing, will be manufactured from carbon steel. The final wellhead and tree material specifications may vary from the information provided at permit submittal, but designs will meet or exceed API requirements. An illustration of the wellhead and tree is provided in **Figure 4-3.** The flow line leading to the wellhead and tree will be equipped with an automatic shutoff valve as required in 40 CFR 146.88(e). Pressure monitoring gauges will be installed on the wellhead that correspond to each annulus.

Table 4-9. Materials Specification of Wellhead and Tree

Section/Assy	Component	Material Class
X-Mas Tree Assy f/ 5-12" Tubing	Blind Flange 5-1/8" 5M x ½" LP tap	HH
	Tee 5-1/8" 5M run x 5-1/8" 5M Outlet	HH
	Hydraulic and Manual Valves 5-1/8" 5M	HH
	Tubing Head Adapter 11" 5M btm x 5-1/8" 5M top w/ Cladded wetted surfaces	EE
	Tubing Hanger 11" x 5-1/2" Tubing, Ported f/ 2 Hyd lines & 3 Gauge Lines	HH
Tubing Head Assy f/ 9-5/8" Production Casing	Tubing Head 13-5/8" 5M btm x 11" 5M top	AA
	Valves 2-1/6" 5M	DD
	DSA 13-5/8" 5M btm & top w/ Gauge Line Port	DD
	9-5/8" Primary Seal Plate Ported f/ Gauge Line	DD
	9-5/8" Casing Hanger Ported f/ Gauge Line	DD
Casing Head Assembly f/13-3/8" Surface Csg	Casing Head 13-5/8" 5M w/ Base Plate	AA
	Valve 2-1/6" 5M	DD

Table 4-10. Material Classes from API 6A (Specification for Wellhead and Tree Equipment)

API Material Class	Body, Bonnet, End & Outlet Connections	Pressure Controlling Parts, Stems & Mandrel Hangers
AA – General Service	Carbon or alloy steel	Carbon or low-alloy steel
BB – General Service	Carbon or low-alloy steel	Stainless steel
CC – General Service	Stainless steel	Stainless steel
DD – Sour Service [a]	Carbon or low-alloy steel [b]	Carbon or low-alloy steel [b]
EE – Sour Service [a]	Carbon or low-alloy steel [b]	Stainless steel [b]
FF – Sour Service [a]	Stainless steel [b]	Stainless steel [b]
HH – Sour Service [a]	Corrosion-resistant alloy [b]	Corrosion-resistant alloy [b]

Source: Cameron Surface Systems, Houston, Texas
(a) As defined by National Association of Corrosion Engineers (NACE) Standards MR075
(b) In compliance with NACE Standard MR0175

M. Injection Well Construction Diagrams

The proposed well construction and wellhead diagrams are provided in **Figures 4-1 through 4-3**.

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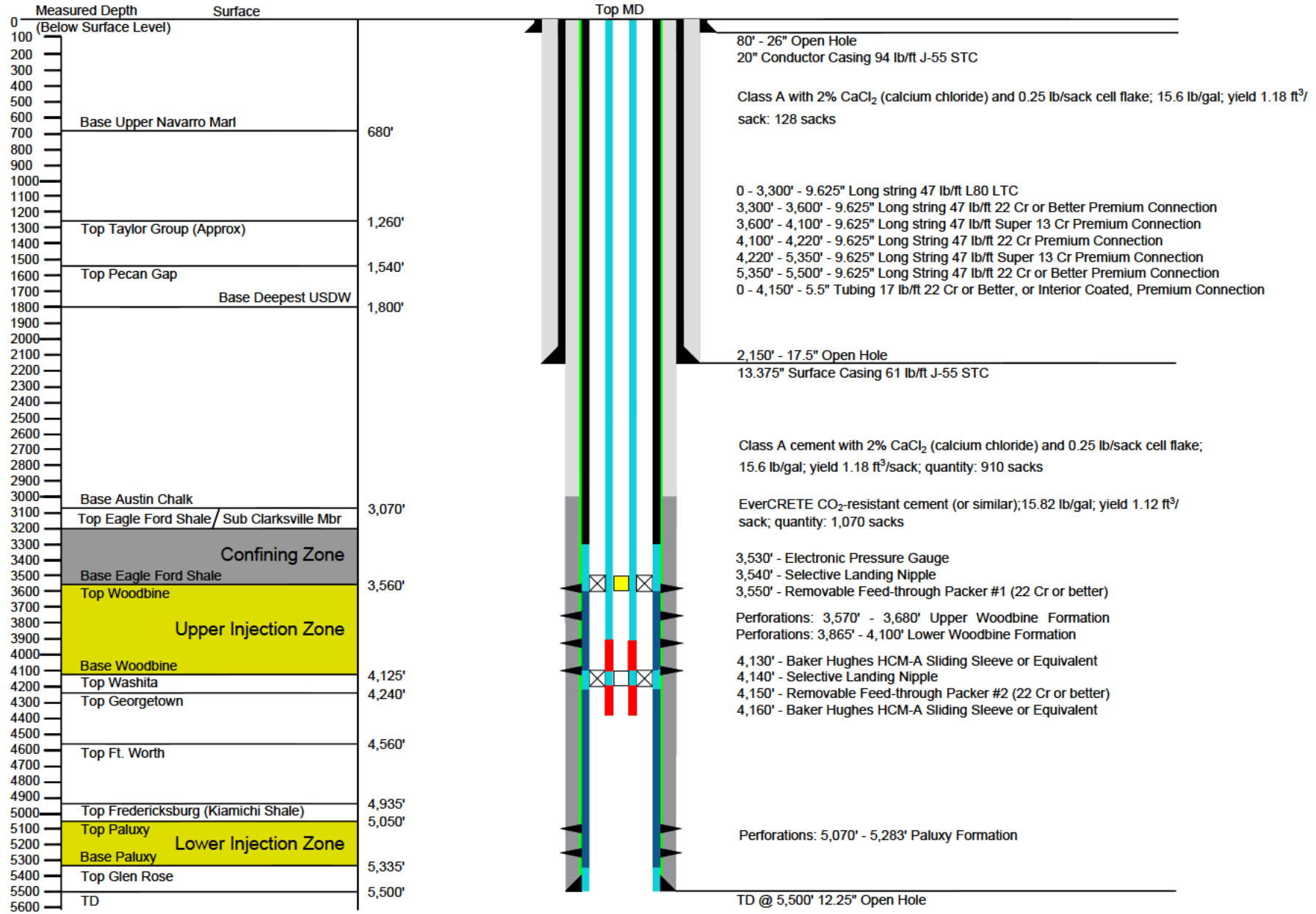
FIGURES



Legend

- Sliding Sleeve
- DAS/DTS Fiber Optic Cable
- Electronic P/T Gauge
- Hydraulic Packer
- Perforations

Cement
- Class A
- EverCRETE

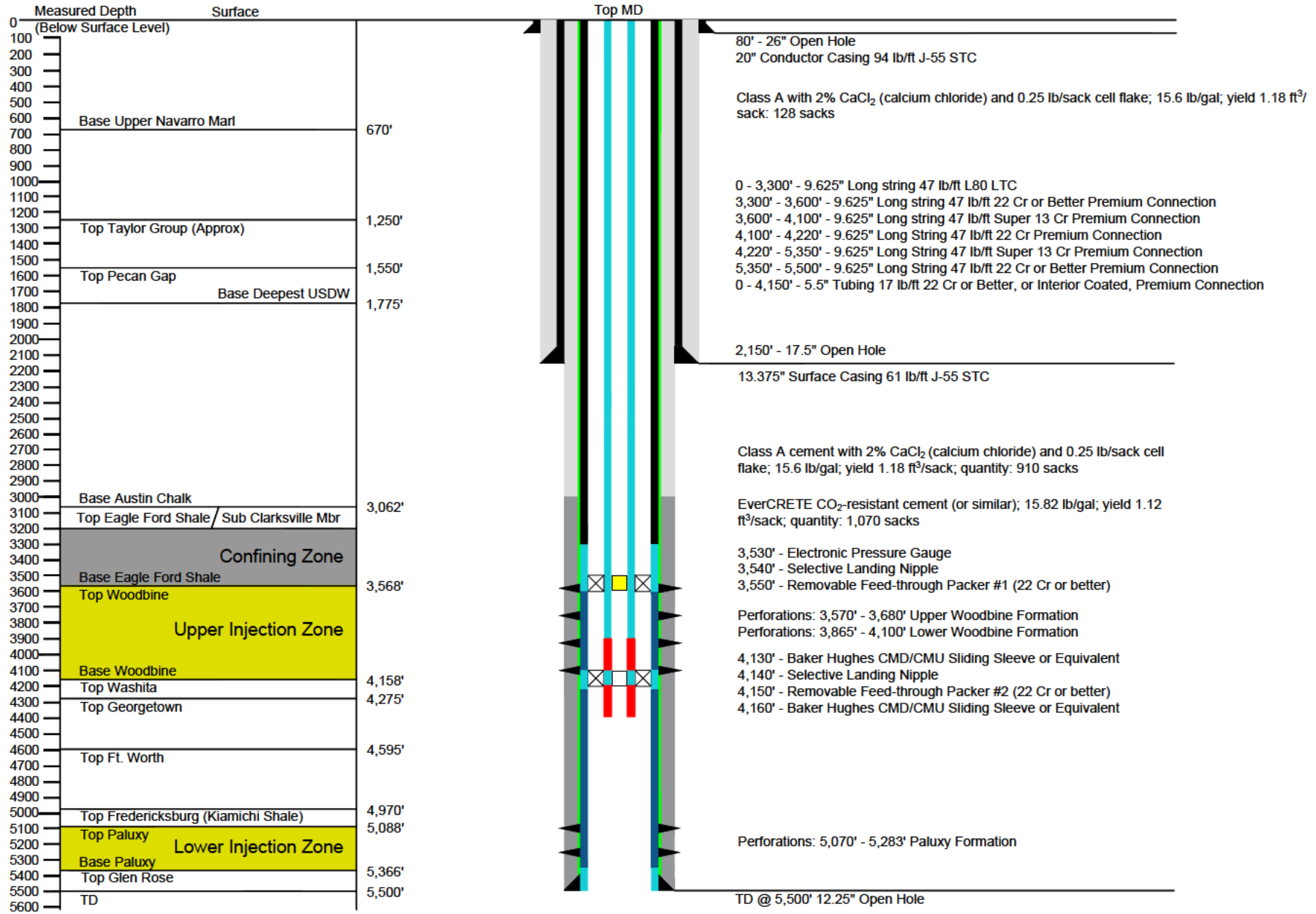
Long String Casing
- L-80
- Super 13 Cr
- 22 Cr or Better

Rock Type
- Injection Zone
- Confining Zone

FIGURE 4-1
PROPOSED WELLBORE DIAGRAM - SB-01 HYDRAULIC SLIDING SLEEVES
SUGARBERRY CCS HUB
SUGARBERRY CCS, LLC
HOPKINS COUNTY, TEXAS

SCS ENGINEERS

Wichita, KS | May 2025



Legend

- Sliding Sleeve
- DAS/DTS Fiber Optic Cable
- Electronic P/T Gauge
- Hydraulic Packer
- Perforations

Cement
- Class A
- EverCRETE

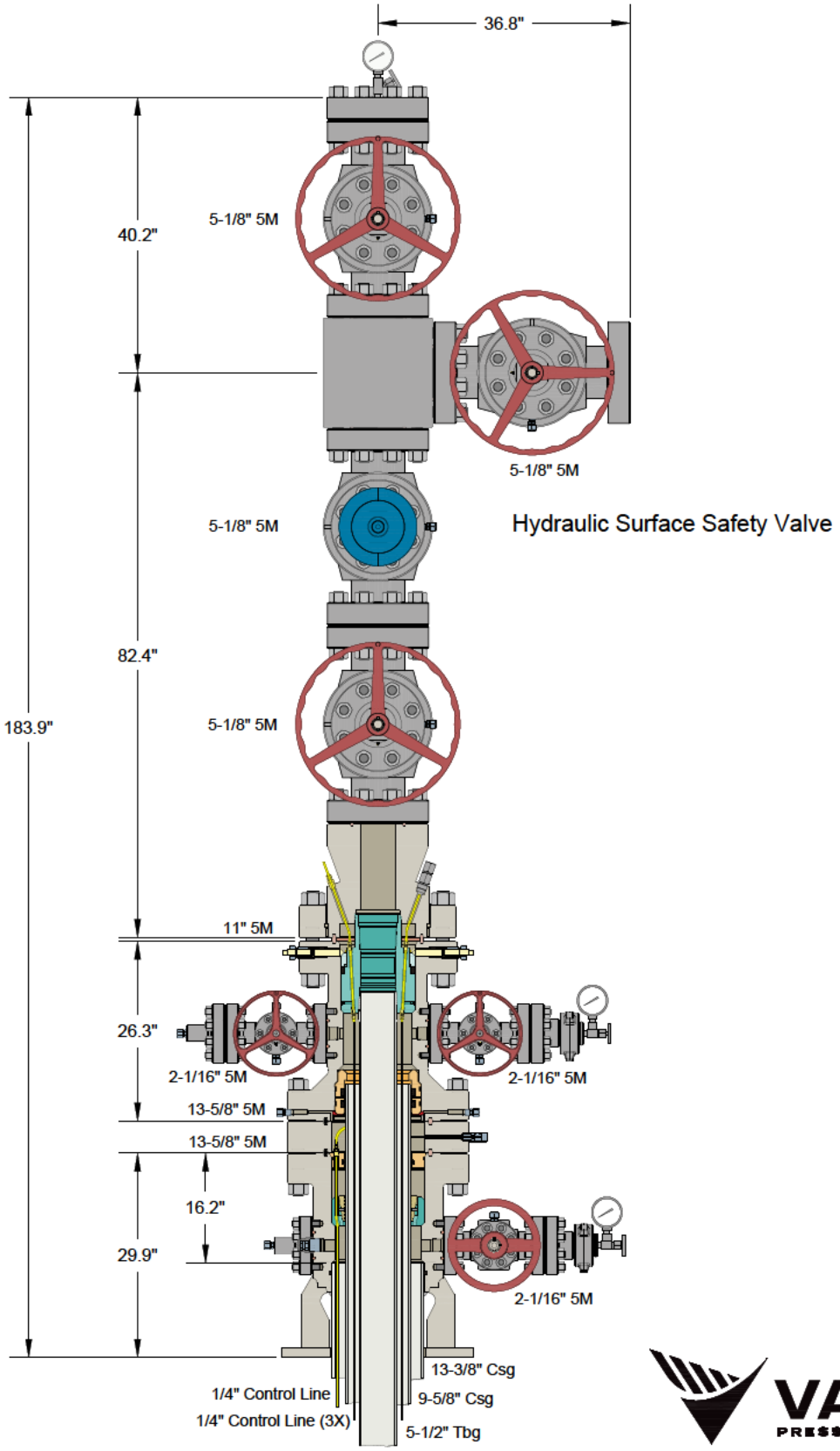
Long String Casing
- L-80
- Super 13 Cr
- 22 Cr or Better

Rock Type
- Injection Zone
- Confining Zone

FIGURE 4-2
PROPOSED WELLBORE DIAGRAM - SB-05 MECHANICAL SLIDING SLEEVES
SUGARBERRY CCS HUB
SUGARBERRY CCS, LLC
HOPKINS COUNTY, TEXAS

SCS ENGINEERS

Wichita, KS | May 2025



VAULT PRESSURE CONTROL

13-3/8" X 9-5/8" X 5-1/2" 5M Conventional Wellhead Assembly, with T-EBS Tubing Head, T-M68-CCL Tubing Hanger and Adapter Flange, with 9-5/8" W1-CCL and DSA-CCL

FIGURE 4-3
WELLHEAD AND CHRISTMAS TREE DESIGN
SUGARBERRY CCS HUB
SUGARBERRY CCS, LLC
HOPKINS COUNTY, TEXAS

SCS ENGINEERS

Wichita, KS	May 2025

APPENDIX A

Calculation Summary
06-0-2 Super13Cr Calculation

Unit Set: Custom

Automatic Chemistry Model
,Aqueous (H+ ion) Databanks:
,,Corrosion (AQ)
,,Aqueous (H+ ion)
,Second Liquid phase
,Redox selected
,Using K-fit Polynomials
,,T-span: 25.0 - 225.0
,,P-span: 1.0 - 1500.0

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Super13Cr stainless steel

Flow Type: Complete Agitation
Scales included - passivating films included.

Calc. elapsed time: 9.839 sec
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mg/L,mg/L
H2O,9.69558e5,9.66585e5
BaCl2,0.173601,0.173601
CaCl2,1221.60,1221.60
CaO,2649.52,2649.52
CO2,1109.73,1109.73
FeCl2,96.6163,96.6163
KCl,198.176,198.176
MgCl2,8044.95,8044.95
NaCl,69850.2,69850.2
SO3,3271.33,3271.33
SrCl2,88.8451,88.8451
BaSO4,195.123,195.123
CaCO3,1214.83,1214.83
FeCO3,212.302,212.302
SrSO4,395.669,395.669

Calculated Rates

Corrosion Rate,1.29625e-3,mm/yr
Corrosion Potential,-0.375137,V (SHE)
Repassivation Potential*,-0.133278,V (SHE)
Corrosion Current Density,1.19447e-3,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaCO3 (Calcite),1.0
,FeCO3 (Siderite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.619503
,CaSO4.0.5H2O (Bassanite),0.264953
,CaSO4.2H2O (Gypsum),0.936165
,CaSO4 (Anhydrite),0.992812
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,1.00065,L
Temperature,43.0000,°C
Pressure,1530.00,psia

Aqueous Properties
pH,5.84280,
Ionic Strength (x-based),0.0289286,mol/mol
Ionic Strength (m-based),1.68919,mol/kg
ORP,-0.0708086,V (SHE)
Osmotic Pressure,1100.66,psia
Specific Electrical Conductivity,1.52175e5,µmho/cm
"Electrical Conductivity, molar",0.0106737,m2/ohm-mol
"Viscosity, absolute",0.753014,cP
"Viscosity, relative",1.21772,
Standard Liquid Volume,1.01667,L
"Volume, Std. Conditions",0.995867,L
"Total Dissolved Solids, Estimated",86624.0,mg/L
Hardness,14572.2,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,4.71394e-4,L

Thermodynamic Properties
 ,Unit,Total,Aqueous,Solid
Density,g/ml,1.05513,1.05400,3.19028

Enthalpy,J,-1.59255e7,-1.59088e7,-16657.8

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
Mole (True),56.4817,56.4677,0.0140297
Mole (App),55.1169,55.1029,0.0140297
,g,g,g
Mass,1055.81,1054.12,1.69865
,L,L,cm3
Volume,1.00065,1.00011,0.532446

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
CaCO3 (Calcite),1.00000,0.0712116
BaSO4 (Barite),1.00000,1626.71
FeCO3 (Siderite),1.00000,0.281937
SrSO4 (Celestine),1.00000,2.97279
CaSO4 (Anhydrite),0.992812,1.15320
CaSO4.2H2O (Gypsum),0.936165,1.05145
CaCO3 (Aragonite),0.619503,0.0441157
Fe2O3 (Hematite),0.614309,4.82516e-5
FeO(OH) (Lepidocrocite),0.608615,5.34790e-3
CaSO4.0.5H2O (Bassanite),0.264953,0.305179
SrCO3 (Strontianite),0.0658101,0.0119942
NaCl (Halite),0.0214673,0.0208317
NaHCO3 (Nahcolite),9.67155e-3,0.0224588
Fe3O4 (Magnetite),8.03798e-3,2.02152e-9
Na2SO4 (Thenardite),5.19801e-3,5.27945e-3
MgCO3 (Magnesite),3.13738e-3,1.80700e-4
MgSO4.7H2O (Epsomite),2.94357e-3,2.45836e-3
MgCO3.3H2O (Nesquehonite),1.68840e-3,9.24622e-5
KCl (Sylvite),1.64300e-4,1.59495e-4
FeSO4.7H2O (Melanterite),1.43439e-4,5.86409e-4
Sr(HCO3)2,7.36530e-5,1.16247e-3

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mg/L,mg/L,mg/L
H2O,9.66424e5,9.66938e5,
Cl-1,49332.2,49358.4,
Na+1,27326.0,27340.6,
SO4-2,2934.56,2936.13,
Ca+2,2395.62,2396.9,

Mg+2,1795.16,1796.11,
CaCO3 (Calcite),939.331,2.11882,937.713
MgSO4,618.109,618.438,0.0
HCO3-1,610.142,610.467,
NaSO4-1,499.663,499.929,
MgHCO3+1,468.913,469.163,
CO2,434.737,434.968,
SrSO4 (Celestine),340.259,8.45492,331.986
FeCO3 (Siderite),233.661,0.329226,233.456
NaHCO3 (Nahcolite),199.957,200.063,0.0
BaSO4 (Barite),195.198,,195.302
CaSO4 (Anhydrite),165.139,165.227,0.0
K+1,100.806,100.86,
Sr+2,75.5373,75.5775,
Fe+2,32.2194,32.2365,
KSO4-1,8.92865,8.9334,
CaHCO3+1,1.96779,1.96884,
KCl (Sylvite),1.03693,1.03748,0.0
MgCO3 (Magnesite),0.45087,0.45111,0.0
CO3-2,0.249586,0.249719,
HSO4-1,0.0802834,0.0803262,
NaCO3-1,0.0742491,0.0742886,
FeCl+1,0.054175,0.0542038,
Ba+2,0.0507904,0.0508174,
CaCl+1,0.0450799,0.0451039,
BaCl(+1),0.0230396,0.0230519,
FeHCO3+1,0.0191221,0.0191323,
FeOH+1,0.0150615,0.0150695,
MgOH+1,6.89614e-3,6.89981e-3,
BaHCO3+1,2.04215e-3,2.04324e-3,
H+1,1.67583e-3,1.67672e-3,
OH-1,6.03533e-4,6.03855e-4,
CaOH+1,5.02635e-4,5.02902e-4,
FeCl2 (Lawrencite),1.47968e-4,1.48047e-4,0.0
Fe(CO3)2-2,8.12707e-5,8.1314e-5,
SrOH+1,3.92907e-6,3.93117e-6,
KHSO4 (Mercallite),2.27296e-6,2.27417e-6,0.0
BaCO3 (Witherite),1.36218e-6,1.3629e-6,0.0
Fe(OH)3 (Bernalite),4.31054e-7,4.31284e-7,0.0
Fe(OH)2+1,7.22791e-8,7.23176e-8,
HCl,6.94225e-8,6.94594e-8,
FeHS+1,1.56314e-8,1.56397e-8,
H2S,9.06131e-9,9.06614e-9,
FeOH+2,4.78088e-9,4.78342e-9,
HS-1,1.94047e-9,1.94151e-9,
HSO3-1,1.4426e-9,1.44336e-9,
Fe(OH)4-1,1.07823e-9,1.0788e-9,
H2,8.70372e-10,8.70835e-10,
SO3-2,3.89554e-10,3.89762e-10,
BaOH+1,2.64919e-10,2.6506e-10,
Fe+3,1.31864e-11,1.31934e-11,
S2O3-2,9.89335e-12,9.89861e-12,
NaS2O3-1,6.57258e-12,6.57608e-12,
HFeO2-1,1.56529e-12,1.56612e-12,

FeCl2+1,5.5679e-13,5.57086e-13,
CaCl2 (Hydrophilite),3.55293e-13,3.55482e-13,0.0
FeCl+2,1.66088e-13,1.66177e-13,
FeSO4+1,1.60046e-13,1.60132e-13,
SO2,9.99863e-14,1.0004e-13,
KS2O3-1,4.98155e-14,4.9842e-14,
FeCl3 (Molysite),1.48554e-14,1.48633e-14,0.0
S-2,2.13427e-15,2.1354e-15,
FeCl4-1,3.14286e-16,3.14453e-16,
H2SO4,2.08774e-18,2.08886e-18,
FeS(HS)-1,1.52284e-20,1.52365e-20,
S2-2,1.43176e-21,1.43252e-21,
SO3,2.77804e-22,2.77952e-22,
Fe2(OH)2+4,1.69176e-24,1.69266e-24,
S2O5-2,4.73798e-27,4.7405e-27,
S2O6-2,7.94006e-28,7.94428e-28,
S3-2,2.73379e-28,2.73525e-28,
S2O4-2,1.42949e-28,1.43025e-28,
Na2S2O4,6.78984e-30,6.79345e-30,0.0
S4-2,2.87115e-35,2.87267e-35,
S5-2,1.75346e-42,1.75439e-42,
FeO4-2,1.06634e-50,1.0669e-50,
HSO5-1,7.14484e-51,7.14864e-51,
S5O6-2,7.8012e-53,7.80536e-53,
O2,9.70262e-59,9.70778e-59,
S2O8-2,7.81073e-63,7.81489e-63,
Total (by phase),1.05513e6,1.054e6,1698.46

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Aqueous,Solid
,mg/L,mg/L,mg/L
H(+1),1.08162e5,1.0822e5,0.0
K(+1),103.933,103.988,0.0
Na(+1),27477.3,27491.9,0.0
Ba(+2),114.926,0.0705549,114.916
Ca(+2),2821.18,2447.19,375.489
Fe(+2),144.906,32.4492,112.534
Mg(+2),2053.67,2054.77,0.0
Fe(+3),2.74342e-7,2.74488e-7,0.0
O(-2),8.62808e5,8.62552e5,715.631
Cl(-1),49332.7,49359.0,0.0
C(+4),470.664,334.18,136.735
S(+4),7.2665e-10,7.27037e-10,0.0
S(+6),1406.06,1322.02,84.788
S(-2),1.60436e-8,1.60521e-8,0.0
S(+2),8.79909e-12,8.80378e-12,0.0
Sr(+2),237.846,79.6106,158.362
H(0),8.70372e-10,8.70835e-10,0.0
O(0),9.70262e-59,9.70778e-59,0.0
S(+8),2.02622e-51,2.0273e-51,0.0

S(+3),7.40503e-29,7.40897e-29,0.0
S(+5),3.18002e-28,3.18172e-28,0.0
S(+7),2.60722e-63,2.60861e-63,0.0
Fe(+6),4.96908e-51,4.97172e-51,0.0
S(0),7.1588e-22,7.16261e-22,0.0

Element Distribution

 ,Total,Total,Aqueous,Solid
,mol,mole %,% of Total,% of Total
H(+1),107.376,65.404,100.0,0.0
K(+1),2.65996e-3,1.62021e-3,100.0,0.0
Na(+1),1.19596,0.72847,100.0,0.0
Ba(+2),8.37399e-4,5.10069e-4,0.061359,99.9386
Ca(+2),0.0704376,0.0429043,86.6974,13.3026
Fe(+2),2.59638e-3,1.58148e-3,22.3813,77.6187
Mg(+2),0.0845505,0.0515006,100.0,0.0
Fe(+3),4.91556e-12,2.99412e-12,100.0,0.0
O(-2),53.9624,32.8691,99.9171,0.082898
Cl(-1),1.39239,0.848122,100.0,0.0
C(+4),0.039211,0.0238838,70.964,29.036
S(+4),2.26757e-14,1.3812e-14,100.0,0.0
S(+6),0.0438772,0.0267261,93.973,6.02698
S(-2),5.00652e-13,3.04952e-13,100.0,0.0
S(+2),2.74583e-16,1.67251e-16,100.0,0.0
Sr(+2),2.71627e-3,1.65451e-3,33.4536,66.5464
H(0),8.64047e-13,5.263e-13,100.0,0.0
O(0),6.06828e-63,3.69625e-63,100.0,0.0
S(+8),6.32298e-56,3.85139e-56,100.0,0.0
S(+3),2.3108e-33,1.40753e-33,100.0,0.0
S(+5),9.92351e-33,6.04452e-33,100.0,0.0
S(+7),8.13604e-68,4.95575e-68,100.0,0.0
Fe(+6),8.9034e-56,5.42316e-56,100.0,0.0
S(0),2.23396e-26,1.36073e-26,100.0,0.0

Calculation Summary
06-0-5 22Cr Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE-SRK (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE-SRK (H3O+ ion)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

MSE-SRK was not designed to work with these components. The results may be in error.
,> FeS2

,> CO2S

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2205

Flow Type: Complete Agitation
Scales included - passivating films included.

The Corrosion databank is not selected and is usually required.
Please add the Corrosion databank unless you know it's not needed.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mg/L,mg/L
H2O,9.69558e5,9.68662e5
BaCl2,0.173601,0.173601
CaCl2,1221.60,1221.60
CaO,2649.52,2649.52
CO2,1109.73,1109.73
FeCl2,96.6163,96.6163
KCl,198.176,198.176
MgCl2,8044.95,8044.95

NaCl,69850.2,69850.2
SO3,3271.33,3271.33
SrCl2,88.8451,88.8451
BaSO4,195.123,195.123
CaCO3,1214.83,1214.83
FeCO3,212.302,212.302
SrSO4,395.669,395.669

Calculated Rates

Corrosion Rate,2.07625e-4,mm/yr
Corrosion Potential,-0.376233,V (SHE)
Repassivation Potential*,-1.27801e-3,V (SHE)
Corrosion Current Density,1.96637e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaCO3 (Calcite),1.0
,FeCO3 (Siderite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.757432
,CaSO4.0.5H2O (Bassanite),0.132193
,CaSO4.2H2O (Gypsum),0.722108
,CaSO4 (Anhydrite),0.789129
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,1.00065,L
Temperature,43.0000,°C
Pressure,1530.00,psia

Liquid 1 Properties
pH,5.88135,
Ionic Strength (x-based),0.0288031,mol/mol
Ionic Strength (m-based),1.68150,mol/kg
Dielectric Constant,55.8822,
ORP,-0.0742417,V (SHE)
Osmotic Pressure,1058.00,psia
Specific Electrical Conductivity,1.51059e5,µmho/cm
"Viscosity, absolute",0.753614,cP
Thermal Conductivity,540.663,cal/hr m °C
Surface Tension,0.0735089,N/m
Standard Liquid Volume,1.01862,L
"Volume, Std. Conditions",0.997009,L

"Total Dissolved Solids, Estimated",86156.9,mg/L
Hardness,14284.4,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,6.05294e-4,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid
Density,g/ml,1.05721,1.05587,3.12736
Enthalpy,J,-1.59592e7,-1.59386e7,-20569.0

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
Mole (True),56.5968,56.5797,0.0171234
Mole (App),55.2292,55.2120,0.0171234
,g,g,g
Mass,1057.90,1055.86,2.03649
,L,L,cm3
Volume,1.00065,0.999994,0.651186

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,1098.54
FeCO3 (Siderite),1.00000,853.641
CaCO3 (Calcite),1.00000,75.1344
SrSO4 (Celestine),1.00000,5.36388
CaSO4 (Anhydrite),0.789129,0.965686
CaCO3 (Aragonite),0.757432,56.9092
CaSO4.2H2O (Gypsum),0.722108,0.882908
H2O,0.630484,0.630212
CaSO4.0.5H2O (Bassanite),0.235603,0.288254
CaSO4.0.5H2O (Bassanite),0.132193,0.161734
SrCO3 (Strontianite),0.0714675,23.5363
Fe2O3 (Hematite),0.0642946,3.92935e5
NaCl (Halite),0.0184516,0.0183911
FeO(OH) (Goethite),0.0176966,43.7388
NaCl.2H2O (hydrohalite),0.0128650,0.0128117
NaHCO3 (Nahcolite),8.91457e-3,0.0231988
Na2SO4.CaSO4 (Glauberite),5.24070e-3,6.78131e-3
Na2SO4 (Thenardite),2.46780e-3,2.60943e-3
Na2SO4.10H2O (Mirabilite),1.80666e-3,1.90212e-3
MgCO3,1.45817e-3,0.0936359
Fe(OH)3 (Bernalite),1.14357e-3,2.82522
Na2SO4.5CaSO4.3H2O,6.06725e-4,1.75835e-3
MgSO4.7H2O (Epsomite),4.41716e-4,4.60589e-4
MgSO4.6H2O (Hexahydrite),3.00885e-4,3.13876e-4
MgSO4.12H2O,1.72244e-4,1.79216e-4

Na2SO4,1.65133e-4,1.74611e-4
MgSO4.5H2O (Pentahydrite),1.48675e-4,1.55162e-4
KCl (sylvite),1.22437e-4,1.22055e-4
Fe3O4 (Magnetite),2.00222e-5,1.00093e6
BaCO3 (Witherite),1.23565e-5,0.833419
Fe(OH)2 (Amakinite),2.60129e-6,0.0212688
Fe0.947O (Wustite),1.91690e-6,8.56804e-3
Mg(OH)2 (Brucite),1.22764e-6,7.55064e-4
FeS2 (Pyrite),9.19122e-8,0.0409511
FeS (Pyrrhotite),4.13634e-8,8.26235e-3
Na2CO3.MgCO3 (Eitelite),2.62454e-8,1.09414e-4
FeS2(marcasite) (Marcasite),2.57884e-8,0.0114899
MgFe2O4 (Magnesioferrite),1.59405e-9,5.99447
FeS (Mackinawite),8.59962e-10,1.71778e-4
CaFe2O4,1.77228e-12,7.79805e-3

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid
,mg/L,mg/L,mg/L
H2O,9.6855e5,9.69181e5,0.0
Cl-1,49332.6,49364.7,
Na+1,27309.1,27326.9,
SO4-2,2920.9,2922.81,
Ca+2,2205.51,2206.95,
Mg+2,1875.13,1876.35,
CaCO3 (Calcite),1229.43,2.83267,1227.4
NaMgSO4+1,1048.48,1049.16,
HCO3-1,758.939,759.434,
CO2,525.116,525.458,
CaSO4 (Anhydrite),418.81,419.082,0.0
SrSO4 (Celestine),402.252,2.5482,399.966
FeCO3 (Siderite),213.745,,213.884
BaSO4 (Barite),195.129,,195.256
K+1,102.939,103.006,
FeCO2+2,67.4114,67.4553,
Sr+2,45.9658,45.9957,
Fe+2,4.14836,4.15106,
KMgSO4+1,4.05583,4.05847,
MgCO3,0.488133,0.488451,0.0
CO3-2,0.344392,0.344617,
CaCl2 (Hydrophilite),0.205223,0.205357,0.0
MgSO4,0.12761,0.127693,0.0
Ba+2,0.110775,0.110847,
FeH(CO3)2-1,0.0587714,0.0588097,
HSO4-1,0.046301,0.0463311,
H3O+1,0.021695,0.0217091,
FeCl+1,4.77742e-3,4.78053e-3,
MgOH+1,4.57931e-3,4.5823e-3,
FeSO4,3.52318e-3,3.52547e-3,0.0
FeOH+1,1.73358e-3,1.73471e-3,

CaOH+1,9.56172e-4,9.56794e-4,
OH-1,8.04856e-4,8.05381e-4,
Na2SO4.NaHSO4,1.03122e-4,1.03189e-4,0.0
BaCO3 (Witherite),6.47772e-6,6.48194e-6,0.0
SrCO3 (Strontianite),3.38587e-6,3.38808e-6,0.0
SrOH+1,2.43362e-6,2.4352e-6,
FeO+1,1.33379e-7,1.33466e-7,
HFeO2,1.19919e-7,1.19997e-7,
NaOH.Na2SO4,4.05045e-8,4.05309e-8,
FeO,3.31784e-8,3.32e-8,
BaOH+1,8.46353e-9,8.46904e-9,
H2S,7.64048e-9,7.64546e-9,
HCl,5.90055e-9,5.90439e-9,
NaOH,3.93635e-9,3.93892e-9,0.0
HS-1,1.44677e-9,1.44771e-9,
H2,1.03301e-9,1.03368e-9,
HSO3-1,8.89336e-10,8.89915e-10,
FeOH+2,6.79287e-10,6.79729e-10,
NaOHCO3-2,4.70137e-10,4.70443e-10,
SO3-2,2.20285e-10,2.20428e-10,
FeS (Pyrrhotite),1.80087e-10,1.80204e-10,0.0
FeO2-1,7.79088e-11,7.79595e-11,
FeHS+1,4.38134e-11,4.38419e-11,
S2O3-2,4.4855e-12,4.48842e-12,
FeCl+2,2.94926e-12,2.95118e-12,
H2SO4,2.22801e-13,2.22946e-13,
HFeO2-1,1.7019e-13,1.70301e-13,
Fe+3,1.08709e-13,1.0878e-13,
MgCl2,1.02062e-13,1.02128e-13,0.0
SO2,6.4532e-14,6.45741e-14,
FeCl2+1,1.51486e-15,1.51584e-15,
HS2O3-1,5.54835e-17,5.55196e-17,
S-2,1.71135e-17,1.71246e-17,
FeHSO4+2,1.44049e-17,1.44143e-17,
CO2S,2.01443e-19,2.01575e-19,
S2-2,3.37818e-22,3.38038e-22,
H2S2O3,2.87046e-22,2.87233e-22,
S2O5-2,4.78486e-24,4.78797e-24,
Fe2(OH)2+4,2.27069e-25,2.27217e-25,
SO3,1.42893e-26,1.42986e-26,
S2O6-2,1.04394e-28,1.04462e-28,
S3-2,4.68767e-29,4.69072e-29,
S2O4-2,2.19271e-29,2.19414e-29,
S4-2,3.57789e-36,3.58022e-36,
S5-2,1.58799e-43,1.58902e-43,
HSO5-1,2.97327e-51,2.97521e-51,
FeO4-2,4.6279e-52,4.63091e-52,
S5O6-2,4.59796e-54,4.60095e-54,
O2,7.36296e-59,7.36776e-59,
S2O8-2,8.78115e-64,8.78687e-64,
S8 (Sulfur),4.81703e-66,4.82017e-66,0.0
Total (by phase),1.05721e6,1.05586e6,2036.51

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

	Total	Liquid-1	Solid
	mg/L	mg/L	mg/L
H(+1)	1.08398e5	1.08468e5	0.0
K(+1)	103.933	104.001	0.0
Na(+1)	27477.3	27495.2	0.0
Ba(+2)	114.926	0.110851	114.89
Ca(+2)	2821.18	2331.53	491.488
Fe(+2)	144.906	41.9009	103.1
Mg(+2)	2053.67	2055.01	0.0
Fe(+3)	1.79622e-7	1.79739e-7	0.0
O(-2)	8.64653e5	8.64346e5	870.119
Cl(-1)	49332.7	49364.8	0.0
C(+4)	470.663	301.5	169.47
S(+4)	4.40011e-10	4.40298e-10	0.0
S(+6)	1406.06	1310.32	96.6491
S(-2)	8.67271e-9	8.67836e-9	0.0
S(+2)	2.56548e-12	2.56715e-12	0.0
Sr(+2)	237.846	47.2113	190.79
H(0)	1.03304e-9	1.03371e-9	0.0
O(0)	7.36296e-59	7.36776e-59	0.0
S(+8)	8.43196e-52	8.43745e-52	0.0
S(+3)	1.09751e-29	1.09822e-29	0.0
S(+5)	4.18103e-29	4.18375e-29	0.0
S(+7)	2.93114e-64	2.93305e-64	0.0
Fe(+6)	2.15658e-52	2.15798e-52	0.0
S(0)	8.50773e-20	8.51327e-20	0.0

Element Distribution

	Total	Total	Liquid-1	Solid
	mol	mole %	% of Total	% of Total
H(+1)	107.607	65.4066	100.0	0.0
K(+1)	2.65996e-3	1.6168e-3	100.0	0.0
Na(+1)	1.19596	0.726937	100.0	0.0
Ba(+2)	8.37399e-4	5.08996e-4	0.0963918	99.9036
Ca(+2)	0.0704376	0.0428141	82.59	17.41
Fe(+2)	2.59638e-3	1.57816e-3	28.897	71.103
Mg(+2)	0.0845505	0.0513923	100.0	0.0
Fe(+3)	3.2184e-12	1.95624e-12	100.0	0.0
O(-2)	54.0777	32.87	99.8994	0.100567
Cl(-1)	1.39239	0.846338	100.0	0.0
C(+4)	0.039211	0.0238336	64.0169	35.9831
S(+4)	1.37309e-14	8.34604e-15	100.0	0.0
S(+6)	0.0438772	0.0266698	93.1307	6.86929
S(-2)	2.70639e-13	1.64502e-13	100.0	0.0
S(+2)	8.00577e-17	4.86614e-17	100.0	0.0
Sr(+2)	2.71627e-3	1.65103e-3	19.8366	80.1634
H(0)	1.0255e-12	6.2333e-13	100.0	0.0
O(0)	4.605e-63	2.79905e-63	100.0	0.0

S(+8),2.63126e-56,1.59936e-56,100.0,0.0
S(+3),3.42486e-34,2.08173e-34,100.0,0.0
S(+5),1.30472e-33,7.93049e-34,100.0,0.0
S(+7),9.14687e-69,5.55974e-69,100.0,0.0
Fe(+6),3.86408e-57,2.3487e-57,100.0,0.0
S(0),2.65491e-24,1.61373e-24,100.0,0.0

Calculation Summary
06-0-6 25Cr Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE-SRK (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE-SRK (H3O+ ion)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

MSE-SRK was not designed to work with these components. The results may be in error.
,> FeS2

,> CO2S

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2507

Flow Type: Complete Agitation
Scales included - passivating films included.

The Corrosion databank is not selected and is usually required.
Please add the Corrosion databank unless you know it's not needed.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mg/L,mg/L
H2O,9.69558e5,9.68662e5
BaCl2,0.173601,0.173601
CaCl2,1221.60,1221.60
CaO,2649.52,2649.52
CO2,1109.73,1109.73
FeCl2,96.6163,96.6163
KCl,198.176,198.176
MgCl2,8044.95,8044.95

NaCl,69850.2,69850.2
SO3,3271.33,3271.33
SrCl2,88.8451,88.8451
BaSO4,195.123,195.123
CaCO3,1214.83,1214.83
FeCO3,212.302,212.302
SrSO4,395.669,395.669

Calculated Rates

Corrosion Rate,2.01744e-4,mm/yr
Corrosion Potential,-0.377194,V (SHE)
Repassivation Potential*,0.299238,V (SHE)
Corrosion Current Density,1.96633e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaCO3 (Calcite),1.0
,FeCO3 (Siderite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.757432
,CaSO4.0.5H2O (Bassanite),0.132193
,CaSO4.2H2O (Gypsum),0.722108
,CaSO4 (Anhydrite),0.789129
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,1.00065,L
Temperature,43.0000,°C
Pressure,1530.00,psia

Liquid 1 Properties
pH,5.88135,
Ionic Strength (x-based),0.0288031,mol/mol
Ionic Strength (m-based),1.68150,mol/kg
Dielectric Constant,55.8822,
ORP,-0.0742417,V (SHE)
Osmotic Pressure,1058.00,psia
Specific Electrical Conductivity,1.51059e5,µmho/cm
"Viscosity, absolute",0.753614,cP
Thermal Conductivity,540.663,cal/hr m °C
Surface Tension,0.0735089,N/m
Standard Liquid Volume,1.01862,L
"Volume, Std. Conditions",0.997009,L

"Total Dissolved Solids, Estimated",86156.9,mg/L
Hardness,14284.4,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,6.05294e-4,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid
Density,g/ml,1.05721,1.05587,3.12736
Enthalpy,J,-1.59592e7,-1.59386e7,-20569.0

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
Mole (True),56.5968,56.5797,0.0171234
Mole (App),55.2292,55.2120,0.0171234
,g,g,g
Mass,1057.90,1055.86,2.03649
,L,L,cm3
Volume,1.00065,0.999994,0.651186

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,1098.54
FeCO3 (Siderite),1.00000,853.641
CaCO3 (Calcite),1.00000,75.1344
SrSO4 (Celestine),1.00000,5.36388
CaSO4 (Anhydrite),0.789129,0.965686
CaCO3 (Aragonite),0.757432,56.9092
CaSO4.2H2O (Gypsum),0.722108,0.882908
H2O,0.630484,0.630212
CaSO4.0.5H2O (Bassanite),0.235603,0.288254
CaSO4.0.5H2O (Bassanite),0.132193,0.161734
SrCO3 (Strontianite),0.0714675,23.5363
Fe2O3 (Hematite),0.0642946,3.92935e5
NaCl (Halite),0.0184516,0.0183911
FeO(OH) (Goethite),0.0176966,43.7388
NaCl.2H2O (hydrohalite),0.0128650,0.0128117
NaHCO3 (Nahcolite),8.91457e-3,0.0231988
Na2SO4.CaSO4 (Glauberite),5.24070e-3,6.78131e-3
Na2SO4 (Thenardite),2.46780e-3,2.60943e-3
Na2SO4.10H2O (Mirabilite),1.80666e-3,1.90212e-3
MgCO3,1.45817e-3,0.0936359
Fe(OH)3 (Bernalite),1.14357e-3,2.82522
Na2SO4.5CaSO4.3H2O,6.06725e-4,1.75835e-3
MgSO4.7H2O (Epsomite),4.41716e-4,4.60589e-4
MgSO4.6H2O (Hexahydrite),3.00885e-4,3.13876e-4
MgSO4.12H2O,1.72244e-4,1.79216e-4

Na2SO4,1.65133e-4,1.74611e-4
MgSO4.5H2O (Pentahydrite),1.48675e-4,1.55162e-4
KCl (sylvite),1.22437e-4,1.22055e-4
Fe3O4 (Magnetite),2.00222e-5,1.00093e6
BaCO3 (Witherite),1.23565e-5,0.833419
Fe(OH)2 (Amakinite),2.60129e-6,0.0212688
Fe0.947O (Wustite),1.91690e-6,8.56804e-3
Mg(OH)2 (Brucite),1.22764e-6,7.55064e-4
FeS2 (Pyrite),9.19122e-8,0.0409511
FeS (Pyrrhotite),4.13634e-8,8.26235e-3
Na2CO3.MgCO3 (Eitelite),2.62454e-8,1.09414e-4
FeS2(marcasite) (Marcasite),2.57884e-8,0.0114899
MgFe2O4 (Magnesioferrite),1.59405e-9,5.99447
FeS (Mackinawite),8.59962e-10,1.71778e-4
CaFe2O4,1.77228e-12,7.79805e-3

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid
,mg/L,mg/L,mg/L
H2O,9.6855e5,9.69181e5,0.0
Cl-1,49332.6,49364.7,
Na+1,27309.1,27326.9,
SO4-2,2920.9,2922.81,
Ca+2,2205.51,2206.95,
Mg+2,1875.13,1876.35,
CaCO3 (Calcite),1229.43,2.83267,1227.4
NaMgSO4+1,1048.48,1049.16,
HCO3-1,758.939,759.434,
CO2,525.116,525.458,
CaSO4 (Anhydrite),418.81,419.082,0.0
SrSO4 (Celestine),402.252,2.5482,399.966
FeCO3 (Siderite),213.745,,213.884
BaSO4 (Barite),195.129,,195.256
K+1,102.939,103.006,
FeCO2+2,67.4114,67.4553,
Sr+2,45.9658,45.9957,
Fe+2,4.14836,4.15106,
KMgSO4+1,4.05583,4.05847,
MgCO3,0.488133,0.488451,0.0
CO3-2,0.344392,0.344617,
CaCl2 (Hydrophilite),0.205223,0.205357,0.0
MgSO4,0.12761,0.127693,0.0
Ba+2,0.110775,0.110847,
FeH(CO3)2-1,0.0587714,0.0588097,
HSO4-1,0.046301,0.0463311,
H3O+1,0.021695,0.0217091,
FeCl+1,4.77742e-3,4.78053e-3,
MgOH+1,4.57931e-3,4.5823e-3,
FeSO4,3.52318e-3,3.52547e-3,0.0
FeOH+1,1.73358e-3,1.73471e-3,

CaOH+1,9.56172e-4,9.56794e-4,
OH-1,8.04856e-4,8.05381e-4,
Na2SO4.NaHSO4,1.03122e-4,1.03189e-4,0.0
BaCO3 (Witherite),6.47772e-6,6.48194e-6,0.0
SrCO3 (Strontianite),3.38587e-6,3.38808e-6,0.0
SrOH+1,2.43362e-6,2.4352e-6,
FeO+1,1.33379e-7,1.33466e-7,
HFeO2,1.19919e-7,1.19997e-7,
NaOH.Na2SO4,4.05045e-8,4.05309e-8,
FeO,3.31784e-8,3.32e-8,
BaOH+1,8.46353e-9,8.46904e-9,
H2S,7.64048e-9,7.64546e-9,
HCl,5.90055e-9,5.90439e-9,
NaOH,3.93635e-9,3.93892e-9,0.0
HS-1,1.44677e-9,1.44771e-9,
H2,1.03301e-9,1.03368e-9,
HSO3-1,8.89336e-10,8.89915e-10,
FeOH+2,6.79287e-10,6.79729e-10,
NaOHCO3-2,4.70137e-10,4.70443e-10,
SO3-2,2.20285e-10,2.20428e-10,
FeS (Pyrrhotite),1.80087e-10,1.80204e-10,0.0
FeO2-1,7.79088e-11,7.79595e-11,
FeHS+1,4.38134e-11,4.38419e-11,
S2O3-2,4.4855e-12,4.48842e-12,
FeCl+2,2.94926e-12,2.95118e-12,
H2SO4,2.22801e-13,2.22946e-13,
HFeO2-1,1.7019e-13,1.70301e-13,
Fe+3,1.08709e-13,1.0878e-13,
MgCl2,1.02062e-13,1.02128e-13,0.0
SO2,6.4532e-14,6.45741e-14,
FeCl2+1,1.51486e-15,1.51584e-15,
HS2O3-1,5.54835e-17,5.55196e-17,
S-2,1.71135e-17,1.71246e-17,
FeHSO4+2,1.44049e-17,1.44143e-17,
CO2S,2.01443e-19,2.01575e-19,
S2-2,3.37818e-22,3.38038e-22,
H2S2O3,2.87046e-22,2.87233e-22,
S2O5-2,4.78486e-24,4.78797e-24,
Fe2(OH)2+4,2.27069e-25,2.27217e-25,
SO3,1.42893e-26,1.42986e-26,
S2O6-2,1.04394e-28,1.04462e-28,
S3-2,4.68767e-29,4.69072e-29,
S2O4-2,2.19271e-29,2.19414e-29,
S4-2,3.57789e-36,3.58022e-36,
S5-2,1.58799e-43,1.58902e-43,
HSO5-1,2.97327e-51,2.97521e-51,
FeO4-2,4.6279e-52,4.63091e-52,
S5O6-2,4.59796e-54,4.60095e-54,
O2,7.36296e-59,7.36776e-59,
S2O8-2,8.78115e-64,8.78687e-64,
S8 (Sulfur),4.81703e-66,4.82017e-66,0.0
Total (by phase),1.05721e6,1.05586e6,2036.51

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

	Total	Liquid-1	Solid
	mg/L	mg/L	mg/L
H(+1)	1.08398e5	1.08468e5	0.0
K(+1)	103.933	104.001	0.0
Na(+1)	27477.3	27495.2	0.0
Ba(+2)	114.926	0.110851	114.89
Ca(+2)	2821.18	2331.53	491.488
Fe(+2)	144.906	41.9009	103.1
Mg(+2)	2053.67	2055.01	0.0
Fe(+3)	1.79622e-7	1.79739e-7	0.0
O(-2)	8.64653e5	8.64346e5	870.119
Cl(-1)	49332.7	49364.8	0.0
C(+4)	470.663	301.5	169.47
S(+4)	4.40011e-10	4.40298e-10	0.0
S(+6)	1406.06	1310.32	96.6491
S(-2)	8.67271e-9	8.67836e-9	0.0
S(+2)	2.56548e-12	2.56715e-12	0.0
Sr(+2)	237.846	47.2113	190.79
H(0)	1.03304e-9	1.03371e-9	0.0
O(0)	7.36296e-59	7.36776e-59	0.0
S(+8)	8.43196e-52	8.43745e-52	0.0
S(+3)	1.09751e-29	1.09822e-29	0.0
S(+5)	4.18103e-29	4.18375e-29	0.0
S(+7)	2.93114e-64	2.93305e-64	0.0
Fe(+6)	2.15658e-52	2.15798e-52	0.0
S(0)	8.50773e-20	8.51327e-20	0.0

Element Distribution

	Total	Total	Liquid-1	Solid
	mol	mole %	% of Total	% of Total
H(+1)	107.607	65.4066	100.0	0.0
K(+1)	2.65996e-3	1.6168e-3	100.0	0.0
Na(+1)	1.19596	0.726937	100.0	0.0
Ba(+2)	8.37399e-4	5.08996e-4	0.0963918	99.9036
Ca(+2)	0.0704376	0.0428141	82.59	17.41
Fe(+2)	2.59638e-3	1.57816e-3	28.897	71.103
Mg(+2)	0.0845505	0.0513923	100.0	0.0
Fe(+3)	3.2184e-12	1.95624e-12	100.0	0.0
O(-2)	54.0777	32.87	99.8994	0.100567
Cl(-1)	1.39239	0.846338	100.0	0.0
C(+4)	0.039211	0.0238336	64.0169	35.9831
S(+4)	1.37309e-14	8.34604e-15	100.0	0.0
S(+6)	0.0438772	0.0266698	93.1307	6.86929
S(-2)	2.70639e-13	1.64502e-13	100.0	0.0
S(+2)	8.00577e-17	4.86614e-17	100.0	0.0
Sr(+2)	2.71627e-3	1.65103e-3	19.8366	80.1634
H(0)	1.0255e-12	6.2333e-13	100.0	0.0
O(0)	4.605e-63	2.79905e-63	100.0	0.0

S(+8),2.63126e-56,1.59936e-56,100.0,0.0
S(+3),3.42486e-34,2.08173e-34,100.0,0.0
S(+5),1.30472e-33,7.93049e-34,100.0,0.0
S(+7),9.14687e-69,5.55974e-69,100.0,0.0
Fe(+6),3.86408e-57,2.3487e-57,100.0,0.0
S(0),2.65491e-24,1.61373e-24,100.0,0.0

Calculation Summary
06-1 Alloy-1 Calculation

Unit Set: Custom

Automatic Chemistry Model
,Aqueous (H+ ion) Databanks:
,,Corrosion (AQ)
,,Aqueous (H+ ion)
,Second Liquid phase
,Redox selected
,Using K-fit Polynomials
,,T-span: 25.0 - 225.0
,,P-span: 1.0 - 1500.0

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Super13Cr stainless steel

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3.1H2O

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,5.33403,5.33403
CO2,0.109039,0.109039
N2,7.77432e-4,7.77432e-4
CO,5.14928e-5,5.14928e-5
O2,2.38930e-6,2.38930e-6
NH3,1.40691e-3,1.40691e-3
CH3OH,5.83154e-4,5.83154e-4
H2S,1.18332e-5,1.18332e-5
SO2,2.22167e-3,2.22167e-3

NO2,2.52557e-5,2.52557e-5
BaCl2,3.19793e-8,3.19793e-8
CaCl2,9.33369e-4,9.33369e-4
CaO,6.11040e-3,6.11040e-3
FeCl2,2.59638e-4,2.59638e-4
KCl,2.65996e-4,2.65996e-4
MgCl2,8.45505e-3,8.45505e-3
NaCl,0.119596,0.119596
SO3,4.07319e-3,4.07319e-3
SrCl2,4.08102e-5,4.08102e-5
BaSO4,8.37079e-5,8.37079e-5
SrSO4,2.30817e-4,2.30817e-4
C6H14O4,1.76328e-5,1.76328e-5

Calculated Rates

Corrosion Rate,7.03717e-4,mm/yr
Corrosion Potential,-0.260145,V (SHE)
Repassivation Potential*,-0.284660,V (SHE)
Corrosion Current Density,6.48462e-4,A/sq-m
Maximum Pit Current Density,0.0240241,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4.2H2O (Gypsum),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.0.5H2O (Bassanite),0.20966
,CaSO4 (Anhydrite),0.843273
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,5.58822,mol
Temperature,80.6085,°F
Pressure,2641.00,psia

Aqueous Properties
pH,3.78737,
Ionic Strength (x-based),0.0288111,mol/mol
Ionic Strength (m-based),1.71435,mol/kg
ORP,0.0267364,V (SHE)
Osmotic Pressure,1472.94,psia
Specific Electrical Conductivity,1.14580e5,µmho/cm
"Electrical Conductivity, molar",4.58645e-3,m2/ohm-mol
"Viscosity, absolute",1.03767,cP

"Viscosity, relative",1.21851,
Standard Liquid Volume,0.104934,L
"Volume, Std. Conditions",0.102328,L
"Total Dissolved Solids, Estimated",86471.8,mg/L
Hardness,14661.0,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,5.01884e-5,L

Second Liquid Properties
Standard Liquid Volume,1.67031e-4,L
"Volume, Std. Conditions",2.49347e-4,L

Thermodynamic Properties
,Unit,Total,Aqueous,Solid,2nd Liquid
Density,g/ml,1.07473,1.07528,3.17463,0.554080
Enthalpy,J,-1.63269e6,-1.62926e6,-1668.63,-1766.18

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid,2nd Liquid
,mol,mol,mol,mol
Mole (True),5.72036,5.71469,1.15155e-3,4.51386e-3
Mole (App),5.58579,5.58013,1.15155e-3,4.51386e-3
,g,g,g,g
Mass,109.794,109.405,0.192998,0.195268
,L,L,cm3,L
Volume,0.102160,0.101746,0.0607938,3.52419e-4

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
S8 (Sulfur),1.00000,1.90212e6
FeS2 (Pyrite),1.00000,6.57954e9
BaSO4 (Barite),1.00000,3573.56
CaSO4.2H2O (Gypsum),1.00000,1.28944
SrSO4 (Celestine),1.00000,4.67214
CaSO4 (Anhydrite),0.843273,1.08969
FeS2(marcasite) (Marcasite),0.260129,1.71153e9
CaSO4.0.5H2O (Bassanite),0.209660,0.270781
NaCl (Halite),0.0216030,0.0215268
Na2SO4.10H2O (Mirabilite),0.0152275,0.0181399
NaHCO3 (Nahcolite),0.0133341,0.0169008
CaCO3 (Calcite),6.63292e-3,0.0112870
Na2SO4 (Thenardite),4.25573e-3,5.12459e-3
MgSO4.7H2O (Epsomite),3.56938e-3,4.14441e-3
CaCO3 (Aragonite),3.13680e-3,5.33778e-3
NH4Cl (Sal ammoniac),4.51249e-4,7.01176e-4
SrCO3 (Strontianite),4.03907e-4,2.48505e-3
KCl (Sylvite),2.18595e-4,2.17038e-4

Sr(HCO3)2,1.31348e-4,8.18737e-4
FeS (Pyrrhotite),1.88314e-9,2.03317
FeCO3 (Siderite),3.48756e-10,0.0314488
FeS(mackinawite) (Mackinawite),3.30367e-11,0.0356687
FeSO4.7H2O (Melanterite),1.27019e-11,8.63249e-4
FeS(amorphous) (FeS amorphous),5.24495e-13,5.66280e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid,2nd Liquid
,mol,mol,mol,mol
H2O,5.33109,5.33103,,5.43564e-5
Cl-1,0.139238,0.139238,,
Na+1,0.117638,0.117638,,
CO2,0.107229,0.102906,,4.32247e-3
Mg+2,7.56111e-3,7.56111e-3,,
Ca+2,6.32612e-3,6.32612e-3,,
SO4-2,2.95209e-3,2.95209e-3,,
NaSO4-1,1.60196e-3,1.60196e-3,,
NH4+1,1.42601e-3,1.42601e-3,,
HCO3-1,9.42655e-4,9.42655e-4,,
N2,7.56347e-4,6.2696e-4,,1.29387e-4
CaSO4.2H2O (Gypsum),5.94085e-4,,5.94085e-4,
CH3OH,5.83154e-4,5.82965e-4,,1.89294e-7
MgHCO3+1,5.11177e-4,5.11177e-4,,
MgSO4,3.82762e-4,3.82762e-4,0.0,
NaHCO3 (Nahcolite),3.55977e-4,3.55977e-4,0.0,
FeS2 (Pyrite),2.59638e-4,,2.59638e-4,
K+1,2.58977e-4,2.58977e-4,,
SrSO4 (Celestine),2.1169e-4,7.11798e-6,2.04572e-4,
CaSO4 (Anhydrite),1.22951e-4,1.22951e-4,0.0,
BaSO4 (Barite),8.37118e-5,,8.37118e-5,
Sr+2,5.99375e-5,5.99375e-5,,
CO,5.14928e-5,4.61062e-5,,5.38667e-6
NH4SO4-1,4.83219e-5,4.83219e-5,,
H+1,1.82293e-5,1.82293e-5,,
C6H14O4,1.76328e-5,1.58653e-5,,1.76749e-6
H2S,1.65046e-5,1.62051e-5,,2.99538e-7
S8 (Sulfur),9.54013e-6,,9.54013e-6,
KSO4-1,5.99701e-6,5.99701e-6,,
HSO4-1,5.50319e-6,5.50319e-6,,
KCl (Sylvite),1.02179e-6,1.02179e-6,0.0,
CaHCO3+1,5.82928e-7,5.82928e-7,,
HS-1,2.30992e-8,2.30992e-8,,
Ba+2,2.02689e-8,2.02689e-8,,
CaCO3 (Calcite),1.59483e-8,1.59483e-8,0.0,
CaCl+1,1.10253e-8,1.10253e-8,,
BaCl(+1),7.52062e-9,7.52062e-9,,
S2O3-2,4.97029e-9,4.97029e-9,,
MgCO3 (Magnesite),3.17585e-9,3.17585e-9,0.0,
CO3-2,2.69647e-9,2.69647e-9,,

NaS2O3-1,2.3838e-9,2.3838e-9,,
NH3,2.18371e-9,2.18357e-9,,1.43404e-13
NaCO3-1,8.13791e-10,8.13791e-10,,
BaHCO3+1,3.42153e-10,3.42153e-10,,
KHSO4 (Mercallite),8.8052e-11,8.8052e-11,0.0,
NH2CO2-1,5.23935e-11,5.23935e-11,,
MgOH+1,4.31085e-11,4.31085e-11,,
KS2O3-1,1.41838e-11,1.41838e-11,,
OH-1,1.04043e-11,1.04043e-11,,
HCl,8.10965e-12,8.09781e-12,,1.18442e-14
Fe+2,4.38985e-12,4.38985e-12,,
CaOH+1,2.00276e-12,2.00276e-12,,
S5-2,8.50315e-13,8.50315e-13,,
HSO3-1,7.41903e-13,7.41903e-13,,
S4-2,2.05072e-13,2.05072e-13,,
H2,1.79315e-13,1.70039e-13,,9.2758e-15
S3-2,2.99086e-14,2.99086e-14,,
FeHS+1,1.04123e-14,1.04123e-14,,
SrOH+1,8.94639e-15,8.94639e-15,,
SO2,5.1895e-15,5.15683e-15,,3.26655e-17
S2-2,2.63881e-15,2.63881e-15,,
FeCl+1,2.62078e-15,2.62078e-15,,
SO3-2,2.52798e-15,2.52798e-15,,
BaCO3 (Witherite),1.83804e-15,1.83804e-15,0.0,
FeHCO3+1,1.10649e-15,1.10649e-15,,
FeCO3 (Siderite),1.50342e-16,1.50342e-16,0.0,
S-2,1.0343e-16,1.0343e-16,,
FeOH+1,5.75601e-18,5.75601e-18,,
FeCl2 (Lawrencite),4.69977e-18,4.69977e-18,0.0,
Fe(NH3)+2,1.80391e-18,1.80391e-18,,
BaOH+1,1.62747e-19,1.62747e-19,,
H2SO4,3.27784e-20,1.79725e-20,,1.48059e-20
CaCl2 (Hydrophilite),2.1981e-21,2.1981e-21,0.0,
FeS(HS)-1,2.33702e-22,2.33702e-22,,
Fe(CO3)2-2,1.48379e-22,1.48379e-22,,
Fe+3,5.2463e-23,5.2463e-23,,
FeOH+2,4.97937e-23,4.97937e-23,,
Fe(NH3)2+2,4.17982e-24,4.17982e-24,,
SO3,2.21755e-24,2.21755e-24,,7.11272e-33
Fe(OH)2+1,2.17292e-24,2.17292e-24,,
FeCl2+1,7.81358e-25,7.81358e-25,,
FeCl+2,2.22925e-25,2.22925e-25,,
FeSO4+1,7.97176e-26,7.97176e-26,,
Fe(OH)3 (Bernalite),6.09124e-26,6.09124e-26,0.0,
FeCl3 (Molysite),2.05764e-26,2.05764e-26,0.0,
S2O5-2,6.79134e-28,6.79134e-28,,
FeCl4-1,5.95252e-28,5.95252e-28,,
S2O4-2,3.53286e-28,3.53286e-28,,
Na2S2O4,1.46635e-29,1.46635e-29,0.0,
S2O6-2,4.3893e-30,4.3893e-30,,
Fe(NH3)3+2,2.39009e-30,2.39009e-30,,
Fe(OH)4-1,2.21313e-31,2.21313e-31,,
S5O6-2,1.90518e-31,1.90518e-31,,
HFeO2-1,4.83348e-33,4.83348e-33,,

N2H5+1,2.37825e-35,2.37825e-35,,
Fe(NH3)4+2,1.61855e-39,1.61855e-39,,
N2H4,6.9438e-40,6.9438e-40,,1.97131e-46
NH2OH,1.9777e-42,1.97768e-42,,1.95893e-47
Fe2(OH)2+4,1.24708e-46,1.24708e-46,,
Fe(NH3)5+2,1.09608e-48,1.09608e-48,,
NO,9.08744e-52,8.53672e-52,,5.5072e-53
N2O,4.21058e-53,3.99886e-53,,2.11724e-54
Fe(NH3)6+2,7.42247e-58,7.42247e-58,,
HSO5-1,3.08676e-59,3.08676e-59,,
NO2-1,2.16825e-61,2.16825e-61,,
HNO2,2.44319e-62,2.35573e-62,,8.74611e-64
S2O8-2,6.61009e-70,6.61009e-70,,
O2,2.38508e-70,2.03148e-70,,3.53596e-71
NO2,6.88195e-76,6.81289e-76,,6.90604e-78
FeO4-2,2.61641e-79,2.61641e-79,,
NO3-1,1.63753e-80,1.63753e-80,,
NaNO3 (Nitratine),7.19916e-82,7.19916e-82,0.0,
Ca(NO3)+1,7.17621e-82,7.17621e-82,,
NH4NO3 (Gwihabaite),5.22173e-82,5.22173e-82,0.0,
SrNO3+1,1.03251e-83,1.03251e-83,,
HNO3,1.51563e-89,1.50808e-89,,7.54745e-92
FeNO3+2,3.63648e-104,3.63648e-104,,
Total (by phase),5.72036,5.71469,1.15155e-3,4.51386e-3

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Aqueous,Solid,2nd Liquid
,mol,mol,mol,mol
H(+1),10.6723,10.6698,2.37634e-3,1.09312e-4
K(+1),2.65996e-4,2.65996e-4,0.0,0.0
Na(+1),0.119596,0.119596,0.0,0.0
N(-3),1.47433e-3,1.47433e-3,0.0,1.43404e-13
Ba(+2),8.37399e-5,2.81317e-8,8.37118e-5,0.0
Ca(+2),7.04376e-3,6.44968e-3,5.94085e-4,0.0
Fe(+2),2.59638e-4,4.40416e-12,2.59638e-4,0.0
Mg(+2),8.45505e-3,8.45505e-3,0.0,0.0
Fe(+3),1.05596e-22,1.05596e-22,0.0,0.0
O(-2),5.57625,5.56283,4.71764e-3,8.70469e-3
Cl(-1),0.139239,0.139239,0.0,1.18442e-14
C(+4),0.109039,0.104717,0.0,4.32247e-3
S(+4),7.49621e-13,7.49588e-13,0.0,3.26655e-17
S(+6),6.00908e-3,5.12671e-3,8.82369e-4,1.48059e-20
S(-2),2.76166e-4,1.62282e-5,2.59638e-4,2.99538e-7
S(+2),1.47366e-8,1.47366e-8,0.0,0.0
N(+3),2.41257e-61,2.40383e-61,0.0,8.74611e-64
N(+5),1.83454e-80,1.83454e-80,0.0,7.54745e-92
Sr(+2),2.71627e-4,6.70554e-5,2.04572e-4,0.0
N(0),1.51269e-3,1.25392e-3,0.0,2.58774e-4
H(0),3.5863e-13,3.40078e-13,0.0,1.85516e-14
O(0),4.77015e-70,4.06296e-70,0.0,7.07192e-71

S(+8),3.08676e-59,3.08676e-59,0.0,0.0
S(+3),7.359e-28,7.359e-28,0.0,0.0
S(+5),8.77859e-30,8.77859e-30,0.0,0.0
S(+7),1.32202e-69,1.32202e-69,0.0,0.0
N(+2),9.08744e-52,8.53672e-52,0.0,5.5072e-53
N(+4),6.88195e-76,6.81289e-76,0.0,6.90604e-78
N(+1),8.42117e-53,7.99772e-53,0.0,4.23449e-54
N(-2),4.75664e-35,4.75664e-35,0.0,3.94263e-46
C(+2),5.14928e-5,4.61062e-5,0.0,5.38667e-6
Fe(+6),2.61641e-79,2.61641e-79,0.0,0.0
S(0),3.35959e-4,4.07893e-12,3.35959e-4,0.0
N(-1),1.9777e-42,1.97768e-42,0.0,1.95893e-47
METHANOL,5.83154e-4,5.82965e-4,0.0,1.89294e-7
TRIETLNGLY,1.76328e-5,1.58653e-5,0.0,1.76749e-6

Element Distribution

,Total,Total,Aqueous,Solid,2nd Liquid
,mol,mole %,% of Total,% of Total,% of Total
H(+1),10.6723,64.1246,99.9767,0.0222664,1.02426e-3
K(+1),2.65996e-4,1.59824e-3,100.0,0.0,0.0
Na(+1),0.119596,0.718591,100.0,0.0,0.0
N(-3),1.47433e-3,8.85854e-3,100.0,0.0,9.72666e-9
Ba(+2),8.37399e-5,5.03151e-4,0.0335941,99.9664,0.0
Ca(+2),7.04376e-3,0.0423225,91.5658,8.4342,0.0
Fe(+2),2.59638e-4,1.56004e-3,1.69627e-6,100.0,0.0
Mg(+2),8.45505e-3,0.0508022,100.0,0.0,0.0
Fe(+3),1.05596e-22,6.34472e-22,100.0,0.0,0.0
O(-2),5.57625,33.5049,99.7593,0.0846024,0.156103
Cl(-1),0.139239,0.836621,100.0,0.0,8.50637e-12
C(+4),0.109039,0.655162,96.0359,0.0,3.96415
S(+4),7.49621e-13,4.5041e-12,99.9956,0.0,4.3576e-3
S(+6),6.00908e-3,0.0361056,85.3161,14.6839,2.46392e-16
S(-2),2.76166e-4,1.65934e-3,5.87625,94.0153,0.108463
S(+2),1.47366e-8,8.85447e-8,100.0,0.0,0.0
N(+3),2.41257e-61,1.44959e-60,99.6375,0.0,0.362522
N(+5),1.83454e-80,1.10228e-79,100.0,0.0,4.11409e-10
Sr(+2),2.71627e-4,1.63207e-3,24.6865,75.3135,0.0
N(0),1.51269e-3,9.08902e-3,82.8932,0.0,17.1068
H(0),3.5863e-13,2.15483e-12,94.8271,0.0,5.17291
O(0),4.77015e-70,2.86615e-69,85.1746,0.0,14.8254
S(+8),3.08676e-59,1.85468e-58,100.0,0.0,0.0
S(+3),7.359e-28,4.42166e-27,100.0,0.0,0.0
S(+5),8.77859e-30,5.27462e-29,100.0,0.0,0.0
S(+7),1.32202e-69,7.94335e-69,100.0,0.0,0.0
N(+2),9.08744e-52,5.46019e-51,93.9398,0.0,6.06023
N(+4),6.88195e-76,4.13502e-75,98.9965,0.0,1.0035
N(+1),8.42117e-53,5.05986e-52,94.9716,0.0,5.02838
N(-2),4.75664e-35,2.85803e-34,100.0,0.0,8.28868e-10
C(+2),5.14928e-5,3.09395e-4,89.539,0.0,10.461
Fe(+6),2.61641e-79,1.57207e-78,100.0,0.0,0.0
S(0),3.35959e-4,2.01861e-3,1.21412e-6,100.0,0.0
N(-1),1.9777e-42,1.1883e-41,99.999,0.0,9.90508e-4

METHANOL,5.83154e-4,3.50388e-3,99.9675,0.0,0.0324604
TRIETLNGLY,1.76328e-5,1.05947e-4,89.9761,0.0,10.0239

Calculation Summary
06-1 Alloy-4 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2205

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3.1H2O

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,5.33403,5.33403
CO2,0.109039,0.109039
N2,7.77432e-4,7.77432e-4
CO,5.14928e-5,5.14928e-5
O2,2.38930e-6,2.38930e-6
NH3,1.40691e-3,1.40691e-3
CH3OH,5.83154e-4,5.83154e-4
H2S,1.18332e-5,1.18332e-5
SO2,2.22167e-3,2.22167e-3
NO2,2.52557e-5,2.52557e-5
BaCl2,3.19793e-8,3.19793e-8

CaCl2,9.33369e-4,9.33369e-4
CaO,6.11040e-3,6.11040e-3
FeCl2,2.59638e-4,2.59638e-4
KCl,2.65996e-4,2.65996e-4
MgCl2,8.45505e-3,8.45505e-3
NaCl,0.119596,0.119596
SO3,4.07319e-3,4.07319e-3
SrCl2,4.08102e-5,4.08102e-5
BaSO4,8.37079e-5,8.37079e-5
SrSO4,2.30817e-4,2.30817e-4
C6H14O4,1.76328e-5,1.76328e-5

Calculated Rates

Corrosion Rate,2.91054e-4,mm/yr
Corrosion Potential,-0.271985,V (SHE)
Repassivation Potential*,-0.186934,V (SHE)
Corrosion Current Density,2.75650e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4.2H2O (Gypsum),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.0.5H2O (Bassanite),0.149208
,CaSO4 (Anhydrite),0.823932
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,5.58822,mol
Temperature,80.6085,°F
Pressure,2641.00,psia

Liquid 1 Properties
pH,4.19759,
Ionic Strength (x-based),0.0282900,mol/mol
Ionic Strength (m-based),1.68405,mol/kg
Dielectric Constant,56.7738,
ORP,-8.05947e-3,V (SHE)
Osmotic Pressure,1555.04,psia
Specific Electrical Conductivity,1.12622e5,µmho/cm
"Viscosity, absolute",1.03353,cP
Thermal Conductivity,525.083,cal/hr m °C
Surface Tension,0.0757696,N/m
Interfacial Tension LLE,5.67754e-7,N/m

Standard Liquid Volume,0.105044,L
"Volume, Std. Conditions",0.102901,L
"Total Dissolved Solids, Estimated",85678.5,mg/L
Hardness,14208.1,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,8.81058e-5,L

Liquid 2 Properties
pH,0.133521,
Ionic Strength (x-based),1.00000,mol/mol
Ionic Strength (m-based),9.72547e12,mol/kg
Dielectric Constant,13.3600,
Standard Liquid Volume,1.37290e-5,L
"Volume, Std. Conditions",8.93311e-6,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid,Liquid-2
Density,g/ml,1.07406,1.07218,2.78289,4.82303
Enthalpy,J,-1.63304e6,-1.63035e6,-2483.49,-207.847

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
Mole (True),5.71816,5.71598,1.39679e-3,7.78914e-4
Mole (App),5.58456,5.58265,1.39679e-3,5.19276e-4
,g,g,g,g
Mass,109.794,109.495,0.255191,0.0443365
,L,L,cm3,L
Volume,0.102224,0.102123,0.0917000,9.19267e-6

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
S8 (Sulfur),1.00000,3251.28
CaSO4.2H2O (Gypsum),1.00000,1.54389
BaSO4 (Barite),1.00000,3367.37
SrSO4 (Celestine),1.00000,9.79066
CaSO4 (Anhydrite),0.823932,1.27332
S8 (Sulfur monoclinic),0.761160,2474.75
H2O,0.705838,0.705490
CaSO4.0.5H2O (Bassanite),0.217324,0.335772
CaSO4.0.5H2O (Bassanite),0.149208,0.230531
CaCO3 (Calcite),0.0415051,0.0430968
CaCO3 (Aragonite),0.0312360,0.0324339
NaHCO3 (Nahcolite),0.0280519,0.0267494
NaCl (Halite),0.0237261,0.0236715
NaCl.2H2O (hydrohalite),0.0215387,0.0214679
Na2SO4.10H2O (Mirabilite),9.93708e-3,0.0133429

Na2SO4.CaSO4 (Glauberite),5.71678e-3,0.0119215
Na2SO4 (Thenardite),2.97886e-3,4.01962e-3
SrCO3 (Strontianite),2.75115e-3,0.0180977
Na2SO4.5CaSO4.3H2O,1.07785e-3,0.0128020
MgSO4.7H2O (Epsomite),6.83394e-4,8.70805e-4
MgSO4.12H2O,5.37595e-4,6.83335e-4
NH4Cl (Sal ammoniac),3.96739e-4,4.95312e-4
MgSO4.6H2O (Hexahydrite),3.25213e-4,4.14602e-4
NH4Cl,2.27822e-4,2.84426e-4
KCl (sylvite),1.92835e-4,1.91578e-4
NH4HCO3 (Ammonium bicarbonate),1.53467e-4,1.83122e-4
Na2SO4,1.44535e-4,1.95033e-4
MgSO4.5H2O (Pentahydrite),1.33024e-4,1.69671e-4
BaCO3 (Witherite),2.90802e-7,6.57938e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H2O,5.33,5.33,0.0,4.44566e-15
Cl-1,0.139239,0.13872,,5.19276e-4
Na+1,0.118119,0.118119,,7.94701e-23
CO2,0.106319,0.106319,,3.36412e-50
Mg+2,6.97297e-3,6.97297e-3,,1.05248e-32
Ca+2,5.57361e-3,5.57361e-3,,1.83891e-28
SO4-2,2.64532e-3,2.64532e-3,,1.6605e-26
HCO3-1,2.46059e-3,2.46059e-3,,5.95276e-59
NaMgSO4+1,1.47635e-3,1.47635e-3,,7.05111e-41
NH4+1,1.43241e-3,1.43241e-3,,2.76366e-15
CaSO4.2H2O (Gypsum),1.00101e-3,,1.00101e-3,
N2,7.77306e-4,7.77306e-4,,9.33804e-14
CH3OH,5.8311e-4,5.8311e-4,,1.03596e-18
CaSO4 (Anhydrite),4.68875e-4,4.68875e-4,0.0,2.69653e-26
K+1,2.60359e-4,2.60359e-4,,5.63643e-19
FeCO2+2,2.59638e-4,1.09936e-31,,2.59638e-4
SrSO4 (Celestine),2.30801e-4,9.05279e-7,2.29896e-4,7.002e-22
BaSO4 (Barite),8.37059e-5,,8.37059e-5,
S8 (Sulfur),8.21905e-5,1.22084e-8,8.21783e-5,8.26125e-16
CO,5.14928e-5,5.14928e-5,,3.98278e-20
H2S,5.05876e-5,5.05876e-5,,8.52247e-19
Sr+2,4.0826e-5,4.0826e-5,,6.61558e-24
C6H14O4,1.76328e-5,1.76328e-5,,1.99685e-24
KMgSO4+1,5.63688e-6,5.63688e-6,,9.59986e-37
H3O+1,3.55077e-6,3.55077e-6,,8.29082e-25
HSO4-1,1.20427e-6,1.20427e-6,,4.60019e-26
HS-1,1.27547e-7,1.27547e-7,,5.03654e-27
CaCO3 (Calcite),1.21388e-7,1.21388e-7,0.0,9.90013e-18
CaCl2 (Hydrophilite),1.05191e-7,1.05191e-7,0.0,5.95773e-37
MgSO4,5.54034e-8,5.54034e-8,0.0,3.10158e-29
CaClCH3OH+1,4.41998e-8,4.41998e-8,,7.68116e-26
Ba+2,3.4029e-8,3.4029e-8,,1.77773e-20

MgCO3,3.06949e-8,3.06949e-8,0.0,2.37414e-23
CO3-2,2.03086e-8,2.03086e-8,,1.65018e-31
S2O3-2,5.69462e-9,5.69462e-9,,2.75138e-33
NH4OH,5.30321e-9,5.30321e-9,,2.24375e-24
NH3,1.51862e-9,1.51862e-9,,7.16382e-23
Na2SO4.NaHSO4,1.43734e-9,1.43734e-9,0.0,3.90819e-31
NH2CO2-1,6.98932e-10,6.98932e-10,,1.34373e-29
MgOH+1,1.28292e-10,1.28292e-10,,5.99909e-22
OH-1,3.85968e-11,3.85968e-11,,9.03659e-24
HO(CH2CH2O)3CO2(-1),2.50233e-11,2.50233e-11,,6.19498e-31
CaOH+1,2.13556e-11,2.13556e-11,,5.05582e-23
MgClCH3OH+1,4.98893e-12,4.98893e-12,,2.09312e-27
S5-2,4.05472e-12,4.05472e-12,,4.06366e-36
HS2O3-1,2.67735e-12,2.67735e-12,,9.32097e-32
S4-2,1.00628e-12,1.00628e-12,,1.0085e-36
H2,4.70817e-13,4.70817e-13,,2.96808e-29
CH5O+1,3.99178e-13,3.99178e-13,,4.97816e-44
HSO3-1,3.75186e-13,3.75186e-13,,1.18667e-32
CH3OH.HCl,2.19045e-13,2.19045e-13,,1.69197e-28
HCl,1.64147e-13,1.64147e-13,,1.61368e-27
S3-2,1.51023e-13,1.51023e-13,,1.51356e-37
BaCO3 (Witherite),6.90259e-14,6.90259e-14,0.0,5.3389e-29
C6H15O4+1,2.60824e-14,2.60824e-14,,2.34461e-34
SrOH+1,1.99778e-14,1.99778e-14,,1.76725e-25
S2-2,1.37118e-14,1.37118e-14,,1.3742e-38
CH3O-1,1.00092e-14,1.00092e-14,,3.4903e-34
SrCO3 (Strontianite),9.53293e-15,9.53293e-15,0.0,7.37337e-30
SO3-2,2.66969e-15,2.66969e-15,,1.35965e-39
SO2,9.63544e-16,9.63544e-16,,1.04937e-29
CO2S,5.92724e-16,5.92724e-16,,4.5845e-31
H2S2O3,4.69468e-16,4.69468e-16,,3.63116e-31
NaOH.Na2SO4,4.11787e-16,4.11787e-16,,1.33848e-44
S1,3.02821e-16,3.02821e-16,,2.34221e-31
S2,2.99296e-16,2.99296e-16,,2.31495e-31
S3,2.95796e-16,2.95796e-16,,2.28788e-31
S4,2.92371e-16,2.92371e-16,,2.26138e-31
S5,2.88996e-16,2.88996e-16,,2.23528e-31
S6,2.85671e-16,2.85671e-16,,2.20956e-31
S7,2.82282e-16,2.82282e-16,,2.18335e-31
H2SO4,7.14273e-17,7.14273e-17,,1.03485e-35
C6H13O4-1,5.31233e-17,5.31233e-17,,1.80778e-36
BaOH+1,2.25441e-17,2.25441e-17,,9.15714e-43
NaOH,2.01232e-17,2.01232e-17,0.0,2.62933e-30
S-2,9.78157e-18,9.78157e-18,,1.04835e-40
NaOHCO3-2,1.60127e-19,1.60127e-19,,1.6048e-43
MgCl2,2.09761e-20,2.09761e-20,0.0,8.15975e-35
S2O5-2,3.96979e-25,3.96979e-25,,3.96677e-49
S2O4-2,6.52858e-29,6.52858e-29,,6.54298e-53
SO3,9.30206e-31,9.30206e-31,,1.52381e-49
S2O6-2,1.59968e-31,1.59968e-31,,1.6032e-55
Fe+2,2.94449e-32,2.94449e-32,,3.10251e-49
S5O6-2,7.37514e-33,7.37514e-33,,7.3914e-57
N2H5+1,2.87871e-35,2.87871e-35,,1.34525e-46
FeHS+1,9.50339e-36,9.50339e-36,,4.44389e-47

FeH(CO3)2-1,7.41251e-36,7.41251e-36,,2.5806e-55
FeCl+1,5.96489e-36,5.96489e-36,,1.85022e-48
FeSO4,4.60865e-36,4.60865e-36,0.0,3.5606e-51
FeS (Pyrrhotite),1.77938e-37,1.77938e-37,0.0,1.37629e-52
FeOH+1,6.12747e-38,6.12747e-38,,2.86528e-49
Fe(NH3)+2,2.20129e-38,2.20129e-38,,6.11469e-53
N2H4,2.323e-39,2.323e-39,,2.42127e-56
NH2OH2+1,2.13326e-39,2.13326e-39,,9.92617e-51
N2H6+2,6.27765e-40,6.27765e-40,,1.13432e-47
NH2OH,2.46162e-41,2.46162e-41,0.0,1.05326e-56
FeO+1,4.37954e-43,4.37954e-43,,2.04792e-54
FeOH+2,2.00368e-43,2.00368e-43,,3.62282e-51
Fe(NH3)2+2,1.63821e-43,1.63821e-43,,4.55058e-58
FeCl+2,3.9718e-44,3.9718e-44,,1.01998e-61
FeO,6.96289e-45,6.96289e-45,,5.38554e-60
Fe+3,3.29789e-45,3.29789e-45,,6.45494e-59
HFeO2,1.92016e-45,1.92016e-45,,1.48517e-60
NH2Cl,9.93973e-47,9.93973e-47,,7.68801e-62
FeCl2+1,9.69919e-48,9.69919e-48,,2.70195e-69
HClO,4.3224e-48,4.3224e-48,,3.34322e-63
FeHSO4+2,3.92765e-48,3.92765e-48,,7.43828e-56
Cl2,6.98941e-49,6.98941e-49,,5.40605e-64
Fe(NH3)3+2,3.00865e-49,3.00865e-49,,8.35738e-64
FeO2-1,1.49296e-50,1.49296e-50,,5.1976e-70
ClO-1,3.39708e-51,3.39708e-51,,1.18266e-70
NO,8.82335e-52,8.82335e-52,,1.30194e-65
HFeO2-1,2.65937e-52,2.65937e-52,,9.25835e-72
N2O,3.61467e-53,3.61467e-53,,1.04545e-66
NH3Cl+1,3.95223e-57,3.95223e-57,,1.84811e-68
Fe(NH3)4+2,6.54367e-58,6.54367e-58,,1.81769e-72
HSO5-1,2.36016e-60,2.36016e-60,,8.21668e-80
NO2-1,1.49446e-61,1.49446e-61,,4.68122e-81
HNO2,1.16594e-62,1.16594e-62,,9.0181e-78
Fe(NH3)5+2,1.42326e-66,1.42326e-66,,3.95351e-81
O2,4.47003e-71,4.47003e-71,,2.79505e-87
S2O8-2,4.73868e-72,4.73868e-72,,4.74912e-96
Fe(NH3)6+2,3.09552e-75,3.09552e-75,,8.59868e-90
NO2,1.1026e-76,1.1026e-76,,9.52813e-90
NO3-1,6.55506e-81,6.55506e-81,,1.24259e-100
HNO3,1.08872e-86,1.08872e-86,,4.35022e-107
Fe2(OH)2+4,9.35783e-87,8.73976e-87,,6.18069e-88
NHCl2,2.47184e-87,2.47184e-87,,1.91187e-102
NH4NO3.(NH4)2SO4,3.707e-91,3.707e-91,0.0,2.86722e-106
ClO2-1,9.14822e-94,9.14822e-94,,3.18487e-113
NH2Cl2+1,8.92961e-95,8.92961e-95,,4.17559e-106
HClO2,3.43483e-96,3.43483e-96,,2.65671e-111
FeO4-2,3.1026e-99,3.1026e-99,,3.10944e-123
ClO2,1.01368e-112,1.01368e-112,,7.84047e-128
ClO3-1,1.43915e-122,1.43915e-122,,0.0
NCl3,4.87314e-129,4.87314e-129,,0.0
N2O3,2.72086e-129,2.72086e-129,,0.0
Total (by phase),5.71816,5.71598,1.39679e-3,7.78914e-4

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H(+1),10.6729,10.6689,4.00403e-3,1.99487e-14
K(+1),2.65996e-4,2.65996e-4,0.0,5.63643e-19
Na(+1),0.119596,0.119596,0.0,7.94701e-23
N(-3),1.43242e-3,1.43242e-3,0.0,2.76366e-15
Ba(+2),8.37399e-5,3.4029e-8,8.37059e-5,1.77773e-20
Ca(+2),7.04376e-3,6.04276e-3,1.00101e-3,9.90018e-18
Fe(+2),2.59638e-4,1.39409e-31,0.0,2.59638e-4
Mg(+2),8.45505e-3,8.45505e-3,0.0,6.23653e-22
Fe(+3),6.83271e-43,6.83271e-43,0.0,3.62494e-51
O(-2),5.57625,5.56847,7.26045e-3,5.19276e-4
Cl(-1),0.139239,0.13872,0.0,5.19276e-4
C(+4),0.109039,0.108779,0.0,2.59638e-4
S(+4),3.78819e-13,3.78819e-13,0.0,1.05055e-29
S(+6),5.91297e-3,4.59836e-3,1.31461e-3,7.0029e-22
S(-2),5.07152e-5,5.07152e-5,0.0,8.52247e-19
S(+2),1.13946e-8,1.13946e-8,0.0,9.18155e-31
N(+3),1.61106e-61,1.61106e-61,0.0,9.02278e-78
N(+5),6.55508e-81,6.55508e-81,0.0,1.2426e-100
Sr(+2),2.71627e-4,4.17313e-5,2.29896e-4,7.06993e-22
N(0),1.55461e-3,1.55461e-3,0.0,1.86761e-13
H(0),9.41634e-13,9.41634e-13,0.0,5.93616e-29
O(0),8.94006e-71,8.94006e-71,0.0,5.5901e-87
S(+8),2.36016e-60,2.36016e-60,0.0,8.21668e-80
Cl(+1),1.04422e-46,1.04422e-46,0.0,8.0764e-62
Cl(+5),1.43915e-122,1.43915e-122,0.0,0.0
S(+3),1.30572e-28,1.30572e-28,0.0,1.3086e-52
S(+5),3.19935e-31,3.19935e-31,0.0,3.20641e-55
S(+7),9.47735e-72,9.47735e-72,0.0,9.49825e-96
N(+2),8.82335e-52,8.82335e-52,0.0,1.30194e-65
N(+4),1.1026e-76,1.1026e-76,0.0,9.52813e-90
Cl(+3),9.18257e-94,9.18257e-94,0.0,2.68856e-111
Cl(+4),1.01368e-112,1.01368e-112,0.0,7.84047e-128
N(+1),7.22934e-53,7.22934e-53,0.0,2.0909e-66
N(-2),5.75801e-35,5.75801e-35,0.0,2.91737e-46
C(+2),5.14928e-5,5.14928e-5,0.0,3.98278e-20
Fe(+6),3.1026e-99,3.1026e-99,0.0,3.10944e-123
S(0),6.57524e-4,9.76868e-8,6.57426e-4,6.609e-15
MeO(-1),5.83154e-4,5.83154e-4,0.0,1.03596e-18
N(-1),2.15788e-39,2.15788e-39,0.0,9.92618e-51
TEGION,1.76328e-5,1.76328e-5,0.0,1.99685e-24

Element Distribution

,Total,Total,Liquid-1,Solid,Liquid-2
,mol,mole %,% of Total,% of Total,% of Total
H(+1),10.6729,64.1259,99.9625,0.0375158,1.8691e-13
K(+1),2.65996e-4,1.59818e-3,100.0,0.0,2.11899e-13

Na(+1),0.119596,0.718565,100.0,0.0,6.6449e-20
N(-3),1.43242e-3,8.60636e-3,100.0,0.0,1.92937e-10
Ba(+2),8.37399e-5,5.03133e-4,0.0406366,99.9594,2.12292e-14
Ca(+2),7.04376e-3,0.042321,85.7888,14.2112,1.40552e-13
Fe(+2),2.59638e-4,1.55998e-3,5.36935e-26,0.0,100.0
Mg(+2),8.45505e-3,0.0508004,100.0,0.0,7.3761e-18
Fe(+3),6.83271e-43,4.10529e-42,100.0,0.0,5.30528e-7
O(-2),5.57625,33.5037,99.8605,0.130203,9.31228e-3
Cl(-1),0.139239,0.83659,99.6271,0.0,0.372937
C(+4),0.109039,0.655138,99.7619,0.0,0.238114
S(+4),3.78819e-13,2.27605e-12,100.0,0.0,2.77323e-15
S(+6),5.91297e-3,0.0355268,77.7674,22.2326,1.18433e-17
S(-2),5.07152e-5,3.04711e-4,100.0,0.0,1.68046e-12
S(+2),1.13946e-8,6.8462e-8,100.0,0.0,8.05781e-21
N(+3),1.61106e-61,9.67968e-61,100.0,0.0,5.60054e-15
N(+5),6.55508e-81,3.93848e-80,100.0,0.0,1.89563e-18
Sr(+2),2.71627e-4,1.63202e-3,15.3634,84.6366,2.6028e-16
N(0),1.55461e-3,9.34056e-3,100.0,0.0,1.20133e-8
H(0),9.41634e-13,5.65761e-12,100.0,0.0,6.3041e-15
O(0),8.94006e-71,5.37145e-70,100.0,0.0,6.25287e-15
S(+8),2.36016e-60,1.41805e-59,100.0,0.0,3.48141e-18
Cl(+1),1.04422e-46,6.27397e-46,100.0,0.0,7.73438e-14
Cl(+5),1.43915e-122,8.64682e-122,100.0,0.0,0.0
S(+3),1.30572e-28,7.84512e-28,100.0,0.0,1.00221e-22
S(+5),3.19935e-31,1.92226e-30,100.0,0.0,1.00221e-22
S(+7),9.47735e-72,5.69426e-71,100.0,0.0,1.00221e-22
N(+2),8.82335e-52,5.30132e-51,100.0,0.0,1.47557e-12
N(+4),1.1026e-76,6.62472e-76,100.0,0.0,8.64154e-12
Cl(+3),9.18257e-94,5.51715e-93,100.0,0.0,2.9279e-16
Cl(+4),1.01368e-112,6.0905e-112,100.0,0.0,7.73463e-14
N(+1),7.22934e-53,4.34359e-52,100.0,0.0,2.89224e-12
N(-2),5.75801e-35,3.45958e-34,100.0,0.0,5.06663e-10
C(+2),5.14928e-5,3.09384e-4,100.0,0.0,7.73463e-14
Fe(+6),3.1026e-99,1.86413e-98,100.0,0.0,1.00221e-22
S(0),6.57524e-4,3.95059e-3,0.0148568,99.9851,1.00513e-9
MeO(-1),5.83154e-4,3.50376e-3,100.0,0.0,1.77648e-13
N(-1),2.15788e-39,1.29651e-38,100.0,0.0,4.59997e-10
TEGION,1.76328e-5,1.05943e-4,100.0,0.0,1.13246e-17

Calculation Summary
06-1 Alloy-5 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2507

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3.1H2O

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,5.33403,5.33403
CO2,0.109039,0.109039
N2,7.77432e-4,7.77432e-4
CO,5.14928e-5,5.14928e-5
O2,2.38930e-6,2.38930e-6
NH3,1.40691e-3,1.40691e-3
CH3OH,5.83154e-4,5.83154e-4
H2S,1.18332e-5,1.18332e-5
SO2,2.22167e-3,2.22167e-3
NO2,2.52557e-5,2.52557e-5
BaCl2,3.19793e-8,3.19793e-8

CaCl2,9.33369e-4,9.33369e-4
CaO,6.11040e-3,6.11040e-3
FeCl2,2.59638e-4,2.59638e-4
KCl,2.65996e-4,2.65996e-4
MgCl2,8.45505e-3,8.45505e-3
NaCl,0.119596,0.119596
SO3,4.07319e-3,4.07319e-3
SrCl2,4.08102e-5,4.08102e-5
BaSO4,8.37079e-5,8.37079e-5
SrSO4,2.30817e-4,2.30817e-4
C6H14O4,1.76328e-5,1.76328e-5

Calculated Rates

Corrosion Rate,2.82721e-4,mm/yr
Corrosion Potential,-0.272071,V (SHE)
Repassivation Potential*,-0.153019,V (SHE)
Corrosion Current Density,2.75558e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4.2H2O (Gypsum),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.0.5H2O (Bassanite),0.149208
,CaSO4 (Anhydrite),0.823932
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,5.58822,mol
Temperature,80.6085,°F
Pressure,2641.00,psia

Liquid 1 Properties
pH,4.19759,
Ionic Strength (x-based),0.0282900,mol/mol
Ionic Strength (m-based),1.68405,mol/kg
Dielectric Constant,56.7738,
ORP,-8.05947e-3,V (SHE)
Osmotic Pressure,1555.04,psia
Specific Electrical Conductivity,1.12622e5,µmho/cm
"Viscosity, absolute",1.03353,cP
Thermal Conductivity,525.083,cal/hr m °C
Surface Tension,0.0757696,N/m
Interfacial Tension LLE,5.67754e-7,N/m

Standard Liquid Volume,0.105044,L
"Volume, Std. Conditions",0.102901,L
"Total Dissolved Solids, Estimated",85678.5,mg/L
Hardness,14208.1,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,8.81058e-5,L

Liquid 2 Properties
pH,0.133521,
Ionic Strength (x-based),1.00000,mol/mol
Ionic Strength (m-based),9.72547e12,mol/kg
Dielectric Constant,13.3600,
Standard Liquid Volume,1.37290e-5,L
"Volume, Std. Conditions",8.93311e-6,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid,Liquid-2
Density,g/ml,1.07406,1.07218,2.78289,4.82303
Enthalpy,J,-1.63304e6,-1.63035e6,-2483.49,-207.847

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
Mole (True),5.71816,5.71598,1.39679e-3,7.78914e-4
Mole (App),5.58456,5.58265,1.39679e-3,5.19276e-4
,g,g,g,g
Mass,109.794,109.495,0.255191,0.0443365
,L,L,cm3,L
Volume,0.102224,0.102123,0.0917000,9.19267e-6

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
S8 (Sulfur),1.00000,3251.28
CaSO4.2H2O (Gypsum),1.00000,1.54389
BaSO4 (Barite),1.00000,3367.37
SrSO4 (Celestine),1.00000,9.79066
CaSO4 (Anhydrite),0.823932,1.27332
S8 (Sulfur monoclinic),0.761160,2474.75
H2O,0.705838,0.705490
CaSO4.0.5H2O (Bassanite),0.217324,0.335772
CaSO4.0.5H2O (Bassanite),0.149208,0.230531
CaCO3 (Calcite),0.0415051,0.0430968
CaCO3 (Aragonite),0.0312360,0.0324339
NaHCO3 (Nahcolite),0.0280519,0.0267494
NaCl (Halite),0.0237261,0.0236715
NaCl.2H2O (hydrohalite),0.0215387,0.0214679
Na2SO4.10H2O (Mirabilite),9.93708e-3,0.0133429

Na2SO4.CaSO4 (Glauberite),5.71678e-3,0.0119215
Na2SO4 (Thenardite),2.97886e-3,4.01962e-3
SrCO3 (Strontianite),2.75115e-3,0.0180977
Na2SO4.5CaSO4.3H2O,1.07785e-3,0.0128020
MgSO4.7H2O (Epsomite),6.83394e-4,8.70805e-4
MgSO4.12H2O,5.37595e-4,6.83335e-4
NH4Cl (Sal ammoniac),3.96739e-4,4.95312e-4
MgSO4.6H2O (Hexahydrite),3.25213e-4,4.14602e-4
NH4Cl,2.27822e-4,2.84426e-4
KCl (sylvite),1.92835e-4,1.91578e-4
NH4HCO3 (Ammonium bicarbonate),1.53467e-4,1.83122e-4
Na2SO4,1.44535e-4,1.95033e-4
MgSO4.5H2O (Pentahydrite),1.33024e-4,1.69671e-4
BaCO3 (Witherite),2.90802e-7,6.57938e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H2O,5.33,5.33,0.0,4.44566e-15
Cl-1,0.139239,0.13872,,5.19276e-4
Na+1,0.118119,0.118119,,7.94701e-23
CO2,0.106319,0.106319,,3.36412e-50
Mg+2,6.97297e-3,6.97297e-3,,1.05248e-32
Ca+2,5.57361e-3,5.57361e-3,,1.83891e-28
SO4-2,2.64532e-3,2.64532e-3,,1.6605e-26
HCO3-1,2.46059e-3,2.46059e-3,,5.95276e-59
NaMgSO4+1,1.47635e-3,1.47635e-3,,7.05111e-41
NH4+1,1.43241e-3,1.43241e-3,,2.76366e-15
CaSO4.2H2O (Gypsum),1.00101e-3,,1.00101e-3,
N2,7.77306e-4,7.77306e-4,,9.33804e-14
CH3OH,5.8311e-4,5.8311e-4,,1.03596e-18
CaSO4 (Anhydrite),4.68875e-4,4.68875e-4,0.0,2.69653e-26
K+1,2.60359e-4,2.60359e-4,,5.63643e-19
FeCO2+2,2.59638e-4,1.09936e-31,,2.59638e-4
SrSO4 (Celestine),2.30801e-4,9.05279e-7,2.29896e-4,7.002e-22
BaSO4 (Barite),8.37059e-5,,8.37059e-5,
S8 (Sulfur),8.21905e-5,1.22084e-8,8.21783e-5,8.26125e-16
CO,5.14928e-5,5.14928e-5,,3.98278e-20
H2S,5.05876e-5,5.05876e-5,,8.52247e-19
Sr+2,4.0826e-5,4.0826e-5,,6.61558e-24
C6H14O4,1.76328e-5,1.76328e-5,,1.99685e-24
KMgSO4+1,5.63688e-6,5.63688e-6,,9.59986e-37
H3O+1,3.55077e-6,3.55077e-6,,8.29082e-25
HSO4-1,1.20427e-6,1.20427e-6,,4.60019e-26
HS-1,1.27547e-7,1.27547e-7,,5.03654e-27
CaCO3 (Calcite),1.21388e-7,1.21388e-7,0.0,9.90013e-18
CaCl2 (Hydrophilite),1.05191e-7,1.05191e-7,0.0,5.95773e-37
MgSO4,5.54034e-8,5.54034e-8,0.0,3.10158e-29
CaClCH3OH+1,4.41998e-8,4.41998e-8,,7.68116e-26
Ba+2,3.4029e-8,3.4029e-8,,1.77773e-20

MgCO3,3.06949e-8,3.06949e-8,0.0,2.37414e-23
CO3-2,2.03086e-8,2.03086e-8,,1.65018e-31
S2O3-2,5.69462e-9,5.69462e-9,,2.75138e-33
NH4OH,5.30321e-9,5.30321e-9,,2.24375e-24
NH3,1.51862e-9,1.51862e-9,,7.16382e-23
Na2SO4.NaHSO4,1.43734e-9,1.43734e-9,0.0,3.90819e-31
NH2CO2-1,6.98932e-10,6.98932e-10,,1.34373e-29
MgOH+1,1.28292e-10,1.28292e-10,,5.99909e-22
OH-1,3.85968e-11,3.85968e-11,,9.03659e-24
HO(CH2CH2O)3CO2(-1),2.50233e-11,2.50233e-11,,6.19498e-31
CaOH+1,2.13556e-11,2.13556e-11,,5.05582e-23
MgClCH3OH+1,4.98893e-12,4.98893e-12,,2.09312e-27
S5-2,4.05472e-12,4.05472e-12,,4.06366e-36
HS2O3-1,2.67735e-12,2.67735e-12,,9.32097e-32
S4-2,1.00628e-12,1.00628e-12,,1.0085e-36
H2,4.70817e-13,4.70817e-13,,2.96808e-29
CH5O+1,3.99178e-13,3.99178e-13,,4.97816e-44
HSO3-1,3.75186e-13,3.75186e-13,,1.18667e-32
CH3OH.HCl,2.19045e-13,2.19045e-13,,1.69197e-28
HCl,1.64147e-13,1.64147e-13,,1.61368e-27
S3-2,1.51023e-13,1.51023e-13,,1.51356e-37
BaCO3 (Witherite),6.90259e-14,6.90259e-14,0.0,5.3389e-29
C6H15O4+1,2.60824e-14,2.60824e-14,,2.34461e-34
SrOH+1,1.99778e-14,1.99778e-14,,1.76725e-25
S2-2,1.37118e-14,1.37118e-14,,1.3742e-38
CH3O-1,1.00092e-14,1.00092e-14,,3.4903e-34
SrCO3 (Strontianite),9.53293e-15,9.53293e-15,0.0,7.37337e-30
SO3-2,2.66969e-15,2.66969e-15,,1.35965e-39
SO2,9.63544e-16,9.63544e-16,,1.04937e-29
CO2S,5.92724e-16,5.92724e-16,,4.5845e-31
H2S2O3,4.69468e-16,4.69468e-16,,3.63116e-31
NaOH.Na2SO4,4.11787e-16,4.11787e-16,,1.33848e-44
S1,3.02821e-16,3.02821e-16,,2.34221e-31
S2,2.99296e-16,2.99296e-16,,2.31495e-31
S3,2.95796e-16,2.95796e-16,,2.28788e-31
S4,2.92371e-16,2.92371e-16,,2.26138e-31
S5,2.88996e-16,2.88996e-16,,2.23528e-31
S6,2.85671e-16,2.85671e-16,,2.20956e-31
S7,2.82282e-16,2.82282e-16,,2.18335e-31
H2SO4,7.14273e-17,7.14273e-17,,1.03485e-35
C6H13O4-1,5.31233e-17,5.31233e-17,,1.80778e-36
BaOH+1,2.25441e-17,2.25441e-17,,9.15714e-43
NaOH,2.01232e-17,2.01232e-17,0.0,2.62933e-30
S-2,9.78157e-18,9.78157e-18,,1.04835e-40
NaOHCO3-2,1.60127e-19,1.60127e-19,,1.6048e-43
MgCl2,2.09761e-20,2.09761e-20,0.0,8.15975e-35
S2O5-2,3.96979e-25,3.96979e-25,,3.96677e-49
S2O4-2,6.52858e-29,6.52858e-29,,6.54298e-53
SO3,9.30206e-31,9.30206e-31,,1.52381e-49
S2O6-2,1.59968e-31,1.59968e-31,,1.6032e-55
Fe+2,2.94449e-32,2.94449e-32,,3.10251e-49
S5O6-2,7.37514e-33,7.37514e-33,,7.3914e-57
N2H5+1,2.87871e-35,2.87871e-35,,1.34525e-46
FeHS+1,9.50339e-36,9.50339e-36,,4.44389e-47

FeH(CO3)2-1,7.41251e-36,7.41251e-36,,2.5806e-55
FeCl+1,5.96489e-36,5.96489e-36,,1.85022e-48
FeSO4,4.60865e-36,4.60865e-36,0.0,3.5606e-51
FeS (Pyrrhotite),1.77938e-37,1.77938e-37,0.0,1.37629e-52
FeOH+1,6.12747e-38,6.12747e-38,,2.86528e-49
Fe(NH3)+2,2.20129e-38,2.20129e-38,,6.11469e-53
N2H4,2.323e-39,2.323e-39,,2.42127e-56
NH2OH2+1,2.13326e-39,2.13326e-39,,9.92617e-51
N2H6+2,6.27765e-40,6.27765e-40,,1.13432e-47
NH2OH,2.46162e-41,2.46162e-41,0.0,1.05326e-56
FeO+1,4.37954e-43,4.37954e-43,,2.04792e-54
FeOH+2,2.00368e-43,2.00368e-43,,3.62282e-51
Fe(NH3)2+2,1.63821e-43,1.63821e-43,,4.55058e-58
FeCl+2,3.9718e-44,3.9718e-44,,1.01998e-61
FeO,6.96289e-45,6.96289e-45,,5.38554e-60
Fe+3,3.29789e-45,3.29789e-45,,6.45494e-59
HFeO2,1.92016e-45,1.92016e-45,,1.48517e-60
NH2Cl,9.93973e-47,9.93973e-47,,7.68801e-62
FeCl2+1,9.69919e-48,9.69919e-48,,2.70195e-69
HClO,4.3224e-48,4.3224e-48,,3.34322e-63
FeHSO4+2,3.92765e-48,3.92765e-48,,7.43828e-56
Cl2,6.98941e-49,6.98941e-49,,5.40605e-64
Fe(NH3)3+2,3.00865e-49,3.00865e-49,,8.35738e-64
FeO2-1,1.49296e-50,1.49296e-50,,5.1976e-70
ClO-1,3.39708e-51,3.39708e-51,,1.18266e-70
NO,8.82335e-52,8.82335e-52,,1.30194e-65
HFeO2-1,2.65937e-52,2.65937e-52,,9.25835e-72
N2O,3.61467e-53,3.61467e-53,,1.04545e-66
NH3Cl+1,3.95223e-57,3.95223e-57,,1.84811e-68
Fe(NH3)4+2,6.54367e-58,6.54367e-58,,1.81769e-72
HSO5-1,2.36016e-60,2.36016e-60,,8.21668e-80
NO2-1,1.49446e-61,1.49446e-61,,4.68122e-81
HNO2,1.16594e-62,1.16594e-62,,9.0181e-78
Fe(NH3)5+2,1.42326e-66,1.42326e-66,,3.95351e-81
O2,4.47003e-71,4.47003e-71,,2.79505e-87
S2O8-2,4.73868e-72,4.73868e-72,,4.74912e-96
Fe(NH3)6+2,3.09552e-75,3.09552e-75,,8.59868e-90
NO2,1.1026e-76,1.1026e-76,,9.52813e-90
NO3-1,6.55506e-81,6.55506e-81,,1.24259e-100
HNO3,1.08872e-86,1.08872e-86,,4.35022e-107
Fe2(OH)2+4,9.35783e-87,8.73976e-87,,6.18069e-88
NHCl2,2.47184e-87,2.47184e-87,,1.91187e-102
NH4NO3.(NH4)2SO4,3.707e-91,3.707e-91,0.0,2.86722e-106
ClO2-1,9.14822e-94,9.14822e-94,,3.18487e-113
NH2Cl2+1,8.92961e-95,8.92961e-95,,4.17559e-106
HClO2,3.43483e-96,3.43483e-96,,2.65671e-111
FeO4-2,3.1026e-99,3.1026e-99,,3.10944e-123
ClO2,1.01368e-112,1.01368e-112,,7.84047e-128
ClO3-1,1.43915e-122,1.43915e-122,,0.0
NCl3,4.87314e-129,4.87314e-129,,0.0
N2O3,2.72086e-129,2.72086e-129,,0.0
Total (by phase),5.71816,5.71598,1.39679e-3,7.78914e-4

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H(+1),10.6729,10.6689,4.00403e-3,1.99487e-14
K(+1),2.65996e-4,2.65996e-4,0.0,5.63643e-19
Na(+1),0.119596,0.119596,0.0,7.94701e-23
N(-3),1.43242e-3,1.43242e-3,0.0,2.76366e-15
Ba(+2),8.37399e-5,3.4029e-8,8.37059e-5,1.77773e-20
Ca(+2),7.04376e-3,6.04276e-3,1.00101e-3,9.90018e-18
Fe(+2),2.59638e-4,1.39409e-31,0.0,2.59638e-4
Mg(+2),8.45505e-3,8.45505e-3,0.0,6.23653e-22
Fe(+3),6.83271e-43,6.83271e-43,0.0,3.62494e-51
O(-2),5.57625,5.56847,7.26045e-3,5.19276e-4
Cl(-1),0.139239,0.13872,0.0,5.19276e-4
C(+4),0.109039,0.108779,0.0,2.59638e-4
S(+4),3.78819e-13,3.78819e-13,0.0,1.05055e-29
S(+6),5.91297e-3,4.59836e-3,1.31461e-3,7.0029e-22
S(-2),5.07152e-5,5.07152e-5,0.0,8.52247e-19
S(+2),1.13946e-8,1.13946e-8,0.0,9.18155e-31
N(+3),1.61106e-61,1.61106e-61,0.0,9.02278e-78
N(+5),6.55508e-81,6.55508e-81,0.0,1.2426e-100
Sr(+2),2.71627e-4,4.17313e-5,2.29896e-4,7.06993e-22
N(0),1.55461e-3,1.55461e-3,0.0,1.86761e-13
H(0),9.41634e-13,9.41634e-13,0.0,5.93616e-29
O(0),8.94006e-71,8.94006e-71,0.0,5.5901e-87
S(+8),2.36016e-60,2.36016e-60,0.0,8.21668e-80
Cl(+1),1.04422e-46,1.04422e-46,0.0,8.0764e-62
Cl(+5),1.43915e-122,1.43915e-122,0.0,0.0
S(+3),1.30572e-28,1.30572e-28,0.0,1.3086e-52
S(+5),3.19935e-31,3.19935e-31,0.0,3.20641e-55
S(+7),9.47735e-72,9.47735e-72,0.0,9.49825e-96
N(+2),8.82335e-52,8.82335e-52,0.0,1.30194e-65
N(+4),1.1026e-76,1.1026e-76,0.0,9.52813e-90
Cl(+3),9.18257e-94,9.18257e-94,0.0,2.68856e-111
Cl(+4),1.01368e-112,1.01368e-112,0.0,7.84047e-128
N(+1),7.22934e-53,7.22934e-53,0.0,2.0909e-66
N(-2),5.75801e-35,5.75801e-35,0.0,2.91737e-46
C(+2),5.14928e-5,5.14928e-5,0.0,3.98278e-20
Fe(+6),3.1026e-99,3.1026e-99,0.0,3.10944e-123
S(0),6.57524e-4,9.76868e-8,6.57426e-4,6.609e-15
MeO(-1),5.83154e-4,5.83154e-4,0.0,1.03596e-18
N(-1),2.15788e-39,2.15788e-39,0.0,9.92618e-51
TEGION,1.76328e-5,1.76328e-5,0.0,1.99685e-24

Element Distribution

,Total,Total,Liquid-1,Solid,Liquid-2
,mol,mole %,% of Total,% of Total,% of Total
H(+1),10.6729,64.1259,99.9625,0.0375158,1.8691e-13
K(+1),2.65996e-4,1.59818e-3,100.0,0.0,2.11899e-13

Na(+1),0.119596,0.718565,100.0,0.0,6.6449e-20
N(-3),1.43242e-3,8.60636e-3,100.0,0.0,1.92937e-10
Ba(+2),8.37399e-5,5.03133e-4,0.0406366,99.9594,2.12292e-14
Ca(+2),7.04376e-3,0.042321,85.7888,14.2112,1.40552e-13
Fe(+2),2.59638e-4,1.55998e-3,5.36935e-26,0.0,100.0
Mg(+2),8.45505e-3,0.0508004,100.0,0.0,7.3761e-18
Fe(+3),6.83271e-43,4.10529e-42,100.0,0.0,5.30528e-7
O(-2),5.57625,33.5037,99.8605,0.130203,9.31228e-3
Cl(-1),0.139239,0.83659,99.6271,0.0,0.372937
C(+4),0.109039,0.655138,99.7619,0.0,0.238114
S(+4),3.78819e-13,2.27605e-12,100.0,0.0,2.77323e-15
S(+6),5.91297e-3,0.0355268,77.7674,22.2326,1.18433e-17
S(-2),5.07152e-5,3.04711e-4,100.0,0.0,1.68046e-12
S(+2),1.13946e-8,6.8462e-8,100.0,0.0,8.05781e-21
N(+3),1.61106e-61,9.67968e-61,100.0,0.0,5.60054e-15
N(+5),6.55508e-81,3.93848e-80,100.0,0.0,1.89563e-18
Sr(+2),2.71627e-4,1.63202e-3,15.3634,84.6366,2.6028e-16
N(0),1.55461e-3,9.34056e-3,100.0,0.0,1.20133e-8
H(0),9.41634e-13,5.65761e-12,100.0,0.0,6.3041e-15
O(0),8.94006e-71,5.37145e-70,100.0,0.0,6.25287e-15
S(+8),2.36016e-60,1.41805e-59,100.0,0.0,3.48141e-18
Cl(+1),1.04422e-46,6.27397e-46,100.0,0.0,7.73438e-14
Cl(+5),1.43915e-122,8.64682e-122,100.0,0.0,0.0
S(+3),1.30572e-28,7.84512e-28,100.0,0.0,1.00221e-22
S(+5),3.19935e-31,1.92226e-30,100.0,0.0,1.00221e-22
S(+7),9.47735e-72,5.69426e-71,100.0,0.0,1.00221e-22
N(+2),8.82335e-52,5.30132e-51,100.0,0.0,1.47557e-12
N(+4),1.1026e-76,6.62472e-76,100.0,0.0,8.64154e-12
Cl(+3),9.18257e-94,5.51715e-93,100.0,0.0,2.9279e-16
Cl(+4),1.01368e-112,6.0905e-112,100.0,0.0,7.73463e-14
N(+1),7.22934e-53,4.34359e-52,100.0,0.0,2.89224e-12
N(-2),5.75801e-35,3.45958e-34,100.0,0.0,5.06663e-10
C(+2),5.14928e-5,3.09384e-4,100.0,0.0,7.73463e-14
Fe(+6),3.1026e-99,1.86413e-98,100.0,0.0,1.00221e-22
S(0),6.57524e-4,3.95059e-3,0.0148568,99.9851,1.00513e-9
MeO(-1),5.83154e-4,3.50376e-3,100.0,0.0,1.77648e-13
N(-1),2.15788e-39,1.29651e-38,100.0,0.0,4.59997e-10
TEGION,1.76328e-5,1.05943e-4,100.0,0.0,1.13246e-17

Calculation Summary
06-2 Alloy-1 Calculation

Unit Set: Custom

Automatic Chemistry Model
,Aqueous (H+ ion) Databanks:
,,Corrosion (AQ)
,,Aqueous (H+ ion)
,Second Liquid phase
,Redox selected
,Using K-fit Polynomials
,,T-span: 25.0 - 225.0
,,P-span: 1.0 - 1500.0

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Super13Cr stainless steel

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,26.8580,26.8580
CO2,0.496331,0.496331
BaCl2,2.64786e-7,2.64786e-7
CaCl2,4.68554e-3,4.68554e-3
CaO,0.0299828,0.0299828
FeCl2,1.29819e-3,1.29819e-3
KCl,1.32998e-3,1.32998e-3
MgCl2,0.0422753,0.0422753
NaCl,0.597978,0.597978
SO3,0.0197968,0.0197968

SrCl2,1.85257e-4,1.85257e-4
BaSO4,4.18435e-4,4.18435e-4
SrSO4,1.17288e-3,1.17288e-3
N2,5.66215e-4,5.66215e-4
CO,2.10063e-4,2.10063e-4
O2,1.05800e-5,1.05800e-5
CH3OH,4.25367e-4,4.25367e-4
H2S,5.01990e-5,5.01990e-5
SO2,9.00972e-4,9.00972e-4
NO2,9.11658e-5,9.11658e-5
C6H14O4,9.05743e-6,9.05743e-6
CaSO4,5.50454e-4,5.50454e-4

Calculated Rates

Corrosion Rate,1.29839e-3,mm/yr
Corrosion Potential,-0.293963,V (SHE)
Repassivation Potential*,-0.133014,V (SHE)
Corrosion Current Density,1.19644e-3,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4 (Anhydrite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.0.5H2O (Bassanite),0.29446
,CaSO4.2H2O (Gypsum),0.922586
,FeCO3 (Siderite),0.187394
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,28.0562,mol
Temperature,43.0000,°C
Pressure,2641.00,psia

Aqueous Properties
pH,4.19488,
Ionic Strength (x-based),0.0287339,mol/mol
Ionic Strength (m-based),1.70660,mol/kg
ORP,0.0227779,V (SHE)
Osmotic Pressure,1472.75,psia
Specific Electrical Conductivity,1.48955e5,µmho/cm
"Electrical Conductivity, molar",6.39956e-3,m2/ohm-mol
"Viscosity, absolute",0.764063,cP
"Viscosity, relative",1.23559,

Standard Liquid Volume,0.526616,L
"Volume, Std. Conditions",0.513826,L
"Total Dissolved Solids, Estimated",85695.7,mg/L
Hardness,14896.0,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,5.17481e-5,L

Thermodynamic Properties
 ,Unit,Total,Aqueous,Solid
Density,g/ml,1.06666,1.06613,3.71837
Enthalpy,J,-8.15795e6,-8.15483e6,-3114.63

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

 ,Total,Aqueous,Solid
 ,mol,mol,mol
Mole (True),28.7298,28.7276,2.25059e-3
Mole (App),28.0560,28.0537,2.25059e-3
 ,g,g,g
Mass,549.239,548.854,0.385094
 ,L,L,cm3
Volume,0.514915,0.514811,0.103565

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
FeS2 (Pyrite),1.00000,2.55092e6
BaSO4 (Barite),1.00000,1770.28
CaSO4 (Anhydrite),1.00000,1.09689
SrSO4 (Celestine),1.00000,2.65686
CaSO4.2H2O (Gypsum),0.922586,1.00981
CaSO4.0.5H2O (Bassanite),0.294460,0.322819
FeS2(marcasite) (Marcasite),0.280070,7.14436e5
FeCO3 (Siderite),0.187394,0.209736
CaCO3 (Calcite),0.0496729,0.0514773
CaCO3 (Aragonite),0.0316558,0.0328057
NaHCO3 (Nahcolite),0.0211529,0.0218644
NaCl (Halite),0.0206550,0.0206104
Na2SO4 (Thenardite),5.07165e-3,5.47579e-3
SrCO3 (Strontianite),3.33672e-3,8.37567e-3
MgSO4.7H2O (Epsomite),2.40337e-3,2.54754e-3
FeO(OH) (Lepidocrocite),8.31691e-4,3.15493e-4
FeSO4.7H2O (Melanterite),5.09046e-4,5.98533e-4
Sr(HCO3)2,4.39617e-4,1.15580e-3
KCl (Sylvite),1.59631e-4,1.58922e-4
MgCO3 (Magnesite),1.36054e-4,1.37278e-4
FeS (Pyrrhotite),3.63196e-5,0.168587
FeS(mackinawite) (Mackinawite),7.81792e-7,3.62889e-3

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
H2O,26.8485,26.8485,
Cl-1,0.696189,0.696189,
Na+1,0.593333,0.593333,
CO2,0.477533,0.477533,
Mg+2,0.0347529,0.0347529,
Ca+2,0.033671,0.033671,
SO4-2,0.0153506,0.0153506,
HCO3-1,0.0110354,0.0110354,
MgHCO3+1,5.15762e-3,5.15762e-3,
NaHCO3 (Nahcolite),2.59927e-3,2.59927e-3,0.0
MgSO4,2.36459e-3,2.36459e-3,0.0
NaSO4-1,2.04597e-3,2.04597e-3,
CaSO4 (Anhydrite),1.5428e-3,6.72275e-4,8.70521e-4
K+1,1.29085e-3,1.29085e-3,
Fe+2,1.17484e-3,1.17484e-3,
SrSO4 (Celestine),8.74724e-4,3.42421e-5,8.40482e-4
N2,5.95053e-4,5.95053e-4,
Sr+2,4.83413e-4,4.83413e-4,
CH3OH,4.25367e-4,4.25367e-4,
BaSO4 (Barite),4.18445e-4,,4.18445e-4
CO,2.10063e-4,2.10063e-4,
FeS2 (Pyrite),1.21147e-4,,1.21147e-4
H+1,3.69495e-5,3.69495e-5,
NH4+1,3.24677e-5,3.24677e-5,
KSO4-1,3.22204e-5,3.22204e-5,
HSO4-1,1.70943e-5,1.70943e-5,
C6H14O4,9.05743e-6,9.05743e-6,
KCl (Sylvite),6.91104e-6,6.91104e-6,0.0
CaHCO3+1,4.03273e-6,4.03273e-6,
FeCl+1,1.18036e-6,1.18036e-6,
NH4SO4-1,1.02105e-6,1.02105e-6,
FeHCO3+1,7.23824e-7,7.23824e-7,
CaCO3 (Calcite),6.62299e-7,6.62299e-7,0.0
CaCl+1,3.27308e-7,3.27308e-7,
FeCO3 (Siderite),2.90283e-7,2.90283e-7,0.0
Ba+2,1.80341e-7,1.80341e-7,
MgCO3 (Magnesite),1.28777e-7,1.28777e-7,0.0
CO3-2,1.14645e-7,1.14645e-7,
BaCl(+1),6.31405e-8,6.31405e-8,
NaCO3-1,2.3712e-8,2.3712e-8,
BaHCO3+1,1.11666e-8,1.11666e-8,
FeOH+1,9.66337e-9,9.66337e-9,
H2S,3.75266e-9,3.75266e-9,
FeCl2 (Lawrencite),2.22564e-9,2.22564e-9,0.0
MgOH+1,1.71528e-9,1.71528e-9,
OH-1,4.16898e-10,4.16898e-10,
NH3,3.56546e-10,3.56546e-10,

KHSO4 (Mercallite),3.47717e-10,3.47717e-10,0.0
FeHS+1,2.37262e-10,2.37262e-10,
CaOH+1,9.88452e-11,9.88452e-11,
HCl,4.11956e-11,4.11956e-11,
HS-1,1.94316e-11,1.94316e-11,
NH2CO2-1,1.3517e-11,1.3517e-11,
Fe(NH3)+2,1.21885e-11,1.21885e-11,
Fe(CO3)2-2,2.52632e-12,2.52632e-12,
S2O3-2,1.27585e-12,1.27585e-12,
HSO3-1,7.33526e-13,7.33526e-13,
NaS2O3-1,6.87045e-13,6.87045e-13,
SrOH+1,4.75355e-13,4.75355e-13,
H2,4.09916e-13,4.09916e-13,
BaCO3 (Witherite),1.7702e-13,1.7702e-13,0.0
FeOH+2,9.52276e-14,9.52276e-14,
Fe(OH)2+1,2.63668e-14,2.63668e-14,
Fe+3,1.6199e-14,1.6199e-14,
SO3-2,4.91273e-15,4.91273e-15,
KS2O3-1,4.78933e-15,4.78933e-15,
SO2,2.90386e-15,2.90386e-15,
Fe(OH)3 (Bernalite),2.60754e-15,2.60754e-15,0.0
FeCl2+1,2.72925e-16,2.72925e-16,
FeCl+2,1.19108e-16,1.19108e-16,
FeSO4+1,5.42286e-17,5.42286e-17,
BaOH+1,1.7047e-17,1.7047e-17,
FeCl3 (Molysite),5.38285e-18,5.38285e-18,0.0
CaCl2 (Hydrophilite),1.68677e-18,1.68677e-18,0.0
Fe(NH3)2+2,6.89253e-19,6.89253e-19,
S-2,5.42679e-19,5.42679e-19,
Fe(OH)4-1,1.34504e-19,1.34504e-19,
FeCl4-1,8.84926e-20,8.84926e-20,
H2SO4,1.95634e-20,1.95634e-20,
FeS(HS)-1,2.69065e-21,2.69065e-21,
S2-2,2.565e-21,2.565e-21,
HFeO2-1,4.26972e-22,4.26972e-22,
S3-2,4.85922e-24,4.85922e-24,
SO3,3.05747e-24,3.05747e-24,
Fe(NH3)3+2,1.03245e-26,1.03245e-26,
S4-2,5.6979e-27,5.6979e-27,
S2O5-2,1.18161e-28,1.18161e-28,
Fe2(OH)2+4,4.63999e-29,4.63999e-29,
S2O6-2,8.86517e-30,8.86517e-30,
S2O4-2,7.989e-30,7.989e-30,
S5-2,4.14421e-30,4.14421e-30,
Na2S2O4,3.04311e-31,3.04311e-31,0.0
N2H5+1,2.3203e-36,2.3203e-36,
Fe(NH3)4+2,2.57493e-37,2.57493e-37,
N2H4,3.83775e-40,3.83775e-40,
NH2OH,1.41248e-40,1.41248e-40,
S5O6-2,1.88584e-42,1.88584e-42,
NO,6.75665e-48,6.75665e-48,
Fe(NH3)5+2,6.42362e-48,6.42362e-48,
N2O,1.00483e-49,1.00483e-49,
HSO5-1,6.34218e-55,6.34218e-55,

NO2-1,4.6714e-56,4.6714e-56,
HNO2,1.44293e-57,1.44293e-57,
Fe(NH3)6+2,1.60205e-58,1.60205e-58,
FeO4-2,9.64316e-63,9.64316e-63,
O2,3.53622e-64,3.53622e-64,
S2O8-2,1.67686e-65,1.67686e-65,
NO2,6.72487e-70,6.72487e-70,
NO3-1,2.68209e-73,2.68209e-73,
NaNO3 (Nitratine),2.3388e-74,2.3388e-74,0.0
Ca(NO3)+1,1.27799e-74,1.27799e-74,
SrNO3+1,2.01766e-76,2.01766e-76,
NH4NO3 (Gwihabaite),7.15182e-77,7.15182e-77,0.0
HNO3,3.33589e-82,3.33589e-82,
FeNO3+2,2.02635e-89,2.02635e-89,
Total (by phase),28.7298,28.7276,2.25059e-3

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
H(+1),53.716,53.716,0.0
K(+1),1.32998e-3,1.32998e-3,0.0
Na(+1),0.597978,0.597978,0.0
N(-3),3.34891e-5,3.34891e-5,0.0
Ba(+2),4.18699e-4,2.54648e-7,4.18445e-4
Ca(+2),0.0352188,0.0343483,8.70521e-4
Fe(+2),1.29819e-3,1.17704e-3,1.21147e-4
Mg(+2),0.0422753,0.0422753,0.0
Fe(+3),1.40853e-13,1.40853e-13,0.0
O(-2),27.9508,27.9423,8.51779e-3
Cl(-1),0.696197,0.696197,0.0
C(+4),0.496331,0.496331,0.0
S(+4),7.41343e-13,7.41343e-13,0.0
S(+6),0.0226475,0.020518,2.12945e-3
S(-2),1.21151e-4,4.00935e-9,1.21147e-4
S(+2),3.93536e-12,3.93536e-12,0.0
N(+3),4.81569e-56,4.81569e-56,0.0
N(+5),3.0465e-73,3.0465e-73,0.0
Sr(+2),1.35814e-3,5.17655e-4,8.40482e-4
N(0),1.19011e-3,1.19011e-3,0.0
H(0),8.19833e-13,8.19833e-13,0.0
O(0),7.07243e-64,7.07243e-64,0.0
S(+8),6.34218e-55,6.34218e-55,0.0
S(+3),1.65866e-29,1.65866e-29,0.0
S(+5),1.77303e-29,1.77303e-29,0.0
S(+7),3.35371e-65,3.35371e-65,0.0
N(+2),6.75665e-48,6.75665e-48,0.0
N(+4),6.72487e-70,6.72487e-70,0.0
N(+1),2.00966e-49,2.00966e-49,0.0
N(-2),4.64137e-36,4.64137e-36,0.0
C(+2),2.10063e-4,2.10063e-4,0.0

Fe(+6),9.64316e-63,9.64316e-63,0.0
S(0),1.21147e-4,2.57474e-21,1.21147e-4
N(-1),1.41248e-40,1.41248e-40,0.0
METHANOL,4.25367e-4,4.25367e-4,0.0
TRIETLNGLY,9.05743e-6,9.05743e-6,0.0

Element Distribution

 ,Total,Total,Aqueous,Solid
,mol,mole %,% of Total,% of Total
H(+1),53.716,64.2813,100.0,0.0
K(+1),1.32998e-3,1.59157e-3,100.0,0.0
Na(+1),0.597978,0.715594,100.0,0.0
N(-3),3.34891e-5,4.0076e-5,100.0,0.0
Ba(+2),4.18699e-4,5.01053e-4,0.0608187,99.9392
Ca(+2),0.0352188,0.042146,97.5283,2.47175
Fe(+2),1.29819e-3,1.55353e-3,90.668,9.33198
Mg(+2),0.0422753,0.0505903,100.0,0.0
Fe(+3),1.40853e-13,1.68557e-13,100.0,0.0
O(-2),27.9508,33.4484,99.9695,0.0304743
Cl(-1),0.696197,0.833131,100.0,0.0
C(+4),0.496331,0.593954,100.0,0.0
S(+4),7.41343e-13,8.87156e-13,100.0,0.0
S(+6),0.0226475,0.027102,90.5974,9.40259
S(-2),1.21151e-4,1.4498e-4,3.30939e-3,99.9967
S(+2),3.93536e-12,4.7094e-12,100.0,0.0
N(+3),4.81569e-56,5.76288e-56,100.0,0.0
N(+5),3.0465e-73,3.64571e-73,100.0,0.0
Sr(+2),1.35814e-3,1.62527e-3,38.1151,61.8849
N(0),1.19011e-3,1.42419e-3,100.0,0.0
H(0),8.19833e-13,9.81085e-13,100.0,0.0
O(0),7.07243e-64,8.4635e-64,100.0,0.0
S(+8),6.34218e-55,7.58961e-55,100.0,0.0
S(+3),1.65866e-29,1.9849e-29,100.0,0.0
S(+5),1.77303e-29,2.12177e-29,100.0,0.0
S(+7),3.35371e-65,4.01335e-65,100.0,0.0
N(+2),6.75665e-48,8.08561e-48,100.0,0.0
N(+4),6.72487e-70,8.04757e-70,100.0,0.0
N(+1),2.00966e-49,2.40494e-49,100.0,0.0
N(-2),4.64137e-36,5.55428e-36,100.0,0.0
C(+2),2.10063e-4,2.5138e-4,100.0,0.0
Fe(+6),9.64316e-63,1.15399e-62,100.0,0.0
S(0),1.21147e-4,1.44975e-4,2.1253e-15,100.0
N(-1),1.41248e-40,1.6903e-40,100.0,0.0
METHANOL,4.25367e-4,5.09032e-4,100.0,0.0
TRIETLNGLY,9.05743e-6,1.08389e-5,100.0,0.0

Calculation Summary
06-2 Alloy-4 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2205

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,26.8580,26.8580
CO2,0.496331,0.496331
BaCl2,2.64786e-7,2.64786e-7
CaCl2,4.68554e-3,4.68554e-3
CaO,0.0299828,0.0299828
FeCl2,1.29819e-3,1.29819e-3
KCl,1.32998e-3,1.32998e-3
MgCl2,0.0422753,0.0422753
NaCl,0.597978,0.597978
SO3,0.0197968,0.0197968
SrCl2,1.85257e-4,1.85257e-4
BaSO4,4.18435e-4,4.18435e-4

SrSO4,1.17288e-3,1.17288e-3
N2,5.66215e-4,5.66215e-4
CO,2.10063e-4,2.10063e-4
O2,1.05800e-5,1.05800e-5
CH3OH,4.25367e-4,4.25367e-4
H2S,5.01990e-5,5.01990e-5
SO2,9.00972e-4,9.00972e-4
NO2,9.11658e-5,9.11658e-5
C6H14O4,9.05743e-6,9.05743e-6
CaSO4,5.50454e-4,5.50454e-4

Calculated Rates

Corrosion Rate,2.07756e-4,mm/yr
Corrosion Potential,-0.290500,V (SHE)
Repassivation Potential*,1.59331e-3,V (SHE)
Corrosion Current Density,1.96761e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4 (Anhydrite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.131726
,CaSO4.0.5H2O (Bassanite),0.194356
,CaCO3 (Calcite),0.172508
,CaSO4.2H2O (Gypsum),0.914166
,FeCO3 (Siderite),0.176107
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,28.0562,mol
Temperature,43.0000,°C
Pressure,2641.00,psia

Liquid 1 Properties
pH,4.39230,
Ionic Strength (x-based),0.0284465,mol/mol
Ionic Strength (m-based),1.68926,mol/kg
Dielectric Constant,53.2439,
ORP,5.01637e-4,V (SHE)
Osmotic Pressure,1554.46,psia
Specific Electrical Conductivity,1.47933e5,µmho/cm
"Viscosity, absolute",0.758908,cP
Thermal Conductivity,543.880,cal/hr m °C

Surface Tension,0.0739733,N/m
Standard Liquid Volume,0.526600,L
"Volume, Std. Conditions",0.513711,L
"Total Dissolved Solids, Estimated",85617.6,mg/L
Hardness,14842.8,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,6.72547e-5,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid
Density,g/ml,1.06680,1.06614,3.66824
Enthalpy,J,-8.15917e6,-8.15521e6,-3957.69

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
Mole (True),28.7259,28.7230,2.83512e-3
Mole (App),28.0554,28.0525,2.83512e-3
,g,g,g
Mass,549.241,548.762,0.478867
,L,L,cm3
Volume,0.514848,0.514717,0.130544

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
FeS2 (Pyrite),1.00000,6.28673e5
BaSO4 (Barite),1.00000,1534.07
CaSO4 (Anhydrite),1.00000,1.20782
SrSO4 (Celestine),1.00000,7.34371
CaSO4.2H2O (Gypsum),0.914166,1.10370
H2O,0.612511,0.612386
CaSO4.0.5H2O (Bassanite),0.282476,0.341146
FeS2(marcasite) (Marcasite),0.280054,1.76062e5
CaSO4.0.5H2O (Bassanite),0.194356,0.234723
FeCO3 (Siderite),0.176107,0.199101
CaCO3 (Calcite),0.172508,0.181932
CaCO3 (Aragonite),0.131726,0.138922
NaHCO3 (Nahcolite),0.0308300,0.0312021
NaCl (Halite),0.0215970,0.0215707
NaCl.2H2O (hydrohalite),0.0146354,0.0146117
SrCO3 (Strontianite),9.67887e-3,0.0620638
Na2SO4.CaSO4 (Glauberite),7.01183e-3,9.92179e-3
Na2SO4 (Thenardite),2.60625e-3,3.05332e-3
Na2SO4.5CaSO4.3H2O,2.11017e-3,6.35069e-3
Na2SO4.10H2O (Mirabilite),1.57568e-3,1.84221e-3
MgSO4.7H2O (Epsomite),4.11903e-4,4.70272e-4
MgSO4.6H2O (Hexahydrite),2.83858e-4,3.24148e-4

MgCO3,2.07321e-4,2.06973e-4
Na2SO4,1.74398e-4,2.04313e-4
MgSO4.12H2O,1.73895e-4,1.98334e-4
MgSO4.5H2O (Pentahydrite),1.45461e-4,1.66141e-4
KCl (sylvite),1.32085e-4,1.31804e-4
FeS (Pyrrhotite),1.21908e-5,0.0259103
BaCO3 (Witherite),1.66883e-6,2.23538e-3
FeS (Mackinawite),2.53453e-7,5.38687e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid
,mol,mol,mol
H2O,26.8485,26.8485,0.0
Cl-1,0.696195,0.696195,
Na+1,0.591641,0.591641,
CO2,0.476496,0.476496,
Mg+2,0.0359165,0.0359165,
Ca+2,0.0315665,0.0315665,
HCO3-1,0.0187589,0.0187589,
SO4-2,0.0110777,0.0110777,
NaMgSO4+1,6.33703e-3,6.33703e-3,
CaSO4 (Anhydrite),3.64821e-3,2.48976e-3,1.15845e-3
K+1,1.30943e-3,1.30943e-3,
SrSO4 (Celestine),1.14275e-3,4.06916e-6,1.13868e-3
FeCO2+2,1.07258e-3,1.07258e-3,
N2,5.91475e-4,5.91475e-4,
CH3OH,4.25326e-4,4.25326e-4,
BaSO4 (Barite),4.18378e-4,,4.18378e-4
Sr+2,2.1539e-4,2.1539e-4,
CO,2.10063e-4,2.10063e-4,
FeS2 (Pyrite),1.19611e-4,,1.19611e-4
Fe+2,1.05825e-4,1.05825e-4,
NH4+1,4.06433e-5,4.06433e-5,
KMgSO4+1,2.05554e-5,2.05554e-5,
H3O+1,1.22413e-5,1.22413e-5,
C6H14O4,9.05739e-6,9.05739e-6,
HSO4-1,5.16673e-6,5.16673e-6,
CaCO3 (Calcite),3.06382e-6,3.06382e-6,0.0
CaCl2 (Hydrophilite),1.02868e-6,1.02868e-6,0.0
MgSO4,6.77491e-7,6.77491e-7,0.0
MgCO3,5.14381e-7,5.14381e-7,0.0
Ba+2,3.21466e-7,3.21466e-7,
CO3-2,3.19964e-7,3.19964e-7,
FeH(CO3)2-1,1.03547e-7,1.03547e-7,
FeCl+1,5.54682e-8,5.54682e-8,
CaClCH3OH+1,4.1388e-8,4.1388e-8,
H2S,1.89783e-8,1.89783e-8,
FeSO4,1.8387e-8,1.8387e-8,0.0
Na2SO4.NaHSO4,6.07612e-9,6.07612e-9,0.0
MgOH+1,3.2421e-9,3.2421e-9,

FeOH+1,9.12544e-10,9.12544e-10,
OH-1,8.58494e-10,8.58494e-10,
NH4OH,6.59562e-10,6.59562e-10,
CaOH+1,6.21027e-10,6.21027e-10,
NH3,2.26261e-10,2.26261e-10,
HS-1,1.08533e-10,1.08533e-10,
NH2CO2-1,9.65895e-11,9.65895e-11,
HO(CH2CH2O)3CO2(-1),3.91461e-11,3.91461e-11,
MgClCH3OH+1,9.89616e-12,9.89616e-12,
BaCO3 (Witherite),2.86433e-12,2.86433e-12,0.0
FeHS+1,2.59456e-12,2.59456e-12,
HCl,2.4826e-12,2.4826e-12,
S2O3-2,2.07674e-12,2.07674e-12,
SrCO3 (Strontianite),1.98715e-12,1.98715e-12,0.0
Fe(NH3)+2,1.70754e-12,1.70754e-12,
H2,1.0481e-12,1.0481e-12,
SrOH+1,6.3289e-13,6.3289e-13,
HSO3-1,4.65372e-13,4.65372e-13,
FeS (Pyrrhotite),3.48723e-13,3.48723e-13,0.0
CH3OH.HCl,2.14785e-13,2.14785e-13,
CH5O+1,2.11895e-13,2.11895e-13,
FeO+1,3.85848e-14,3.85848e-14,
CH3O-1,3.07887e-14,3.07887e-14,
C6H15O4+1,2.62595e-14,2.62595e-14,
FeOH+2,5.7187e-15,5.7187e-15,
SO3-2,4.18728e-15,4.18728e-15,
NaOH.Na2SO4,4.16818e-15,4.16818e-15,
NaOH,1.84916e-15,1.84916e-15,0.0
BaOH+1,1.42467e-15,1.42467e-15,
SO2,1.21293e-15,1.21293e-15,
HFeO2,8.09806e-16,8.09806e-16,
HS2O3-1,7.91283e-16,7.91283e-16,
H2SO4,6.19362e-16,6.19362e-16,
FeCl+2,5.72822e-16,5.72822e-16,
FeO,5.72288e-16,5.72288e-16,
C6H13O4-1,2.26132e-16,2.26132e-16,
Fe+3,3.85028e-17,3.85028e-17,
NaOHCO3-2,1.08292e-17,1.08292e-17,
CO2S,4.58835e-18,4.58835e-18,
S1,2.84911e-18,2.84911e-18,
MgCl2,8.30499e-19,8.30499e-19,0.0
Fe(NH3)2+2,2.42437e-19,2.42437e-19,
FeCl2+1,1.86326e-19,1.86326e-19,
H2S2O3,1.20311e-19,1.20311e-19,
S-2,4.85643e-20,4.85643e-20,
FeHSO4+2,3.65631e-20,3.65631e-20,
FeO2-1,1.76168e-20,1.76168e-20,
S2-2,1.59588e-20,1.59588e-20,
S2,9.73637e-22,9.73637e-22,
HFeO2-1,7.86564e-23,7.86564e-23,
S3-2,5.39857e-23,5.39857e-23,
S3,3.32707e-25,3.32707e-25,
S2O5-2,1.29736e-25,1.29736e-25,
S4-2,1.1304e-25,1.1304e-25,

Fe(NH3)3+2,9.11768e-27,9.11768e-27,
S5-2,1.46812e-28,1.46812e-28,
S4,1.13704e-28,1.13704e-28,
SO3,5.01199e-29,5.01199e-29,
S2O4-2,2.30836e-30,2.30836e-30,
Fe2(OH)2+4,9.1435e-31,9.1435e-31,
S2O6-2,5.86263e-31,5.86263e-31,
S5,3.88599e-32,3.88599e-32,
S8 (Sulfur),3.6428e-35,3.6428e-35,0.0
S6,1.32815e-35,1.32815e-35,
N2H5+1,2.82993e-36,2.82993e-36,
Fe(NH3)4+2,5.70913e-37,5.70913e-37,
NH2OH2+1,2.51409e-38,2.51409e-38,
S7,4.53774e-39,4.53774e-39,
NH2OH,9.52041e-40,9.52041e-40,0.0
N2H4,8.93604e-40,8.93604e-40,
N2H6+2,3.5251e-41,3.5251e-41,
S5O6-2,8.4774e-43,8.4774e-43,
HClO,2.52215e-44,2.52215e-44,
NH2Cl,3.97599e-45,3.97599e-45,
Cl2,1.59528e-45,1.59528e-45,
ClO-1,3.89391e-47,3.89391e-47,
Fe(NH3)5+2,3.57586e-47,3.57586e-47,
NO,6.25566e-48,6.25566e-48,
N2O,7.71373e-50,7.71373e-50,
NH3Cl+1,3.54969e-55,3.54969e-55,
HSO5-1,7.24919e-56,7.24919e-56,
NO2-1,1.86399e-56,1.86399e-56,
Fe(NH3)6+2,2.23906e-57,2.23906e-57,
HNO2,7.29524e-58,7.29524e-58,
FeO4-2,2.71174e-64,2.71174e-64,
O2,9.23353e-65,9.23353e-65,
S2O8-2,2.52721e-67,2.52721e-67,
NO2,9.77676e-71,9.77676e-71,
NO3-1,6.91282e-74,6.91282e-74,
HNO3,7.94713e-80,7.94713e-80,
NHCl2,4.70641e-83,4.70641e-83,
ClO2-1,1.71213e-86,1.71213e-86,
HClO2,5.74853e-89,5.74853e-89,
NH2Cl2+1,2.20622e-90,2.20622e-90,
NH4NO3.(NH4)2SO4,4.56905e-91,4.56905e-91,0.0
ClO2,2.71156e-104,2.71156e-104,
ClO3-1,8.93415e-113,8.93415e-113,
N2O3,2.28767e-120,2.28767e-120,
NCl3,5.06905e-122,5.06905e-122,
NHCl3+1,1.39579e-126,1.39579e-126,
Total (by phase),28.7259,28.723,2.83512e-3

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid

,mol,mol,mol
H(+1),53.7164,53.7164,0.0
K(+1),1.32998e-3,1.32998e-3,0.0
Na(+1),0.597978,0.597978,0.0
N(-3),4.06443e-5,4.06443e-5,0.0
Ba(+2),4.18699e-4,3.21469e-7,4.18378e-4
Ca(+2),0.0352188,0.0340604,1.15845e-3
Fe(+2),1.29819e-3,1.17858e-3,1.19611e-4
Mg(+2),0.0422753,0.0422753,0.0
Fe(+3),4.57249e-14,4.57249e-14,0.0
O(-2),27.9508,27.9399,0.010862
Cl(-1),0.696197,0.696197,0.0
C(+4),0.496331,0.496331,0.0
S(+4),4.70773e-13,4.70773e-13,0.0
S(+6),0.0226505,0.019935,2.71551e-3
S(-2),1.1963e-4,1.90898e-8,1.19611e-4
S(+2),4.15506e-12,4.15506e-12,0.0
N(+3),1.93694e-56,1.93694e-56,0.0
N(+5),6.91282e-74,6.91282e-74,0.0
Sr(+2),1.35814e-3,2.19459e-4,1.13868e-3
N(0),1.18295e-3,1.18295e-3,0.0
H(0),2.09621e-12,2.09621e-12,0.0
O(0),1.84671e-64,1.84671e-64,0.0
S(+8),7.24919e-56,7.24919e-56,0.0
Cl(+1),3.08317e-44,3.08317e-44,0.0
Cl(+5),8.93415e-113,8.93415e-113,0.0
S(+3),4.61673e-30,4.61673e-30,0.0
S(+5),1.17253e-30,1.17253e-30,0.0
S(+7),5.05441e-67,5.05441e-67,0.0
N(+2),6.25566e-48,6.25566e-48,0.0
N(+4),9.77676e-71,9.77676e-71,0.0
Cl(+3),1.71788e-86,1.71788e-86,0.0
Cl(+4),2.71156e-104,2.71156e-104,0.0
N(+1),1.54275e-49,1.54275e-49,0.0
N(-2),5.66173e-36,5.66173e-36,0.0
C(+2),2.10063e-4,2.10063e-4,0.0
Fe(+6),2.71174e-64,2.71174e-64,0.0
S(0),1.19611e-4,7.45547e-18,1.19611e-4
MeO(-1),4.25367e-4,4.25367e-4,0.0
N(-1),2.6093e-38,2.6093e-38,0.0
TEGION,9.05743e-6,9.05743e-6,0.0

Element Distribution

 ,Total,Total,Liquid-1,Solid
,mol,mole %,% of Total,% of Total
H(+1),53.7164,64.2815,100.0,0.0
K(+1),1.32998e-3,1.59156e-3,100.0,0.0
Na(+1),0.597978,0.71559,100.0,0.0
N(-3),4.06443e-5,4.86383e-5,100.0,0.0
Ba(+2),4.18699e-4,5.0105e-4,0.076778,99.9232
Ca(+2),0.0352188,0.0421457,96.7107,3.28929
Fe(+2),1.29819e-3,1.55352e-3,90.7863,9.21367

Mg(+2),0.0422753,0.05059,100.0,0.0
Fe(+3),4.57249e-14,5.47182e-14,100.0,0.0
O(-2),27.9508,33.4482,99.9611,0.0388613
Cl(-1),0.696197,0.833127,100.0,0.0
C(+4),0.496331,0.593951,100.0,0.0
S(+4),4.70773e-13,5.63365e-13,100.0,0.0
S(+6),0.0226505,0.0271055,88.0113,11.9887
S(-2),1.1963e-4,1.43159e-4,0.0159574,99.984
S(+2),4.15506e-12,4.97229e-12,100.0,0.0
N(+3),1.93694e-56,2.3179e-56,100.0,0.0
N(+5),6.91282e-74,8.27245e-74,100.0,0.0
Sr(+2),1.35814e-3,1.62526e-3,16.1588,83.8412
N(0),1.18295e-3,1.41562e-3,100.0,0.0
H(0),2.09621e-12,2.5085e-12,100.0,0.0
O(0),1.84671e-64,2.20992e-64,100.0,0.0
S(+8),7.24919e-56,8.67497e-56,100.0,0.0
Cl(+1),3.08317e-44,3.68957e-44,100.0,0.0
Cl(+5),8.93415e-113,1.06913e-112,100.0,0.0
S(+3),4.61673e-30,5.52476e-30,100.0,0.0
S(+5),1.17253e-30,1.40314e-30,100.0,0.0
S(+7),5.05441e-67,6.04852e-67,100.0,0.0
N(+2),6.25566e-48,7.48603e-48,100.0,0.0
N(+4),9.77676e-71,1.16997e-70,100.0,0.0
Cl(+3),1.71788e-86,2.05576e-86,100.0,0.0
Cl(+4),2.71156e-104,3.24488e-104,100.0,0.0
N(+1),1.54275e-49,1.84618e-49,100.0,0.0
N(-2),5.66173e-36,6.77529e-36,100.0,0.0
C(+2),2.10063e-4,2.51379e-4,100.0,0.0
Fe(+6),2.71174e-64,3.24509e-64,100.0,0.0
S(0),1.19611e-4,1.43136e-4,6.2331e-12,100.0
MeO(-1),4.25367e-4,5.09029e-4,100.0,0.0
N(-1),2.6093e-38,3.1225e-38,100.0,0.0
TEGION,9.05743e-6,1.08389e-5,100.0,0.0

Calculation Summary
06-2 Alloy-5 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2507

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,26.8580,26.8580
CO2,0.496331,0.496331
BaCl2,2.64786e-7,2.64786e-7
CaCl2,4.68554e-3,4.68554e-3
CaO,0.0299828,0.0299828
FeCl2,1.29819e-3,1.29819e-3
KCl,1.32998e-3,1.32998e-3
MgCl2,0.0422753,0.0422753
NaCl,0.597978,0.597978
SO3,0.0197968,0.0197968
SrCl2,1.85257e-4,1.85257e-4
BaSO4,4.18435e-4,4.18435e-4

SrSO4,1.17288e-3,1.17288e-3
N2,5.66215e-4,5.66215e-4
CO,2.10063e-4,2.10063e-4
O2,1.05800e-5,1.05800e-5
CH3OH,4.25367e-4,4.25367e-4
H2S,5.01990e-5,5.01990e-5
SO2,9.00972e-4,9.00972e-4
NO2,9.11658e-5,9.11658e-5
C6H14O4,9.05743e-6,9.05743e-6
CaSO4,5.50454e-4,5.50454e-4

Calculated Rates

Corrosion Rate,2.01837e-4,mm/yr
Corrosion Potential,-0.290738,V (SHE)
Repassivation Potential*,0.297744,V (SHE)
Corrosion Current Density,1.96724e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4 (Anhydrite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.131726
,CaSO4.0.5H2O (Bassanite),0.194356
,CaCO3 (Calcite),0.172508
,CaSO4.2H2O (Gypsum),0.914166
,FeCO3 (Siderite),0.176107
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,28.0562,mol
Temperature,43.0000,°C
Pressure,2641.00,psia

Liquid 1 Properties
pH,4.39230,
Ionic Strength (x-based),0.0284465,mol/mol
Ionic Strength (m-based),1.68926,mol/kg
Dielectric Constant,53.2439,
ORP,5.01637e-4,V (SHE)
Osmotic Pressure,1554.46,psia
Specific Electrical Conductivity,1.47933e5,µmho/cm
"Viscosity, absolute",0.758908,cP
Thermal Conductivity,543.880,cal/hr m °C

Surface Tension,0.0739733,N/m
Standard Liquid Volume,0.526600,L
"Volume, Std. Conditions",0.513711,L
"Total Dissolved Solids, Estimated",85617.6,mg/L
Hardness,14842.8,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,6.72547e-5,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid
Density,g/ml,1.06680,1.06614,3.66824
Enthalpy,J,-8.15917e6,-8.15521e6,-3957.69

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
Mole (True),28.7259,28.7230,2.83512e-3
Mole (App),28.0554,28.0525,2.83512e-3
,g,g,g
Mass,549.241,548.762,0.478867
,L,L,cm3
Volume,0.514848,0.514717,0.130544

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
FeS2 (Pyrite),1.00000,6.28673e5
BaSO4 (Barite),1.00000,1534.07
CaSO4 (Anhydrite),1.00000,1.20782
SrSO4 (Celestine),1.00000,7.34371
CaSO4.2H2O (Gypsum),0.914166,1.10370
H2O,0.612511,0.612386
CaSO4.0.5H2O (Bassanite),0.282476,0.341146
FeS2(marcasite) (Marcasite),0.280054,1.76062e5
CaSO4.0.5H2O (Bassanite),0.194356,0.234723
FeCO3 (Siderite),0.176107,0.199101
CaCO3 (Calcite),0.172508,0.181932
CaCO3 (Aragonite),0.131726,0.138922
NaHCO3 (Nahcolite),0.0308300,0.0312021
NaCl (Halite),0.0215970,0.0215707
NaCl.2H2O (hydrohalite),0.0146354,0.0146117
SrCO3 (Strontianite),9.67887e-3,0.0620638
Na2SO4.CaSO4 (Glauberite),7.01183e-3,9.92179e-3
Na2SO4 (Thenardite),2.60625e-3,3.05332e-3
Na2SO4.5CaSO4.3H2O,2.11017e-3,6.35069e-3
Na2SO4.10H2O (Mirabilite),1.57568e-3,1.84221e-3
MgSO4.7H2O (Epsomite),4.11903e-4,4.70272e-4
MgSO4.6H2O (Hexahydrite),2.83858e-4,3.24148e-4

MgCO3,2.07321e-4,2.06973e-4
Na2SO4,1.74398e-4,2.04313e-4
MgSO4.12H2O,1.73895e-4,1.98334e-4
MgSO4.5H2O (Pentahydrite),1.45461e-4,1.66141e-4
KCl (sylvite),1.32085e-4,1.31804e-4
FeS (Pyrrhotite),1.21908e-5,0.0259103
BaCO3 (Witherite),1.66883e-6,2.23538e-3
FeS (Mackinawite),2.53453e-7,5.38687e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid
,mol,mol,mol
H2O,26.8485,26.8485,0.0
Cl-1,0.696195,0.696195,
Na+1,0.591641,0.591641,
CO2,0.476496,0.476496,
Mg+2,0.0359165,0.0359165,
Ca+2,0.0315665,0.0315665,
HCO3-1,0.0187589,0.0187589,
SO4-2,0.0110777,0.0110777,
NaMgSO4+1,6.33703e-3,6.33703e-3,
CaSO4 (Anhydrite),3.64821e-3,2.48976e-3,1.15845e-3
K+1,1.30943e-3,1.30943e-3,
SrSO4 (Celestine),1.14275e-3,4.06916e-6,1.13868e-3
FeCO2+2,1.07258e-3,1.07258e-3,
N2,5.91475e-4,5.91475e-4,
CH3OH,4.25326e-4,4.25326e-4,
BaSO4 (Barite),4.18378e-4,,4.18378e-4
Sr+2,2.1539e-4,2.1539e-4,
CO,2.10063e-4,2.10063e-4,
FeS2 (Pyrite),1.19611e-4,,1.19611e-4
Fe+2,1.05825e-4,1.05825e-4,
NH4+1,4.06433e-5,4.06433e-5,
KMgSO4+1,2.05554e-5,2.05554e-5,
H3O+1,1.22413e-5,1.22413e-5,
C6H14O4,9.05739e-6,9.05739e-6,
HSO4-1,5.16673e-6,5.16673e-6,
CaCO3 (Calcite),3.06382e-6,3.06382e-6,0.0
CaCl2 (Hydrophilite),1.02868e-6,1.02868e-6,0.0
MgSO4,6.77491e-7,6.77491e-7,0.0
MgCO3,5.14381e-7,5.14381e-7,0.0
Ba+2,3.21466e-7,3.21466e-7,
CO3-2,3.19964e-7,3.19964e-7,
FeH(CO3)2-1,1.03547e-7,1.03547e-7,
FeCl+1,5.54682e-8,5.54682e-8,
CaClCH3OH+1,4.1388e-8,4.1388e-8,
H2S,1.89783e-8,1.89783e-8,
FeSO4,1.8387e-8,1.8387e-8,0.0
Na2SO4.NaHSO4,6.07612e-9,6.07612e-9,0.0
MgOH+1,3.2421e-9,3.2421e-9,

FeOH+1,9.12544e-10,9.12544e-10,
OH-1,8.58494e-10,8.58494e-10,
NH4OH,6.59562e-10,6.59562e-10,
CaOH+1,6.21027e-10,6.21027e-10,
NH3,2.26261e-10,2.26261e-10,
HS-1,1.08533e-10,1.08533e-10,
NH2CO2-1,9.65895e-11,9.65895e-11,
HO(CH2CH2O)3CO2(-1),3.91461e-11,3.91461e-11,
MgClCH3OH+1,9.89616e-12,9.89616e-12,
BaCO3 (Witherite),2.86433e-12,2.86433e-12,0.0
FeHS+1,2.59456e-12,2.59456e-12,
HCl,2.4826e-12,2.4826e-12,
S2O3-2,2.07674e-12,2.07674e-12,
SrCO3 (Strontianite),1.98715e-12,1.98715e-12,0.0
Fe(NH3)+2,1.70754e-12,1.70754e-12,
H2,1.0481e-12,1.0481e-12,
SrOH+1,6.3289e-13,6.3289e-13,
HSO3-1,4.65372e-13,4.65372e-13,
FeS (Pyrrhotite),3.48723e-13,3.48723e-13,0.0
CH3OH.HCl,2.14785e-13,2.14785e-13,
CH5O+1,2.11895e-13,2.11895e-13,
FeO+1,3.85848e-14,3.85848e-14,
CH3O-1,3.07887e-14,3.07887e-14,
C6H15O4+1,2.62595e-14,2.62595e-14,
FeOH+2,5.7187e-15,5.7187e-15,
SO3-2,4.18728e-15,4.18728e-15,
NaOH.Na2SO4,4.16818e-15,4.16818e-15,
NaOH,1.84916e-15,1.84916e-15,0.0
BaOH+1,1.42467e-15,1.42467e-15,
SO2,1.21293e-15,1.21293e-15,
HFeO2,8.09806e-16,8.09806e-16,
HS2O3-1,7.91283e-16,7.91283e-16,
H2SO4,6.19362e-16,6.19362e-16,
FeCl+2,5.72822e-16,5.72822e-16,
FeO,5.72288e-16,5.72288e-16,
C6H13O4-1,2.26132e-16,2.26132e-16,
Fe+3,3.85028e-17,3.85028e-17,
NaOHCO3-2,1.08292e-17,1.08292e-17,
CO2S,4.58835e-18,4.58835e-18,
S1,2.84911e-18,2.84911e-18,
MgCl2,8.30499e-19,8.30499e-19,0.0
Fe(NH3)2+2,2.42437e-19,2.42437e-19,
FeCl2+1,1.86326e-19,1.86326e-19,
H2S2O3,1.20311e-19,1.20311e-19,
S-2,4.85643e-20,4.85643e-20,
FeHSO4+2,3.65631e-20,3.65631e-20,
FeO2-1,1.76168e-20,1.76168e-20,
S2-2,1.59588e-20,1.59588e-20,
S2,9.73637e-22,9.73637e-22,
HFeO2-1,7.86564e-23,7.86564e-23,
S3-2,5.39857e-23,5.39857e-23,
S3,3.32707e-25,3.32707e-25,
S2O5-2,1.29736e-25,1.29736e-25,
S4-2,1.1304e-25,1.1304e-25,

Fe(NH3)3+2,9.11768e-27,9.11768e-27,
S5-2,1.46812e-28,1.46812e-28,
S4,1.13704e-28,1.13704e-28,
SO3,5.01199e-29,5.01199e-29,
S2O4-2,2.30836e-30,2.30836e-30,
Fe2(OH)2+4,9.1435e-31,9.1435e-31,
S2O6-2,5.86263e-31,5.86263e-31,
S5,3.88599e-32,3.88599e-32,
S8 (Sulfur),3.6428e-35,3.6428e-35,0.0
S6,1.32815e-35,1.32815e-35,
N2H5+1,2.82993e-36,2.82993e-36,
Fe(NH3)4+2,5.70913e-37,5.70913e-37,
NH2OH2+1,2.51409e-38,2.51409e-38,
S7,4.53774e-39,4.53774e-39,
NH2OH,9.52041e-40,9.52041e-40,0.0
N2H4,8.93604e-40,8.93604e-40,
N2H6+2,3.5251e-41,3.5251e-41,
S5O6-2,8.4774e-43,8.4774e-43,
HClO,2.52215e-44,2.52215e-44,
NH2Cl,3.97599e-45,3.97599e-45,
Cl2,1.59528e-45,1.59528e-45,
ClO-1,3.89391e-47,3.89391e-47,
Fe(NH3)5+2,3.57586e-47,3.57586e-47,
NO,6.25566e-48,6.25566e-48,
N2O,7.71373e-50,7.71373e-50,
NH3Cl+1,3.54969e-55,3.54969e-55,
HSO5-1,7.24919e-56,7.24919e-56,
NO2-1,1.86399e-56,1.86399e-56,
Fe(NH3)6+2,2.23906e-57,2.23906e-57,
HNO2,7.29524e-58,7.29524e-58,
FeO4-2,2.71174e-64,2.71174e-64,
O2,9.23353e-65,9.23353e-65,
S2O8-2,2.52721e-67,2.52721e-67,
NO2,9.77676e-71,9.77676e-71,
NO3-1,6.91282e-74,6.91282e-74,
HNO3,7.94713e-80,7.94713e-80,
NHCl2,4.70641e-83,4.70641e-83,
ClO2-1,1.71213e-86,1.71213e-86,
HClO2,5.74853e-89,5.74853e-89,
NH2Cl2+1,2.20622e-90,2.20622e-90,
NH4NO3.(NH4)2SO4,4.56905e-91,4.56905e-91,0.0
ClO2,2.71156e-104,2.71156e-104,
ClO3-1,8.93415e-113,8.93415e-113,
N2O3,2.28767e-120,2.28767e-120,
NCl3,5.06905e-122,5.06905e-122,
NHCl3+1,1.39579e-126,1.39579e-126,
Total (by phase),28.7259,28.723,2.83512e-3

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid

,mol,mol,mol
H(+1),53.7164,53.7164,0.0
K(+1),1.32998e-3,1.32998e-3,0.0
Na(+1),0.597978,0.597978,0.0
N(-3),4.06443e-5,4.06443e-5,0.0
Ba(+2),4.18699e-4,3.21469e-7,4.18378e-4
Ca(+2),0.0352188,0.0340604,1.15845e-3
Fe(+2),1.29819e-3,1.17858e-3,1.19611e-4
Mg(+2),0.0422753,0.0422753,0.0
Fe(+3),4.57249e-14,4.57249e-14,0.0
O(-2),27.9508,27.9399,0.010862
Cl(-1),0.696197,0.696197,0.0
C(+4),0.496331,0.496331,0.0
S(+4),4.70773e-13,4.70773e-13,0.0
S(+6),0.0226505,0.019935,2.71551e-3
S(-2),1.1963e-4,1.90898e-8,1.19611e-4
S(+2),4.15506e-12,4.15506e-12,0.0
N(+3),1.93694e-56,1.93694e-56,0.0
N(+5),6.91282e-74,6.91282e-74,0.0
Sr(+2),1.35814e-3,2.19459e-4,1.13868e-3
N(0),1.18295e-3,1.18295e-3,0.0
H(0),2.09621e-12,2.09621e-12,0.0
O(0),1.84671e-64,1.84671e-64,0.0
S(+8),7.24919e-56,7.24919e-56,0.0
Cl(+1),3.08317e-44,3.08317e-44,0.0
Cl(+5),8.93415e-113,8.93415e-113,0.0
S(+3),4.61673e-30,4.61673e-30,0.0
S(+5),1.17253e-30,1.17253e-30,0.0
S(+7),5.05441e-67,5.05441e-67,0.0
N(+2),6.25566e-48,6.25566e-48,0.0
N(+4),9.77676e-71,9.77676e-71,0.0
Cl(+3),1.71788e-86,1.71788e-86,0.0
Cl(+4),2.71156e-104,2.71156e-104,0.0
N(+1),1.54275e-49,1.54275e-49,0.0
N(-2),5.66173e-36,5.66173e-36,0.0
C(+2),2.10063e-4,2.10063e-4,0.0
Fe(+6),2.71174e-64,2.71174e-64,0.0
S(0),1.19611e-4,7.45547e-18,1.19611e-4
MeO(-1),4.25367e-4,4.25367e-4,0.0
N(-1),2.6093e-38,2.6093e-38,0.0
TEGION,9.05743e-6,9.05743e-6,0.0

Element Distribution

 ,Total,Total,Liquid-1,Solid
,mol,mole %,% of Total,% of Total
H(+1),53.7164,64.2815,100.0,0.0
K(+1),1.32998e-3,1.59156e-3,100.0,0.0
Na(+1),0.597978,0.71559,100.0,0.0
N(-3),4.06443e-5,4.86383e-5,100.0,0.0
Ba(+2),4.18699e-4,5.0105e-4,0.076778,99.9232
Ca(+2),0.0352188,0.0421457,96.7107,3.28929
Fe(+2),1.29819e-3,1.55352e-3,90.7863,9.21367

Mg(+2),0.0422753,0.05059,100.0,0.0
Fe(+3),4.57249e-14,5.47182e-14,100.0,0.0
O(-2),27.9508,33.4482,99.9611,0.0388613
Cl(-1),0.696197,0.833127,100.0,0.0
C(+4),0.496331,0.593951,100.0,0.0
S(+4),4.70773e-13,5.63365e-13,100.0,0.0
S(+6),0.0226505,0.0271055,88.0113,11.9887
S(-2),1.1963e-4,1.43159e-4,0.0159574,99.984
S(+2),4.15506e-12,4.97229e-12,100.0,0.0
N(+3),1.93694e-56,2.3179e-56,100.0,0.0
N(+5),6.91282e-74,8.27245e-74,100.0,0.0
Sr(+2),1.35814e-3,1.62526e-3,16.1588,83.8412
N(0),1.18295e-3,1.41562e-3,100.0,0.0
H(0),2.09621e-12,2.5085e-12,100.0,0.0
O(0),1.84671e-64,2.20992e-64,100.0,0.0
S(+8),7.24919e-56,8.67497e-56,100.0,0.0
Cl(+1),3.08317e-44,3.68957e-44,100.0,0.0
Cl(+5),8.93415e-113,1.06913e-112,100.0,0.0
S(+3),4.61673e-30,5.52476e-30,100.0,0.0
S(+5),1.17253e-30,1.40314e-30,100.0,0.0
S(+7),5.05441e-67,6.04852e-67,100.0,0.0
N(+2),6.25566e-48,7.48603e-48,100.0,0.0
N(+4),9.77676e-71,1.16997e-70,100.0,0.0
Cl(+3),1.71788e-86,2.05576e-86,100.0,0.0
Cl(+4),2.71156e-104,3.24488e-104,100.0,0.0
N(+1),1.54275e-49,1.84618e-49,100.0,0.0
N(-2),5.66173e-36,6.77529e-36,100.0,0.0
C(+2),2.10063e-4,2.51379e-4,100.0,0.0
Fe(+6),2.71174e-64,3.24509e-64,100.0,0.0
S(0),1.19611e-4,1.43136e-4,6.2331e-12,100.0
MeO(-1),4.25367e-4,5.09029e-4,100.0,0.0
N(-1),2.6093e-38,3.1225e-38,100.0,0.0
TEGION,9.05743e-6,1.08389e-5,100.0,0.0

Calculation Summary
06-3 Alloy-1 Calculation

Unit Set: Custom

Automatic Chemistry Model
,Aqueous (H+ ion) Databanks:
,,Corrosion (AQ)
,,Aqueous (H+ ion)
,Second Liquid phase
,Redox selected
,Using K-fit Polynomials
,,T-span: 25.0 - 225.0
,,P-span: 1.0 - 1500.0

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Super13Cr stainless steel

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,48.4202,48.4202
CO2,0.838171,0.838171
BaCl2,4.89505e-7,4.89505e-7
CaCl2,8.42726e-3,8.42726e-3
CaO,0.0543687,0.0543687
FeCl2,2.33674e-3,2.33674e-3
KCl,2.39397e-3,2.39397e-3
MgCl2,0.0760955,0.0760955
NaCl,1.07636,1.07636

SO3,0.0360339,0.0360339
SrCl2,3.40157e-4,3.40157e-4
BaSO4,7.53170e-4,7.53170e-4
SrSO4,2.10449e-3,2.10449e-3
N2,8.01811e-3,8.01811e-3
CO,4.23411e-4,4.23411e-4
O2,2.52702e-5,2.52702e-5
NH3,1.32721e-4,1.32721e-4
CH3OH,8.47631e-5,8.47631e-5
H2S,5.07330e-5,5.07330e-5
SO2,2.02298e-4,2.02298e-4
NO2,1.20612e-4,1.20612e-4
C6H14O4,1.69979e-6,1.69979e-6
CaSO4,5.97925e-4,5.97925e-4

Calculated Rates

Corrosion Rate,1.29826e-3,mm/yr
Corrosion Potential,-0.297707,V (SHE)
Repassivation Potential*,-0.132948,V (SHE)
Corrosion Current Density,1.19632e-3,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4 (Anhydrite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.0.5H2O (Bassanite),0.294604
,CaSO4.2H2O (Gypsum),0.924384
,FeCO3 (Siderite),0.255297
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,50.5272,mol
Temperature,109.400,°F
Pressure,2641.00,psia

Aqueous Properties
pH,4.25671,
Ionic Strength (x-based),0.0287461,mol/mol
Ionic Strength (m-based),1.70553,mol/kg
ORP,0.0184708,V (SHE)
Osmotic Pressure,1452.13,psia
Specific Electrical Conductivity,1.49011e5,µmho/cm
"Electrical Conductivity, molar",6.55140e-3,m2/ohm-mol

"Viscosity, absolute",0.764432,cP
"Viscosity, relative",1.23618,
Standard Liquid Volume,0.947426,L
"Volume, Std. Conditions",0.924646,L
"Total Dissolved Solids, Estimated",85904.7,mg/L
Hardness,14980.5,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,5.96509e-5,L

Thermodynamic Properties
,Unit,Total,Aqueous,Solid
Density,g/ml,1.06597,1.06552,3.84913
Enthalpy,J,-1.46828e7,-1.46783e7,-4496.97

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
Mole (True),51.7382,51.7351,3.09868e-3
Mole (App),50.5275,50.5244,3.09868e-3
,g,g,g
Mass,987.648,987.082,0.566544
,L,L,cm3
Volume,0.926529,0.926382,0.147187

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
FeS2 (Pyrite),1.00000,1.34775e6
BaSO4 (Barite),1.00000,1683.36
CaSO4 (Anhydrite),1.00000,1.05944
SrSO4 (Celestine),1.00000,2.62383
CaSO4.2H2O (Gypsum),0.924384,0.977163
CaSO4.0.5H2O (Bassanite),0.294604,0.311942
FeS2(marcasite) (Marcasite),0.280070,3.77465e5
FeCO3 (Siderite),0.255297,0.440273
CaCO3 (Calcite),0.0623383,0.107081
CaCO3 (Aragonite),0.0397273,0.0682411
NaHCO3 (Nahcolite),0.0227575,0.0301904
NaCl (Halite),0.0206099,0.0204946
Na2SO4 (Thenardite),5.00224e-3,5.25453e-3
SrCO3 (Strontianite),4.18750e-3,0.0178145
MgSO4.7H2O (Epsomite),2.37082e-3,2.37425e-3
FeO(OH) (Lepidocrocite),1.19513e-3,7.06768e-4
FeSO4.7H2O (Melanterite),5.56382e-4,5.87219e-4
Sr(HCO3)2,5.15906e-4,2.26791e-3
MgCO3 (Magnesite),1.67288e-4,2.73743e-4
KCl (Sylvite),1.59380e-4,1.58468e-4
MgCO3.3H2O (Nesquehonite),8.75347e-5,1.42763e-4

FeS (Pyrrhotite),4.45325e-5,0.188069
FeS(mackinawite) (Mackinawite),9.58578e-7,4.04824e-3

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Aqueous,Solid
,mol,mol,mol
H2O,48.4019,48.4019,
Cl-1,1.25314,1.25314,
Na+1,1.06766,1.06766,
CO2,0.801751,0.801751,
Mg+2,0.0620027,0.0620027,
Ca+2,0.0613453,0.0613453,
SO4-2,0.0274342,0.0274342,
HCO3-1,0.0214505,0.0214505,
MgHCO3+1,9.91499e-3,9.91499e-3,
N2,8.06954e-3,8.06954e-3,
NaHCO3 (Nahcolite),5.0425e-3,5.0425e-3,0.0
MgSO4,4.17746e-3,4.17746e-3,0.0
NaSO4-1,3.65726e-3,3.65726e-3,
K+1,2.32408e-3,2.32408e-3,
Fe+2,2.31972e-3,2.31972e-3,
CaSO4 (Anhydrite),2.03855e-3,1.21223e-3,8.26319e-4
SrSO4 (Celestine),1.56851e-3,6.17446e-5,1.50677e-3
Sr+2,8.76136e-4,8.76136e-4,
BaSO4 (Barite),7.53194e-4,,7.53194e-4
CO,4.23411e-4,4.23411e-4,
NH4+1,1.45912e-4,1.45912e-4,
CH3OH,8.47631e-5,8.47631e-5,
H+1,5.77782e-5,5.77782e-5,
KSO4-1,5.74455e-5,5.74455e-5,
HSO4-1,2.64736e-5,2.64736e-5,
KCl (Sylvite),1.24422e-5,1.24422e-5,0.0
FeS2 (Pyrite),1.24046e-5,,1.24046e-5
CaHCO3+1,7.9188e-6,7.9188e-6,
NH4SO4-1,4.54632e-6,4.54632e-6,
FeCl+1,2.33242e-6,2.33242e-6,
C6H14O4,1.69979e-6,1.69979e-6,
FeHCO3+1,1.54216e-6,1.54216e-6,
CaCO3 (Calcite),1.49875e-6,1.49875e-6,0.0
FeCO3 (Siderite),7.13101e-7,7.13101e-7,0.0
CaCl+1,5.96623e-7,5.96623e-7,
Ba+2,3.28292e-7,3.28292e-7,
MgCO3 (Magnesite),2.85516e-7,2.85516e-7,0.0
CO3-2,2.57218e-7,2.57218e-7,
BaCl(+1),1.15069e-7,1.15069e-7,
NaCO3-1,5.30254e-8,5.30254e-8,
FeOH+1,2.20393e-8,2.20393e-8,
BaHCO3+1,2.19025e-8,2.19025e-8,
H2S,5.6945e-9,5.6945e-9,
FeCl2 (Lawrencite),4.39781e-9,4.39781e-9,0.0

MgOH+1,3.53074e-9,3.53074e-9,
NH3,1.84848e-9,1.84848e-9,
OH-1,8.67425e-10,8.67425e-10,
KHSO4 (Mercallite),5.37836e-10,5.37836e-10,0.0
FeHS+1,4.53903e-10,4.53903e-10,
CaOH+1,2.07608e-10,2.07608e-10,
NH2CO2-1,7.54853e-11,7.54853e-11,
Fe(NH3)+2,6.93744e-11,6.93744e-11,
HCl,6.44238e-11,6.44238e-11,
HS-1,3.40013e-11,3.40013e-11,
Fe(CO3)2-2,7.70984e-12,7.70984e-12,
S2O3-2,1.9159e-12,1.9159e-12,
HSO3-1,1.17148e-12,1.17148e-12,
NaS2O3-1,1.02963e-12,1.02963e-12,
SrOH+1,9.98336e-13,9.98336e-13,
H2,7.62742e-13,7.62742e-13,
BaCO3 (Witherite),4.00586e-13,4.00586e-13,0.0
FeOH+2,1.85633e-13,1.85633e-13,
Fe(OH)2+1,5.92537e-14,5.92537e-14,
Fe+3,2.73351e-14,2.73351e-14,
SO3-2,9.04373e-15,9.04373e-15,
KS2O3-1,7.17936e-15,7.17936e-15,
Fe(OH)3 (Bernalite),6.76312e-15,6.76312e-15,0.0
SO2,4.01827e-15,4.01827e-15,
FeCl2+1,4.60287e-16,4.60287e-16,
FeCl+2,2.01172e-16,2.01172e-16,
FeSO4+1,9.05991e-17,9.05991e-17,
BaOH+1,3.58044e-17,3.58044e-17,
Fe(NH3)2+2,1.12794e-17,1.12794e-17,
FeCl3 (Molysite),9.08089e-18,9.08089e-18,0.0
CaCl2 (Hydrophilite),3.07031e-18,3.07031e-18,0.0
S-2,1.09595e-18,1.09595e-18,
Fe(OH)4-1,4.02509e-19,4.02509e-19,
FeCl4-1,1.49239e-19,1.49239e-19,
H2SO4,2.62851e-20,2.62851e-20,
FeS(HS)-1,5.77086e-21,5.77086e-21,
S2-2,4.2186e-21,4.2186e-21,
HFeO2-1,1.29543e-21,1.29543e-21,
S3-2,6.51795e-24,6.51795e-24,
SO3,4.10397e-24,4.10397e-24,
Fe(NH3)3+2,4.85777e-25,4.85777e-25,
S4-2,6.23337e-27,6.23337e-27,
S2O5-2,1.66899e-28,1.66899e-28,
Fe2(OH)2+4,9.82039e-29,9.82039e-29,
S2O6-2,1.2145e-29,1.2145e-29,
S2O4-2,1.16317e-29,1.16317e-29,
S5-2,3.69755e-30,3.69755e-30,
Na2S2O4,4.41404e-31,4.41404e-31,0.0
Fe(NH3)4+2,3.48333e-35,3.48333e-35,
N2H5+1,2.90592e-35,2.90592e-35,
N2H4,5.5436e-39,5.5436e-39,
NH2OH,7.1033e-40,7.1033e-40,
S5O6-2,1.40172e-42,1.40172e-42,
Fe(NH3)5+2,2.49843e-45,2.49843e-45,

NO,3.2415e-47,3.2415e-47,
N2O,1.32221e-48,1.32221e-48,
HSO5-1,9.52763e-55,9.52763e-55,
NO2-1,2.54613e-55,2.54613e-55,
Fe(NH3)6+2,1.79153e-55,1.79153e-55,
HNO2,6.8212e-57,6.8212e-57,
FeO4-2,3.17331e-62,3.17331e-62,
O2,5.99981e-64,5.99981e-64,
S2O8-2,2.16155e-65,2.16155e-65,
NO2,3.12952e-69,3.12952e-69,
NO3-1,1.41952e-72,1.41952e-72,
NaNO3 (Nitratine),1.23427e-73,1.23427e-73,0.0
Ca(NO3)+1,6.81914e-74,6.81914e-74,
SrNO3+1,1.07657e-75,1.07657e-75,
NH4NO3 (Gwihabaite),9.42912e-76,9.42912e-76,0.0
HNO3,1.5297e-81,1.5297e-81,
FeNO3+2,1.0018e-88,1.0018e-88,
Total (by phase),51.7382,51.7351,3.09868e-3

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
H(+1),96.8408,96.8408,0.0
K(+1),2.39397e-3,2.39397e-3,0.0
Na(+1),1.07636,1.07636,0.0
N(-3),1.50461e-4,1.50461e-4,0.0
Ba(+2),7.53659e-4,4.65264e-7,7.53194e-4
Ca(+2),0.0633939,0.0625676,8.26319e-4
Fe(+2),2.33674e-3,2.32434e-3,1.24046e-5
Mg(+2),0.0760955,0.0760955,0.0
Fe(+3),2.79747e-13,2.79747e-13,0.0
O(-2),50.2739,50.2616,0.0123451
Cl(-1),1.25315,1.25315,0.0
C(+4),0.838171,0.838171,0.0
S(+4),1.18454e-12,1.18454e-12,0.0
S(+6),0.0397177,0.0366314,3.08628e-3
S(-2),1.24108e-5,6.18241e-9,1.24046e-5
S(+2),5.90542e-12,5.90542e-12,0.0
N(+3),2.61434e-55,2.61434e-55,0.0
N(+5),1.61315e-72,1.61315e-72,0.0
Sr(+2),2.44465e-3,9.3788e-4,1.50677e-3
N(0),0.0161391,0.0161391,0.0
H(0),1.52548e-12,1.52548e-12,0.0
O(0),1.19996e-63,1.19996e-63,0.0
S(+8),9.52763e-55,9.52763e-55,0.0
S(+3),2.41461e-29,2.41461e-29,0.0
S(+5),2.42899e-29,2.42899e-29,0.0
S(+7),4.32309e-65,4.32309e-65,0.0
N(+2),3.2415e-47,3.2415e-47,0.0
N(+4),3.12952e-69,3.12952e-69,0.0

N(+1),2.64443e-48,2.64443e-48,0.0
N(-2),5.81294e-35,5.81294e-35,0.0
C(+2),4.23411e-4,4.23411e-4,0.0
Fe(+6),3.17331e-62,3.17331e-62,0.0
S(0),1.24046e-5,4.23165e-21,1.24046e-5
N(-1),7.1033e-40,7.1033e-40,0.0
METHANOL,8.47631e-5,8.47631e-5,0.0
TRIETLNGLY,1.69979e-6,1.69979e-6,0.0

Element Distribution

,Total,Total,Aqueous,Solid
,mol,mole %,% of Total,% of Total
H(+1),96.8408,64.3519,100.0,0.0
K(+1),2.39397e-3,1.59082e-3,100.0,0.0
Na(+1),1.07636,0.715254,100.0,0.0
N(-3),1.50461e-4,9.99828e-5,100.0,0.0
Ba(+2),7.53659e-4,5.00815e-4,0.061734,99.9383
Ca(+2),0.0633939,0.042126,98.6965,1.30347
Fe(+2),2.33674e-3,1.55279e-3,99.4692,0.53085
Mg(+2),0.0760955,0.0505663,100.0,0.0
Fe(+3),2.79747e-13,1.85895e-13,100.0,0.0
O(-2),50.2739,33.4076,99.9754,0.0245557
Cl(-1),1.25315,0.832736,100.0,0.0
C(+4),0.838171,0.556975,100.0,0.0
S(+4),1.18454e-12,7.8714e-13,100.0,0.0
S(+6),0.0397177,0.0263929,92.2295,7.77054
S(-2),1.24108e-5,8.2471e-6,0.0498149,99.9502
S(+2),5.90542e-12,3.92422e-12,100.0,0.0
N(+3),2.61434e-55,1.73726e-55,100.0,0.0
N(+5),1.61315e-72,1.07196e-72,100.0,0.0
Sr(+2),2.44465e-3,1.6245e-3,38.3646,61.6354
N(0),0.0161391,0.0107246,100.0,0.0
H(0),1.52548e-12,1.0137e-12,100.0,0.0
O(0),1.19996e-63,7.97389e-64,100.0,0.0
S(+8),9.52763e-55,6.33123e-55,100.0,0.0
S(+3),2.41461e-29,1.60454e-29,100.0,0.0
S(+5),2.42899e-29,1.61409e-29,100.0,0.0
S(+7),4.32309e-65,2.87274e-65,100.0,0.0
N(+2),3.2415e-47,2.15401e-47,100.0,0.0
N(+4),3.12952e-69,2.0796e-69,100.0,0.0
N(+1),2.64443e-48,1.75725e-48,100.0,0.0
N(-2),5.81294e-35,3.86277e-35,100.0,0.0
C(+2),4.23411e-4,2.81362e-4,100.0,0.0
Fe(+6),3.17331e-62,2.1087e-62,100.0,0.0
S(0),1.24046e-5,8.24299e-6,3.41136e-14,100.0
N(-1),7.1033e-40,4.72023e-40,100.0,0.0
METHANOL,8.47631e-5,5.63261e-5,100.0,0.0
TRIETLNGLY,1.69979e-6,1.12953e-6,100.0,0.0

Calculation Summary
06-3 Alloy-4 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2205

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,48.4202,48.4202
CO2,0.838171,0.838171
BaCl2,4.89505e-7,4.89505e-7
CaCl2,8.42726e-3,8.42726e-3
CaO,0.0543687,0.0543687
FeCl2,2.33674e-3,2.33674e-3
KCl,2.39397e-3,2.39397e-3
MgCl2,0.0760955,0.0760955
NaCl,1.07636,1.07636
SO3,0.0360339,0.0360339
SrCl2,3.40157e-4,3.40157e-4

BaSO4,7.53170e-4,7.53170e-4
SrSO4,2.10449e-3,2.10449e-3
N2,8.01811e-3,8.01811e-3
CO,4.23411e-4,4.23411e-4
O2,2.52702e-5,2.52702e-5
NH3,1.32721e-4,1.32721e-4
CH3OH,8.47631e-5,8.47631e-5
H2S,5.07330e-5,5.07330e-5
SO2,2.02298e-4,2.02298e-4
NO2,1.20612e-4,1.20612e-4
C6H14O4,1.69979e-6,1.69979e-6
CaSO4,5.97925e-4,5.97925e-4

Calculated Rates

Corrosion Rate,2.07630e-4,mm/yr
Corrosion Potential,-0.295807,V (SHE)
Repassivation Potential*,1.49075e-3,V (SHE)
Corrosion Current Density,1.96642e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4 (Anhydrite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.166622
,CaSO4.0.5H2O (Bassanite),0.194665
,CaCO3 (Calcite),0.218207
,CaSO4.2H2O (Gypsum),0.920004
,FeCO3 (Siderite),0.110752
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,50.5272,mol
Temperature,109.400,°F
Pressure,2641.00,psia

Liquid 1 Properties
pH,4.49015,
Ionic Strength (x-based),0.0285798,mol/mol
Ionic Strength (m-based),1.69323,mol/kg
Dielectric Constant,53.6199,
ORP,0.0484882,V (SHE)
Osmotic Pressure,1486.67,psia
Specific Electrical Conductivity,1.48146e5,µmho/cm

"Viscosity, absolute",0.759325,cP
Thermal Conductivity,543.924,cal/hr m °C
Surface Tension,0.0739887,N/m
Interfacial Tension LLE,1.63016e-6,N/m
Standard Liquid Volume,0.944888,L
"Volume, Std. Conditions",0.925568,L
"Total Dissolved Solids, Estimated",85943.4,mg/L
Hardness,15035.0,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,5.39711e-5,L

Liquid 2 Properties
pH,4.92164,
Ionic Strength (x-based),0.0386571,mol/mol
Ionic Strength (m-based),355.156,mol/kg
Dielectric Constant,4.02929,
Specific Electrical Conductivity,44639.6,µmho/cm
"Viscosity, absolute",0.684260,cP
Surface Tension,0.0739955,N/m
Thermal Conductivity,531.483,cal/hr m °C
Standard Liquid Volume,2.54332e-3,L
"Volume, Std. Conditions",4.73181e-3,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid,Liquid-2
Density,g/ml,1.06394,1.06461,3.91272,0.785610
Enthalpy,J,-1.46846e7,-1.46525e7,-4989.85,-27143.1

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
Mole (True),51.7350,51.6607,3.42803e-3,0.0707962
Mole (App),50.5271,50.4544,3.42803e-3,0.0693391
,g,g,g,g
Mass,987.652,983.941,0.636811,3.07447
,L,L,cm3,L
Volume,0.928301,0.924225,0.162754,3.91347e-3

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
CaSO4 (Anhydrite),1.00000,1.14706
BaSO4 (Barite),1.00000,1434.58
SrSO4 (Celestine),1.00000,6.78656
CaSO4.2H2O (Gypsum),0.920004,1.05168
H2O,0.614464,0.613407
CaSO4.0.5H2O (Bassanite),0.282926,0.324255
CaCO3 (Calcite),0.218207,0.212764

CaSO4.0.5H2O (Bassanite),0.194665,0.223102
CaCO3 (Aragonite),0.166622,0.162465
FeCO3 (Siderite),0.110752,1.97699e-28
NaHCO3 (Nahcolite),0.0318636,0.0323963
NaCl (Halite),0.0210292,0.0213033
NaCl.2H2O (hydrohalite),0.0143417,0.0144787
SrCO3 (Strontianite),0.0122429,0.0706279
Na2SO4.CaSO4 (Glauberite),6.90775e-3,8.94106e-3
Na2SO4 (Thenardite),2.56756e-3,2.89725e-3
Na2SO4.5CaSO4.3H2O,2.09879e-3,4.67876e-3
Na2SO4.10H2O (Mirabilite),1.60249e-3,1.77739e-3
MgSO4.7H2O (Epsomite),4.14116e-4,4.54133e-4
MgSO4.6H2O (Hexahydrite),2.84476e-4,3.12503e-4
MgCO3,2.57843e-4,2.43271e-4
MgSO4.12H2O,1.77633e-4,1.93128e-4
Na2SO4,1.71809e-4,1.93870e-4
MgSO4.5H2O (Pentahydrite),1.45314e-4,1.59906e-4
KCl (sylvite),1.29950e-4,1.30939e-4
FeO(OH) (Goethite),1.00559e-4,
BaCO3 (Witherite),2.11092e-6,2.57417e-3

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H2O,48.4022,48.4018,0.0,4.27737e-4
Cl-1,1.25315,1.25156,,1.58841e-3
Na+1,1.06568,1.06568,,4.39568e-13
CO2,0.80065,0.73503,,0.0656204
Mg+2,0.0653752,0.0653752,,1.35177e-22
Ca+2,0.0583123,0.0583123,,2.81885e-22
HCO3-1,0.0359643,0.0359364,,2.79573e-5
SO4-2,0.0211448,0.0211442,,5.78211e-7
NaMgSO4+1,0.0106829,0.0106787,,4.15545e-6
N2,8.04059e-3,6.03778e-3,,2.00281e-3
CaSO4 (Anhydrite),5.07276e-3,4.43058e-3,6.3724e-4,4.93826e-6
K+1,2.35894e-3,2.35894e-3,,8.74326e-14
SrSO4 (Celestine),2.04499e-3,7.25027e-6,2.03773e-3,7.79247e-9
FeCO2+2,1.3401e-3,1.3401e-3,,1.95821e-103
Fe+2,9.96454e-4,8.57798e-5,,9.10674e-4
BaSO4 (Barite),7.53057e-4,,7.53057e-4,
CO,4.23411e-4,4.22957e-4,,4.54587e-7
Sr+2,3.99657e-4,3.99657e-4,,5.8724e-24
NH2CO2-1,2.07992e-4,1.0933e-12,,2.07992e-4
CH3OH,8.47553e-5,8.47141e-5,,4.11683e-8
KMgSO4+1,3.50291e-5,3.50133e-5,,1.58407e-8
H3O+1,1.85653e-5,1.85653e-5,,3.40614e-19
HSO4-1,7.83042e-6,7.83021e-6,,2.08511e-10
CaCO3 (Calcite),6.91243e-6,6.90744e-6,0.0,4.99666e-9
CaCl2 (Hydrophilite),1.88979e-6,1.88979e-6,0.0,2.03075e-22
C6H14O4,1.69979e-6,1.69978e-6,,5.56752e-12

MgSO4,1.18698e-6,1.18559e-6,0.0,1.38545e-9
MgCO3,1.14107e-6,1.13984e-6,0.0,1.22509e-9
CO3-2,7.78117e-7,7.75896e-7,,2.22181e-9
Ba+2,6.02344e-7,6.02344e-7,,3.46876e-29
NH4+1,3.7279e-7,3.7279e-7,,8.3691e-14
FeH(CO3)2-1,1.24981e-7,1.24594e-7,,3.86542e-10
FeCl+1,4.67669e-8,4.67469e-8,,1.99878e-11
FeSO4,1.63063e-8,1.62888e-8,0.0,1.74988e-11
Na2SO4.NaHSO4,9.00637e-9,9.00637e-9,0.0,7.39421e-18
CaClCH3OH+1,7.84299e-9,7.83909e-9,,3.90543e-12
MgOH+1,6.71489e-9,6.71203e-9,,2.85476e-12
OH-1,1.91992e-9,1.91768e-9,,2.23808e-12
CaOH+1,1.3084e-9,1.3081e-9,,3.00782e-13
FeOH+1,9.55718e-10,9.55312e-10,,4.06313e-13
HO(CH2CH2O)3CO2(-1),8.37581e-12,8.35695e-12,,1.886e-14
NH4OH,7.4978e-12,7.49641e-12,,1.38719e-15
BaCO3 (Witherite),6.46248e-12,6.45554e-12,0.0,6.93831e-15
SrCO3 (Strontianite),4.4834e-12,4.47859e-12,0.0,4.81351e-15
HCl,3.63434e-12,3.5479e-12,,8.64359e-14
NH3,2.59456e-12,2.59416e-12,,4.03595e-16
MgClCH3OH+1,1.85475e-12,1.85365e-12,,1.10649e-15
SrOH+1,1.3081e-12,1.30694e-12,,1.1627e-15
FeO+1,2.9465e-13,2.94525e-13,,1.25267e-16
H2,3.51638e-14,3.51182e-14,,4.55942e-17
FeOH+2,3.48968e-14,3.48893e-14,,7.51401e-18
CH3OH.HCl,3.45163e-14,3.44793e-14,,3.70571e-17
CH5O+1,3.37126e-14,3.36947e-14,,1.78377e-17
HSO3-1,1.3245e-14,1.32055e-14,,3.95426e-17
NaOH.Na2SO4,9.40879e-15,9.40879e-15,,4.27912e-29
Fe(NH3)+2,9.02288e-15,9.02087e-15,,2.00679e-18
HFeO2,7.77633e-15,7.76798e-15,,8.34889e-18
CH3O-1,7.69386e-15,7.67005e-15,,2.38135e-17
C6H15O4+1,4.17464e-15,4.1728e-15,,1.84205e-18
NaOH,4.01757e-15,4.01744e-15,0.0,1.27328e-19
BaOH+1,2.99645e-15,2.99602e-15,,4.35311e-19
H2S,2.87157e-15,2.77499e-15,,9.65804e-17
FeCl+2,2.82211e-15,2.82193e-15,,1.82517e-19
H2SO4,7.64596e-16,7.64596e-16,,3.96479e-24
FeO,7.51298e-16,7.50491e-16,,8.06616e-19
Fe+3,1.89516e-16,1.89495e-16,,2.16034e-20
SO3-2,1.49961e-16,1.49024e-16,,9.36763e-19
C6H13O4-1,5.6546e-17,5.63727e-17,,1.73265e-19
NaOHCO3-2,3.17937e-17,3.14335e-17,,3.60195e-19
SO2,2.78219e-17,2.75228e-17,,2.99088e-19
HS-1,2.03602e-17,2.02876e-17,,7.25532e-20
MgCl2,1.40401e-18,1.39707e-18,0.0,6.94054e-21
FeCl2+1,9.26868e-19,9.26817e-19,,5.05774e-23
S2O3-2,3.31002e-19,3.29072e-19,,1.93028e-21
FeHS+1,2.26847e-19,2.2675e-19,,9.64414e-23
FeO2-1,2.12352e-19,2.11696e-19,,6.56767e-22
FeHSO4+2,1.50365e-19,1.50331e-19,,3.37024e-23
FeS (Pyrrhotite),3.82182e-20,3.81772e-20,0.0,4.10322e-23
HFeO2-1,1.30032e-22,1.2963e-22,,4.02166e-25
HS2O3-1,1.00229e-22,9.9919e-23,,3.0999e-25

CO2S,3.11364e-23,3.1103e-23,,3.3429e-26
S1,2.2627e-23,2.26027e-23,,2.42931e-26
Fe(NH3)2+2,8.10778e-24,8.10597e-24,,1.80326e-27
S-2,1.25469e-26,1.13614e-26,,1.18552e-27
H2S2O3,1.21403e-26,1.21273e-26,,1.30342e-29
SO3,6.14622e-29,6.14622e-29,,2.22209e-35
S2O5-2,5.91189e-29,5.84491e-29,,6.69765e-31
Fe2(OH)2+4,1.91964e-29,1.91942e-29,,2.2206e-33
S2,3.44286e-32,3.43916e-32,,3.69635e-35
S2-2,1.68508e-32,1.66599e-32,,1.90905e-34
S2O6-2,1.42487e-32,1.40872e-32,,1.61425e-34
Fe(NH3)3+2,1.92981e-33,1.92939e-33,,4.29213e-37
S2O4-2,1.97227e-35,1.94992e-35,,2.23441e-37
NH2OH2+1,1.2079e-38,1.20739e-38,,5.11213e-42
N2H5+1,8.57472e-39,8.57108e-39,,3.64476e-42
NH2OH,5.75513e-40,5.75181e-40,0.0,3.31623e-43
S3-2,2.53807e-40,2.50931e-40,,2.87541e-42
S3,5.23825e-41,5.23263e-41,,5.62394e-44
N2H4,3.49605e-42,3.49598e-42,,6.58665e-47
N2H6+2,8.5352e-44,8.53336e-44,,1.83745e-47
NO,1.61599e-45,1.4192e-45,,1.96786e-46
Fe(NH3)4+2,7.64769e-46,7.64599e-46,,1.70094e-49
N2O,4.59013e-47,4.37792e-47,,2.12203e-48
S4-2,2.36623e-48,2.33943e-48,,2.68074e-50
S4,7.97079e-50,7.96224e-50,,8.55768e-53
NO2-1,3.99333e-53,3.98197e-53,,1.13567e-55
HSO5-1,5.86635e-54,5.8482e-54,,1.81435e-56
HNO2,1.24547e-54,1.24413e-54,,1.33717e-57
S5-2,1.36833e-56,1.35283e-56,,1.5502e-58
Fe(NH3)5+2,3.03158e-58,3.03091e-58,,6.74259e-62
S5,1.21292e-58,1.21162e-58,,1.30223e-61
S5O6-2,1.81867e-60,1.79806e-60,,2.06039e-62
FeO4-2,1.61278e-60,1.59451e-60,,1.82714e-62
O2,4.81232e-61,4.55379e-61,,2.58525e-62
S2O8-2,1.7472e-65,1.72741e-65,,1.97942e-67
NO2,1.22631e-66,1.16705e-66,,5.92609e-68
S6,1.84578e-67,1.84379e-67,,1.98168e-70
NO3-1,7.89057e-69,7.8899e-69,,6.63434e-73
Fe(NH3)6+2,1.20139e-70,1.20112e-70,,2.67203e-74
HNO3,7.27456e-75,7.27456e-75,,5.87289e-81
S7,2.80786e-76,2.80484e-76,,3.0146e-79
S8 (Sulfur),3.00833e-77,9.87318e-78,0.0,2.02101e-77
NH4NO3.(NH4)2SO4,7.14713e-93,7.13945e-93,0.0,7.67337e-96
N2O3,1.04318e-110,3.60423e-114,,1.04282e-110
Total (by phase),51.735,51.6607,3.42803e-3,0.0707962

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H(+1),96.8409,96.8396,0.0,1.29946e-3

K(+1),2.39397e-3,2.39395e-3,0.0,1.58408e-8
Na(+1),1.07636,1.07636,0.0,4.15545e-6
N(-3),2.08365e-4,3.72801e-7,0.0,2.07992e-4
Ba(+2),7.53659e-4,6.0235e-7,7.53057e-4,6.93874e-15
Ca(+2),0.0633939,0.0627517,6.3724e-4,4.94326e-6
Fe(+2),2.33674e-3,1.42607e-3,0.0,9.10675e-4
Mg(+2),0.0760955,0.0760913,0.0,4.1739e-6
Fe(+3),3.40336e-13,3.40195e-13,0.0,1.41335e-16
O(-2),50.2739,50.128,0.0137121,0.132208
Cl(-1),1.25315,1.25157,0.0,1.58841e-3
C(+4),0.838171,0.772315,0.0,0.0658564
S(+4),1.34228e-14,1.3382e-14,0.0,4.07784e-17
S(+6),0.0397425,0.0363048,3.42803e-3,9.69716e-6
S(-2),2.89219e-15,2.79554e-15,0.0,9.66531e-17
S(+2),6.62204e-19,6.58343e-19,0.0,3.86117e-21
N(+3),4.11787e-53,4.10638e-53,0.0,1.14904e-55
N(+5),7.89057e-69,7.88991e-69,0.0,6.63434e-73
Sr(+2),2.44465e-3,4.06907e-4,2.03773e-3,7.79248e-9
N(0),0.0160812,0.0120756,0.0,4.00562e-3
H(0),7.03276e-14,7.02364e-14,0.0,9.11885e-17
O(0),9.62463e-61,9.10758e-61,0.0,5.1705e-62
S(+8),5.86635e-54,5.8482e-54,0.0,1.81435e-56
S(+3),3.94454e-35,3.89985e-35,0.0,4.46882e-37
S(+5),2.84973e-32,2.81745e-32,0.0,3.2285e-34
S(+7),3.4944e-65,3.45481e-65,0.0,3.95885e-67
N(+2),1.61599e-45,1.4192e-45,0.0,1.96786e-46
N(+4),1.22631e-66,1.16705e-66,0.0,5.92609e-68
N(+1),9.18026e-47,8.75585e-47,0.0,4.24406e-48
N(-2),1.71566e-38,1.71493e-38,0.0,7.28969e-42
C(+2),4.23411e-4,4.22957e-4,0.0,4.54587e-7
Fe(+6),1.61278e-60,1.59451e-60,0.0,1.82714e-62
S(0),5.37635e-23,5.37058e-23,0.0,5.7722e-26
MeO(-1),8.47631e-5,8.4722e-5,0.0,4.11722e-8
N(-1),1.26545e-38,1.2649e-38,0.0,5.44375e-42
TEGION,1.69979e-6,1.69979e-6,0.0,5.58639e-12

Element Distribution

 ,Total,Total,Liquid-1,Solid,Liquid-2
,mol,mole %,% of Total,% of Total,% of Total
H(+1),96.8409,64.3519,99.9987,0.0,1.34185e-3
K(+1),2.39397e-3,1.59082e-3,99.9993,0.0,6.61697e-4
Na(+1),1.07636,0.715254,99.9996,0.0,3.86065e-4
N(-3),2.08365e-4,1.38461e-4,0.178917,0.0,99.8211
Ba(+2),7.53659e-4,5.00815e-4,0.0799234,99.9201,9.20674e-10
Ca(+2),0.0633939,0.042126,98.987,1.00521,7.79769e-3
Fe(+2),2.33674e-3,1.55279e-3,61.028,0.0,38.972
Mg(+2),0.0760955,0.0505663,99.9945,0.0,5.48509e-3
Fe(+3),3.40336e-13,2.26157e-13,99.9585,0.0,0.0415281
O(-2),50.2739,33.4076,99.7098,0.0272748,0.262975
Cl(-1),1.25315,0.832736,99.8732,0.0,0.126753
C(+4),0.838171,0.556975,92.1429,0.0,7.85715
S(+4),1.34228e-14,8.91961e-15,99.6962,0.0,0.303799

S(+6),0.0397425,0.0264093,91.35,8.6256,0.0244
S(-2),2.89219e-15,1.9219e-15,96.6581,0.0,3.34186
S(+2),6.62204e-19,4.40042e-19,99.4169,0.0,0.583079
N(+3),4.11787e-53,2.73638e-53,99.721,0.0,0.279037
N(+5),7.89057e-69,5.24338e-69,99.9916,0.0,8.40793e-3
Sr(+2),2.44465e-3,1.6245e-3,16.6448,83.3549,3.18757e-4
N(0),0.0160812,0.0106861,75.0913,0.0,24.9087
H(0),7.03276e-14,4.67335e-14,99.8703,0.0,0.129663
O(0),9.62463e-61,6.39568e-61,94.6279,0.0,5.37215
S(+8),5.86635e-54,3.89826e-54,99.6907,0.0,0.309282
S(+3),3.94454e-35,2.62119e-35,98.8671,0.0,1.13291
S(+5),2.84973e-32,1.89368e-32,98.8671,0.0,1.13291
S(+7),3.4944e-65,2.32207e-65,98.8671,0.0,1.13291
N(+2),1.61599e-45,1.07384e-45,87.8225,0.0,12.1775
N(+4),1.22631e-66,8.14897e-67,95.1675,0.0,4.83246
N(+1),9.18026e-47,6.10038e-47,95.377,0.0,4.62303
N(-2),1.71566e-38,1.14008e-38,99.9575,0.0,0.0424891
C(+2),4.23411e-4,2.81362e-4,99.8926,0.0,0.107363
Fe(+6),1.61278e-60,1.07171e-60,98.8671,0.0,1.13291
S(0),5.37635e-23,3.57264e-23,99.8926,0.0,0.107363
MeO(-1),8.47631e-5,5.63261e-5,99.9514,0.0,0.0485732
N(-1),1.26545e-38,8.40905e-39,99.957,0.0,0.0430183
TEGION,1.69979e-6,1.12953e-6,99.9997,0.0,3.28651e-4

Calculation Summary
06-3 Alloy-5 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2507

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,48.4202,48.4202
CO2,0.838171,0.838171
BaCl2,4.89505e-7,4.89505e-7
CaCl2,8.42726e-3,8.42726e-3
CaO,0.0543687,0.0543687
FeCl2,2.33674e-3,2.33674e-3
KCl,2.39397e-3,2.39397e-3
MgCl2,0.0760955,0.0760955
NaCl,1.07636,1.07636
SO3,0.0360339,0.0360339
SrCl2,3.40157e-4,3.40157e-4

BaSO4,7.53170e-4,7.53170e-4
SrSO4,2.10449e-3,2.10449e-3
N2,8.01811e-3,8.01811e-3
CO,4.23411e-4,4.23411e-4
O2,2.52702e-5,2.52702e-5
NH3,1.32721e-4,1.32721e-4
CH3OH,8.47631e-5,8.47631e-5
H2S,5.07330e-5,5.07330e-5
SO2,2.02298e-4,2.02298e-4
NO2,1.20612e-4,1.20612e-4
C6H14O4,1.69979e-6,1.69979e-6
CaSO4,5.97925e-4,5.97925e-4

Calculated Rates

Corrosion Rate,2.01723e-4,mm/yr
Corrosion Potential,-0.296045,V (SHE)
Repassivation Potential*,0.303989,V (SHE)
Corrosion Current Density,1.96613e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaSO4 (Anhydrite),1.0
,SrSO4 (Celestine),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.166622
,CaSO4.0.5H2O (Bassanite),0.194665
,CaCO3 (Calcite),0.218207
,CaSO4.2H2O (Gypsum),0.920004
,FeCO3 (Siderite),0.110752
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,50.5272,mol
Temperature,109.400,°F
Pressure,2641.00,psia

Liquid 1 Properties
pH,4.49015,
Ionic Strength (x-based),0.0285798,mol/mol
Ionic Strength (m-based),1.69323,mol/kg
Dielectric Constant,53.6199,
ORP,0.0484882,V (SHE)
Osmotic Pressure,1486.67,psia
Specific Electrical Conductivity,1.48146e5,µmho/cm

"Viscosity, absolute",0.759325,cP
Thermal Conductivity,543.924,cal/hr m °C
Surface Tension,0.0739887,N/m
Interfacial Tension LLE,1.63016e-6,N/m
Standard Liquid Volume,0.944888,L
"Volume, Std. Conditions",0.925568,L
"Total Dissolved Solids, Estimated",85943.4,mg/L
Hardness,15035.0,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,5.39711e-5,L

Liquid 2 Properties
pH,4.92164,
Ionic Strength (x-based),0.0386571,mol/mol
Ionic Strength (m-based),355.156,mol/kg
Dielectric Constant,4.02929,
Specific Electrical Conductivity,44639.6,µmho/cm
"Viscosity, absolute",0.684260,cP
Surface Tension,0.0739955,N/m
Thermal Conductivity,531.483,cal/hr m °C
Standard Liquid Volume,2.54332e-3,L
"Volume, Std. Conditions",4.73181e-3,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid,Liquid-2
Density,g/ml,1.06394,1.06461,3.91272,0.785610
Enthalpy,J,-1.46846e7,-1.46525e7,-4989.85,-27143.1

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
Mole (True),51.7350,51.6607,3.42803e-3,0.0707962
Mole (App),50.5271,50.4544,3.42803e-3,0.0693391
,g,g,g,g
Mass,987.652,983.941,0.636811,3.07447
,L,L,cm3,L
Volume,0.928301,0.924225,0.162754,3.91347e-3

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
CaSO4 (Anhydrite),1.00000,1.14706
BaSO4 (Barite),1.00000,1434.58
SrSO4 (Celestine),1.00000,6.78656
CaSO4.2H2O (Gypsum),0.920004,1.05168
H2O,0.614464,0.613407
CaSO4.0.5H2O (Bassanite),0.282926,0.324255
CaCO3 (Calcite),0.218207,0.212764

CaSO4.0.5H2O (Bassanite),0.194665,0.223102
CaCO3 (Aragonite),0.166622,0.162465
FeCO3 (Siderite),0.110752,1.97699e-28
NaHCO3 (Nahcolite),0.0318636,0.0323963
NaCl (Halite),0.0210292,0.0213033
NaCl.2H2O (hydrohalite),0.0143417,0.0144787
SrCO3 (Strontianite),0.0122429,0.0706279
Na2SO4.CaSO4 (Glauberite),6.90775e-3,8.94106e-3
Na2SO4 (Thenardite),2.56756e-3,2.89725e-3
Na2SO4.5CaSO4.3H2O,2.09879e-3,4.67876e-3
Na2SO4.10H2O (Mirabilite),1.60249e-3,1.77739e-3
MgSO4.7H2O (Epsomite),4.14116e-4,4.54133e-4
MgSO4.6H2O (Hexahydrite),2.84476e-4,3.12503e-4
MgCO3,2.57843e-4,2.43271e-4
MgSO4.12H2O,1.77633e-4,1.93128e-4
Na2SO4,1.71809e-4,1.93870e-4
MgSO4.5H2O (Pentahydrite),1.45314e-4,1.59906e-4
KCl (sylvite),1.29950e-4,1.30939e-4
FeO(OH) (Goethite),1.00559e-4,
BaCO3 (Witherite),2.11092e-6,2.57417e-3

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H2O,48.4022,48.4018,0.0,4.27737e-4
Cl-1,1.25315,1.25156,,1.58841e-3
Na+1,1.06568,1.06568,,4.39568e-13
CO2,0.80065,0.73503,,0.0656204
Mg+2,0.0653752,0.0653752,,1.35177e-22
Ca+2,0.0583123,0.0583123,,2.81885e-22
HCO3-1,0.0359643,0.0359364,,2.79573e-5
SO4-2,0.0211448,0.0211442,,5.78211e-7
NaMgSO4+1,0.0106829,0.0106787,,4.15545e-6
N2,8.04059e-3,6.03778e-3,,2.00281e-3
CaSO4 (Anhydrite),5.07276e-3,4.43058e-3,6.3724e-4,4.93826e-6
K+1,2.35894e-3,2.35894e-3,,8.74326e-14
SrSO4 (Celestine),2.04499e-3,7.25027e-6,2.03773e-3,7.79247e-9
FeCO2+2,1.3401e-3,1.3401e-3,,1.95821e-103
Fe+2,9.96454e-4,8.57798e-5,,9.10674e-4
BaSO4 (Barite),7.53057e-4,,7.53057e-4,
CO,4.23411e-4,4.22957e-4,,4.54587e-7
Sr+2,3.99657e-4,3.99657e-4,,5.8724e-24
NH2CO2-1,2.07992e-4,1.0933e-12,,2.07992e-4
CH3OH,8.47553e-5,8.47141e-5,,4.11683e-8
KMgSO4+1,3.50291e-5,3.50133e-5,,1.58407e-8
H3O+1,1.85653e-5,1.85653e-5,,3.40614e-19
HSO4-1,7.83042e-6,7.83021e-6,,2.08511e-10
CaCO3 (Calcite),6.91243e-6,6.90744e-6,0.0,4.99666e-9
CaCl2 (Hydrophilite),1.88979e-6,1.88979e-6,0.0,2.03075e-22
C6H14O4,1.69979e-6,1.69978e-6,,5.56752e-12

MgSO4,1.18698e-6,1.18559e-6,0.0,1.38545e-9
MgCO3,1.14107e-6,1.13984e-6,0.0,1.22509e-9
CO3-2,7.78117e-7,7.75896e-7,,2.22181e-9
Ba+2,6.02344e-7,6.02344e-7,,3.46876e-29
NH4+1,3.7279e-7,3.7279e-7,,8.3691e-14
FeH(CO3)2-1,1.24981e-7,1.24594e-7,,3.86542e-10
FeCl+1,4.67669e-8,4.67469e-8,,1.99878e-11
FeSO4,1.63063e-8,1.62888e-8,0.0,1.74988e-11
Na2SO4.NaHSO4,9.00637e-9,9.00637e-9,0.0,7.39421e-18
CaClCH3OH+1,7.84299e-9,7.83909e-9,,3.90543e-12
MgOH+1,6.71489e-9,6.71203e-9,,2.85476e-12
OH-1,1.91992e-9,1.91768e-9,,2.23808e-12
CaOH+1,1.3084e-9,1.3081e-9,,3.00782e-13
FeOH+1,9.55718e-10,9.55312e-10,,4.06313e-13
HO(CH2CH2O)3CO2(-1),8.37581e-12,8.35695e-12,,1.886e-14
NH4OH,7.4978e-12,7.49641e-12,,1.38719e-15
BaCO3 (Witherite),6.46248e-12,6.45554e-12,0.0,6.93831e-15
SrCO3 (Strontianite),4.4834e-12,4.47859e-12,0.0,4.81351e-15
HCl,3.63434e-12,3.5479e-12,,8.64359e-14
NH3,2.59456e-12,2.59416e-12,,4.03595e-16
MgClCH3OH+1,1.85475e-12,1.85365e-12,,1.10649e-15
SrOH+1,1.3081e-12,1.30694e-12,,1.1627e-15
FeO+1,2.9465e-13,2.94525e-13,,1.25267e-16
H2,3.51638e-14,3.51182e-14,,4.55942e-17
FeOH+2,3.48968e-14,3.48893e-14,,7.51401e-18
CH3OH.HCl,3.45163e-14,3.44793e-14,,3.70571e-17
CH5O+1,3.37126e-14,3.36947e-14,,1.78377e-17
HSO3-1,1.3245e-14,1.32055e-14,,3.95426e-17
NaOH.Na2SO4,9.40879e-15,9.40879e-15,,4.27912e-29
Fe(NH3)+2,9.02288e-15,9.02087e-15,,2.00679e-18
HFeO2,7.77633e-15,7.76798e-15,,8.34889e-18
CH3O-1,7.69386e-15,7.67005e-15,,2.38135e-17
C6H15O4+1,4.17464e-15,4.1728e-15,,1.84205e-18
NaOH,4.01757e-15,4.01744e-15,0.0,1.27328e-19
BaOH+1,2.99645e-15,2.99602e-15,,4.35311e-19
H2S,2.87157e-15,2.77499e-15,,9.65804e-17
FeCl+2,2.82211e-15,2.82193e-15,,1.82517e-19
H2SO4,7.64596e-16,7.64596e-16,,3.96479e-24
FeO,7.51298e-16,7.50491e-16,,8.06616e-19
Fe+3,1.89516e-16,1.89495e-16,,2.16034e-20
SO3-2,1.49961e-16,1.49024e-16,,9.36763e-19
C6H13O4-1,5.6546e-17,5.63727e-17,,1.73265e-19
NaOHCO3-2,3.17937e-17,3.14335e-17,,3.60195e-19
SO2,2.78219e-17,2.75228e-17,,2.99088e-19
HS-1,2.03602e-17,2.02876e-17,,7.25532e-20
MgCl2,1.40401e-18,1.39707e-18,0.0,6.94054e-21
FeCl2+1,9.26868e-19,9.26817e-19,,5.05774e-23
S2O3-2,3.31002e-19,3.29072e-19,,1.93028e-21
FeHS+1,2.26847e-19,2.2675e-19,,9.64414e-23
FeO2-1,2.12352e-19,2.11696e-19,,6.56767e-22
FeHSO4+2,1.50365e-19,1.50331e-19,,3.37024e-23
FeS (Pyrrhotite),3.82182e-20,3.81772e-20,0.0,4.10322e-23
HFeO2-1,1.30032e-22,1.2963e-22,,4.02166e-25
HS2O3-1,1.00229e-22,9.9919e-23,,3.0999e-25

CO2S,3.11364e-23,3.1103e-23,,3.3429e-26
S1,2.2627e-23,2.26027e-23,,2.42931e-26
Fe(NH3)2+2,8.10778e-24,8.10597e-24,,1.80326e-27
S-2,1.25469e-26,1.13614e-26,,1.18552e-27
H2S2O3,1.21403e-26,1.21273e-26,,1.30342e-29
SO3,6.14622e-29,6.14622e-29,,2.22209e-35
S2O5-2,5.91189e-29,5.84491e-29,,6.69765e-31
Fe2(OH)2+4,1.91964e-29,1.91942e-29,,2.2206e-33
S2,3.44286e-32,3.43916e-32,,3.69635e-35
S2-2,1.68508e-32,1.66599e-32,,1.90905e-34
S2O6-2,1.42487e-32,1.40872e-32,,1.61425e-34
Fe(NH3)3+2,1.92981e-33,1.92939e-33,,4.29213e-37
S2O4-2,1.97227e-35,1.94992e-35,,2.23441e-37
NH2OH2+1,1.2079e-38,1.20739e-38,,5.11213e-42
N2H5+1,8.57472e-39,8.57108e-39,,3.64476e-42
NH2OH,5.75513e-40,5.75181e-40,0.0,3.31623e-43
S3-2,2.53807e-40,2.50931e-40,,2.87541e-42
S3,5.23825e-41,5.23263e-41,,5.62394e-44
N2H4,3.49605e-42,3.49598e-42,,6.58665e-47
N2H6+2,8.5352e-44,8.53336e-44,,1.83745e-47
NO,1.61599e-45,1.4192e-45,,1.96786e-46
Fe(NH3)4+2,7.64769e-46,7.64599e-46,,1.70094e-49
N2O,4.59013e-47,4.37792e-47,,2.12203e-48
S4-2,2.36623e-48,2.33943e-48,,2.68074e-50
S4,7.97079e-50,7.96224e-50,,8.55768e-53
NO2-1,3.99333e-53,3.98197e-53,,1.13567e-55
HSO5-1,5.86635e-54,5.8482e-54,,1.81435e-56
HNO2,1.24547e-54,1.24413e-54,,1.33717e-57
S5-2,1.36833e-56,1.35283e-56,,1.5502e-58
Fe(NH3)5+2,3.03158e-58,3.03091e-58,,6.74259e-62
S5,1.21292e-58,1.21162e-58,,1.30223e-61
S5O6-2,1.81867e-60,1.79806e-60,,2.06039e-62
FeO4-2,1.61278e-60,1.59451e-60,,1.82714e-62
O2,4.81232e-61,4.55379e-61,,2.58525e-62
S2O8-2,1.7472e-65,1.72741e-65,,1.97942e-67
NO2,1.22631e-66,1.16705e-66,,5.92609e-68
S6,1.84578e-67,1.84379e-67,,1.98168e-70
NO3-1,7.89057e-69,7.8899e-69,,6.63434e-73
Fe(NH3)6+2,1.20139e-70,1.20112e-70,,2.67203e-74
HNO3,7.27456e-75,7.27456e-75,,5.87289e-81
S7,2.80786e-76,2.80484e-76,,3.0146e-79
S8 (Sulfur),3.00833e-77,9.87318e-78,0.0,2.02101e-77
NH4NO3.(NH4)2SO4,7.14713e-93,7.13945e-93,0.0,7.67337e-96
N2O3,1.04318e-110,3.60423e-114,,1.04282e-110
Total (by phase),51.735,51.6607,3.42803e-3,0.0707962

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H(+1),96.8409,96.8396,0.0,1.29946e-3

K(+1),2.39397e-3,2.39395e-3,0.0,1.58408e-8
Na(+1),1.07636,1.07636,0.0,4.15545e-6
N(-3),2.08365e-4,3.72801e-7,0.0,2.07992e-4
Ba(+2),7.53659e-4,6.0235e-7,7.53057e-4,6.93874e-15
Ca(+2),0.0633939,0.0627517,6.3724e-4,4.94326e-6
Fe(+2),2.33674e-3,1.42607e-3,0.0,9.10675e-4
Mg(+2),0.0760955,0.0760913,0.0,4.1739e-6
Fe(+3),3.40336e-13,3.40195e-13,0.0,1.41335e-16
O(-2),50.2739,50.128,0.0137121,0.132208
Cl(-1),1.25315,1.25157,0.0,1.58841e-3
C(+4),0.838171,0.772315,0.0,0.0658564
S(+4),1.34228e-14,1.3382e-14,0.0,4.07784e-17
S(+6),0.0397425,0.0363048,3.42803e-3,9.69716e-6
S(-2),2.89219e-15,2.79554e-15,0.0,9.66531e-17
S(+2),6.62204e-19,6.58343e-19,0.0,3.86117e-21
N(+3),4.11787e-53,4.10638e-53,0.0,1.14904e-55
N(+5),7.89057e-69,7.88991e-69,0.0,6.63434e-73
Sr(+2),2.44465e-3,4.06907e-4,2.03773e-3,7.79248e-9
N(0),0.0160812,0.0120756,0.0,4.00562e-3
H(0),7.03276e-14,7.02364e-14,0.0,9.11885e-17
O(0),9.62463e-61,9.10758e-61,0.0,5.1705e-62
S(+8),5.86635e-54,5.8482e-54,0.0,1.81435e-56
S(+3),3.94454e-35,3.89985e-35,0.0,4.46882e-37
S(+5),2.84973e-32,2.81745e-32,0.0,3.2285e-34
S(+7),3.4944e-65,3.45481e-65,0.0,3.95885e-67
N(+2),1.61599e-45,1.4192e-45,0.0,1.96786e-46
N(+4),1.22631e-66,1.16705e-66,0.0,5.92609e-68
N(+1),9.18026e-47,8.75585e-47,0.0,4.24406e-48
N(-2),1.71566e-38,1.71493e-38,0.0,7.28969e-42
C(+2),4.23411e-4,4.22957e-4,0.0,4.54587e-7
Fe(+6),1.61278e-60,1.59451e-60,0.0,1.82714e-62
S(0),5.37635e-23,5.37058e-23,0.0,5.7722e-26
MeO(-1),8.47631e-5,8.4722e-5,0.0,4.11722e-8
N(-1),1.26545e-38,1.2649e-38,0.0,5.44375e-42
TEGION,1.69979e-6,1.69979e-6,0.0,5.58639e-12

Element Distribution

 ,Total,Total,Liquid-1,Solid,Liquid-2
,mol,mole %,% of Total,% of Total,% of Total
H(+1),96.8409,64.3519,99.9987,0.0,1.34185e-3
K(+1),2.39397e-3,1.59082e-3,99.9993,0.0,6.61697e-4
Na(+1),1.07636,0.715254,99.9996,0.0,3.86065e-4
N(-3),2.08365e-4,1.38461e-4,0.178917,0.0,99.8211
Ba(+2),7.53659e-4,5.00815e-4,0.0799234,99.9201,9.20674e-10
Ca(+2),0.0633939,0.042126,98.987,1.00521,7.79769e-3
Fe(+2),2.33674e-3,1.55279e-3,61.028,0.0,38.972
Mg(+2),0.0760955,0.0505663,99.9945,0.0,5.48509e-3
Fe(+3),3.40336e-13,2.26157e-13,99.9585,0.0,0.0415281
O(-2),50.2739,33.4076,99.7098,0.0272748,0.262975
Cl(-1),1.25315,0.832736,99.8732,0.0,0.126753
C(+4),0.838171,0.556975,92.1429,0.0,7.85715
S(+4),1.34228e-14,8.91961e-15,99.6962,0.0,0.303799

S(+6),0.0397425,0.0264093,91.35,8.6256,0.0244
S(-2),2.89219e-15,1.9219e-15,96.6581,0.0,3.34186
S(+2),6.62204e-19,4.40042e-19,99.4169,0.0,0.583079
N(+3),4.11787e-53,2.73638e-53,99.721,0.0,0.279037
N(+5),7.89057e-69,5.24338e-69,99.9916,0.0,8.40793e-3
Sr(+2),2.44465e-3,1.6245e-3,16.6448,83.3549,3.18757e-4
N(0),0.0160812,0.0106861,75.0913,0.0,24.9087
H(0),7.03276e-14,4.67335e-14,99.8703,0.0,0.129663
O(0),9.62463e-61,6.39568e-61,94.6279,0.0,5.37215
S(+8),5.86635e-54,3.89826e-54,99.6907,0.0,0.309282
S(+3),3.94454e-35,2.62119e-35,98.8671,0.0,1.13291
S(+5),2.84973e-32,1.89368e-32,98.8671,0.0,1.13291
S(+7),3.4944e-65,2.32207e-65,98.8671,0.0,1.13291
N(+2),1.61599e-45,1.07384e-45,87.8225,0.0,12.1775
N(+4),1.22631e-66,8.14897e-67,95.1675,0.0,4.83246
N(+1),9.18026e-47,6.10038e-47,95.377,0.0,4.62303
N(-2),1.71566e-38,1.14008e-38,99.9575,0.0,0.0424891
C(+2),4.23411e-4,2.81362e-4,99.8926,0.0,0.107363
Fe(+6),1.61278e-60,1.07171e-60,98.8671,0.0,1.13291
S(0),5.37635e-23,3.57264e-23,99.8926,0.0,0.107363
MeO(-1),8.47631e-5,5.63261e-5,99.9514,0.0,0.0485732
N(-1),1.26545e-38,8.40905e-39,99.957,0.0,0.0430183
TEGION,1.69979e-6,1.12953e-6,99.9997,0.0,3.28651e-4

Calculation Summary
06-0-2 Super13Cr Calculation

Unit Set: Custom

Automatic Chemistry Model
,Aqueous (H+ ion) Databanks:
,,Corrosion (AQ)
,,Aqueous (H+ ion)
,Second Liquid phase
,Redox selected
,Using K-fit Polynomials
,,T-span: 25.0 - 225.0
,,P-span: 1.0 - 1500.0

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Super13Cr stainless steel

Flow Type: Complete Agitation
Scales included - passivating films included.

Calc. elapsed time: 6.828 sec
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mg/L,mg/L
H2O,9.74892e5,9.73511e5
BaCl2,1.42242,1.42242
CaCl2,2903.43,2903.43
CaO,363.788,363.788
CO2,194.219,194.219
FeCl2,8.55693,8.55693
MgCl2,1339.62,1339.62
NaCl,63023.6,63023.6
SO3,369.435,369.435
BaSO4,137.754,137.754
CaCO3,135.897,135.897
FeCO3,8.77356,8.77356

Calculated Rates

Corrosion Rate,1.77571e-3,mm/yr
Corrosion Potential,-0.410030,V (SHE)
Repassivation Potential*,-0.135766,V (SHE)
Corrosion Current Density,1.63629e-3,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaCO3 (Calcite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.699178
,FeCO3 (Siderite),0.283778
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,1.00008,L
Temperature,50.0000,°C
Pressure,3398.00,psia

Aqueous Properties
pH,6.56214,
Ionic Strength (x-based),0.0216692,mol/mol
Ionic Strength (m-based),1.25383,mol/kg
ORP,-0.169402,V (SHE)
Osmotic Pressure,890.030,psia
Specific Electrical Conductivity,1.46695e5,µmho/cm
"Electrical Conductivity, molar",0.0129098,m2/ohm-mol
"Viscosity, absolute",0.628452,cP
"Viscosity, relative",1.14845,
Standard Liquid Volume,1.01645,L
"Volume, Std. Conditions",0.997701,L
"Total Dissolved Solids, Estimated",68240.7,mg/L
Hardness,4693.13,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,6.17790e-5,L

Thermodynamic Properties
,Unit,Total,Aqueous,Solid
Density,g/ml,1.04200,1.04181,3.46596
Enthalpy,J,-1.58116e7,-1.58093e7,-2323.39

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid

,mol,mol,mol
Mole (True),56.3343,56.3325,1.81152e-3
Mole (App),55.1789,55.1771,1.81152e-3
,g,g,g
Mass,1042.08,1041.82,0.262250
,L,L,cm3
Volume,1.00008,1.00001,0.0756645

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
Fe2O3 (Hematite),1.00000,1.80461e-9
FeS2 (Pyrite),1.00000,2.56865e-14
CaCO3 (Calcite),1.00000,1.70701e-3
BaSO4 (Barite),1.00000,203.036
FeO(OH) (Lepidocrocite),0.758086,3.18913e-5
CaCO3 (Aragonite),0.699178,1.19350e-3
FeS2(marcasite) (Marcasite),0.288259,7.40435e-15
FeCO3 (Siderite),0.283778,8.29085e-4
Fe3O4 (Magnetite),0.0982986,2.81830e-16
CaSO4 (Anhydrite),0.0904426,0.104314
CaSO4.2H2O (Gypsum),0.0795792,0.0882602
CaSO4.0.5H2O (Bassanite),0.0306866,0.0350482
NaCl (Halite),0.0149473,0.0143370
FeS (Pyrrhotite),9.45375e-3,7.14248e-14
NaHCO3 (Nahcolite),2.44421e-3,4.21606e-3
MgCO3 (Magnesite),1.45045e-3,2.35830e-6
Na2SO4 (Thenardite),7.18080e-4,8.00540e-4
MgCO3.3H2O (Nesquehonite),6.79000e-4,1.04102e-6
FeS(mackinawite) (Mackinawite),2.21139e-4,1.67075e-15
Fe(OH)3 (Bernalite),1.76710e-4,7.28978e-9
FeO (Wustite),1.58456e-4,2.51752e-10
Fe(OH)2 (Amakinite),1.50205e-4,2.34017e-10

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mg/L,mg/L,mg/L
H2O,9.73474e5,9.73548e5,
Cl-1,41089.5,41092.6,
Na+1,24768.1,24770.0,
Ca+2,1308.55,1308.65,
SO4-2,372.867,372.895,
Mg+2,331.092,331.117,
HCO3-1,192.269,192.284,
BaSO4 (Barite),138.58,,138.59
CaCO3 (Calcite),122.068,3.4644,118.613
NaHCO3 (Nahcolite),51.9603,51.9642,0.0
NaSO4-1,49.2667,49.2704,

CO2,25.1634,25.1653,
MgHCO3+1,23.3107,23.3124,
MgSO4,20.6942,20.6958,0.0
CaSO4 (Anhydrite),18.4215,18.4229,0.0
Fe2O3 (Hematite),4.55543,,4.55577
Fe+2,4.51748,4.51782,
FeS2 (Pyrite),0.488752,,0.488789
CO3-2,0.455565,0.455599,
Ba+2,0.332369,0.332395,
MgCO3 (Magnesite),0.189467,0.189482,0.0
BaCl(+1),0.145403,0.145414,
NaCO3-1,0.120706,0.120715,
FeCO3 (Siderite),0.100979,0.100987,0.0
CaCl+1,0.0422639,0.0422671,
CaHCO3+1,0.0215113,0.0215129,
FeOH+1,0.0183901,0.0183915,
MgOH+1,0.0107684,0.0107692,
FeCl+1,7.97739e-3,7.97799e-3,
BaHCO3+1,5.85133e-3,5.85178e-3,
OH-1,5.42325e-3,5.42366e-3,
HSO4-1,2.79807e-3,2.79828e-3,
CaOH+1,2.40689e-3,2.40707e-3,
FeHCO3+1,9.37354e-4,9.37425e-4,
H+1,3.33267e-4,3.33292e-4,
HS-1,4.45707e-5,4.45741e-5,
Fe(CO3)2-2,4.17432e-5,4.17464e-5,
FeHS+1,3.32229e-5,3.32254e-5,
H2S,3.28953e-5,3.28978e-5,
BaCO3 (Witherite),2.58687e-5,2.58707e-5,0.0
FeCl2 (Lawrencite),1.9115e-5,1.91165e-5,0.0
Fe(OH)3 (Bernalite),8.20732e-7,8.20794e-7,0.0
H2,4.41276e-8,4.4131e-8,
Fe(OH)2+1,2.34722e-8,2.3474e-8,
Fe(OH)4-1,2.07626e-8,2.07641e-8,
BaOH+1,1.69055e-8,1.69067e-8,
HCl,1.68812e-8,1.68825e-8,
S2O3-2,4.47771e-9,4.47804e-9,
NaS2O3-1,3.34546e-9,3.34572e-9,
SO3-2,2.62264e-9,2.62284e-9,
HSO3-1,2.0453e-9,2.04546e-9,
S-2,3.49462e-10,3.49488e-10,
FeOH+2,1.87382e-10,1.87396e-10,
HFeO2-1,1.28337e-10,1.28347e-10,
FeS(HS)-1,5.05766e-12,5.05805e-12,
CaCl2 (Hydrophilite),1.09132e-12,1.09141e-12,0.0
Fe+3,5.20441e-14,5.2048e-14,
SO2,3.2835e-14,3.28375e-14,
S2-2,1.86903e-14,1.86917e-14,
FeCl2+1,2.03257e-15,2.03272e-15,
FeCl+2,9.04101e-16,9.04169e-16,
FeSO4+1,1.31149e-16,1.31159e-16,
FeCl3 (Molysite),4.11533e-17,4.11564e-17,0.0
FeCl4-1,4.5635e-19,4.56385e-19,
S3-2,3.2685e-19,3.26874e-19,

H2SO4,1.37182e-20,1.37193e-20,
S4-2,3.17482e-24,3.17506e-24,
SO3,1.84958e-24,1.84972e-24,
S2O5-2,6.94338e-27,6.9439e-27,
S2O4-2,6.20314e-27,6.20361e-27,
Fe2(OH)2+4,1.44618e-27,1.44629e-27,
Na2S2O4,3.61594e-28,3.61622e-28,0.0
S2O6-2,4.95538e-29,4.95576e-29,
S5-2,1.81177e-29,1.81191e-29,
S5O6-2,3.9668e-48,3.9671e-48,
FeO4-2,8.18661e-50,8.18723e-50,
HSO5-1,1.17974e-52,1.17983e-52,
O2,3.94793e-60,3.94823e-60,
S2O8-2,4.61239e-66,4.61274e-66,
Total (by phase),1.042e6,1.04181e6,262.248

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mg/L,mg/L,mg/L
H(+1),1.08937e5,1.08945e5,0.0
Na(+1),24791.9,24793.7,0.0
Ba(+2),81.9932,0.452041,81.5473
Ca(+2),1362.89,1315.49,47.4963
Fe(+2),4.81312,4.58597,0.227518
Mg(+2),341.972,341.997,0.0
Fe(+3),3.18622,4.53019e-7,3.18646
O(-2),8.65146e5,8.65115e5,96.2539
Cl(-1),41089.6,41092.7,0.0
C(+4),70.2241,55.9951,14.2343
S(+4),1.85936e-9,1.8595e-9,0.0
S(+6),166.625,147.596,19.041
S(-2),0.130712,8.61494e-5,0.130635
S(+2),4.14885e-9,4.14916e-9,0.0
H(0),4.41276e-8,4.4131e-8,0.0
O(0),3.94793e-60,3.94823e-60,0.0
S(+8),3.34566e-53,3.34591e-53,0.0
S(+3),3.23802e-27,3.23826e-27,0.0
S(+5),1.98465e-29,1.9848e-29,0.0
S(+7),1.53962e-66,1.53973e-66,0.0
Fe(+6),3.81492e-50,3.81521e-50,0.0
S(0),0.130626,9.34607e-15,0.130635

Element Distribution

,Total,Total,Aqueous,Solid
,mol,mole %,% of Total,% of Total
H(+1),108.085,65.7208,100.0,0.0
Na(+1),1.07847,0.655761,100.0,0.0
Ba(+2),5.97102e-4,3.63067e-4,0.551273,99.4487

Ca(+2),0.0340087,0.020679,96.5153,3.48471
Fe(+2),8.61912e-5,5.24085e-5,95.2733,4.72668
Mg(+2),0.0140712,8.55597e-3,100.0,0.0
Fe(+3),5.70573e-5,3.46937e-5,1.4217e-5,100.0
O(-2),54.0782,32.8822,99.9889,0.0111249
Cl(-1),1.15908,0.70478,100.0,0.0
C(+4),5.84708e-3,3.55531e-3,79.7317,20.2683
S(+4),5.79903e-14,3.5261e-14,100.0,0.0
S(+6),5.19673e-3,3.15987e-3,88.5734,11.4266
S(-2),4.07667e-6,2.47882e-6,0.0659029,99.9341
S(+2),1.29395e-13,7.86787e-14,100.0,0.0
H(0),4.37823e-11,2.66218e-11,100.0,0.0
O(0),2.46775e-64,1.50052e-64,100.0,0.0
S(+8),1.04345e-57,6.3447e-58,100.0,0.0
S(+3),1.00988e-31,6.14057e-32,100.0,0.0
S(+5),6.18977e-34,3.76369e-34,100.0,0.0
S(+7),4.80179e-71,2.91972e-71,100.0,0.0
Fe(+6),6.83159e-55,4.15394e-55,100.0,0.0
S(0),4.07399e-6,2.47718e-6,7.15431e-12,100.0

Calculation Summary
06-0-5 22Cr Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE-SRK (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE-SRK (H3O+ ion)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

MSE-SRK was not designed to work with these components. The results may be in error.
,> FeS2

,> CO2S

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2205

Flow Type: Complete Agitation
Scales included - passivating films included.

The Corrosion databank is not selected and is usually required.
Please add the Corrosion databank unless you know it's not needed.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mg/L,mg/L
H2O,9.74892e5,9.75449e5
BaCl2,1.42242,1.42242
CaCl2,2903.43,2903.43
CaO,363.788,363.788
CO2,194.219,194.219
FeCl2,8.55693,8.55693
MgCl2,1339.62,1339.62
NaCl,63023.6,63023.6

SO3,369.435,369.435
BaSO4,137.754,137.754
CaCO3,135.897,135.897
FeCO3,8.77356,8.77356

Calculated Rates

Corrosion Rate,2.51002e-4,mm/yr
Corrosion Potential,-0.422311,V (SHE)
Repassivation Potential*,-0.0186557,V (SHE)
Corrosion Current Density,2.37718e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaCO3 (Calcite),1.0
,FeCO3 (Siderite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.772189
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,1.00008,L
Temperature,50.0000,°C
Pressure,3398.00,psia

Liquid 1 Properties
pH,6.56158,
Ionic Strength (x-based),0.0216280,mol/mol
Ionic Strength (m-based),1.25136,mol/kg
Dielectric Constant,56.3345,
ORP,-0.169570,V (SHE)
Osmotic Pressure,871.861,psia
Specific Electrical Conductivity,1.45176e5,µmho/cm
"Viscosity, absolute",0.632398,cP
Thermal Conductivity,554.991,cal/hr m °C
Surface Tension,0.0710685,N/m
Standard Liquid Volume,1.01839,L
"Volume, Std. Conditions",0.998916,L
"Total Dissolved Solids, Estimated",68213.3,mg/L
Hardness,4676.55,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,7.16797e-5,L

Thermodynamic Properties

,Unit,Total,Liquid-1,Solid
Density,g/ml,1.04394,1.04374,3.40023
Enthalpy,J,-1.58427e7,-1.58402e7,-2553.31

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
Mole (True),56.4426,56.4405,2.01695e-3
Mole (App),55.2863,55.2843,2.01695e-3
,g,g,g
Mass,1044.03,1043.74,0.281735
,L,L,cm3
Volume,1.00008,1.00000,0.0828575

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
FeCO3 (Siderite),1.00000,7.64936e-3
CaCO3 (Calcite),1.00000,0.0108418
BaSO4 (Barite),1.00000,147.046
Fe2O3 (Hematite),1.00000,1.25460e-7
CaCO3 (Aragonite),0.772189,8.37191e-3
H2O,0.592637,0.592466
FeS2 (Pyrite),0.273409,3.10519e9
FeS2(marcasite) (Marcasite),0.0788064,8.95028e8
FeO(OH) (Goethite),0.0782743,2.77144e-5
CaSO4 (Anhydrite),0.0752298,0.133100
CaSO4.2H2O (Gypsum),0.0668603,0.118224
CaSO4.0.5H2O (Bassanite),0.0215167,0.0380629
CaSO4.0.5H2O (Bassanite),0.0169798,0.0300372
NaCl (Halite),0.0127226,0.0127665
Fe3O4 (Magnetite),9.66591e-3,1.33749e-12
NaCl.2H2O (hydrohalite),8.19690e-3,8.22044e-3
Fe(OH)3 (Bernalite),5.22680e-3,1.85011e-6
FeS (Pyrrhotite),2.06594e-3,22.7662
NaHCO3 (Nahcolite),1.97075e-3,5.31798e-4
MgCO3,5.53372e-4,5.72547e-6
Na2SO4 (Thenardite),2.70960e-4,4.64156e-4
BaCO3 (Witherite),1.57714e-4,1.42114e-4
Na2SO4.10H2O (Mirabilite),1.11666e-4,1.90733e-4
Na2SO4.CaSO4 (Glauberite),5.81173e-5,1.76138e-4
FeS (Mackinawite),4.72230e-5,0.520386
FeS(amorphous) (FeS amorphous),1.75500e-6,0.0193397
Fe3S4 (Greigite),3.67086e-20,0.0506277

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mg/L,mg/L,mg/L
H2O,9.75416e5,9.75497e5,0.0
Cl-1,41089.5,41092.9,
Na+1,24785.6,24787.7,
Ca+2,1291.28,1291.38,
SO4-2,378.73,378.761,
Mg+2,335.309,335.336,
HCO3-1,223.805,223.823,
CaCO3 (Calcite),138.697,3.48028,135.228
BaSO4 (Barite),137.724,,137.736
CaSO4 (Anhydrite),54.4281,54.4326,0.0
NaMgSO4+1,38.9934,38.9967,
CO2,30.1471,30.1496,
FeCO3 (Siderite),8.76852,,8.76925
Fe+2,2.56854,2.56876,
FeCO2+2,2.1263,2.12647,
Ba+2,0.955366,0.955445,
CO3-2,0.52952,0.529563,
MgCO3,0.162486,0.162499,0.0
CaCl2 (Hydrophilite),0.124752,0.124763,0.0
FeH(CO3)2-1,0.01794,0.0179415,
FeOH+1,7.97431e-3,7.97497e-3,
MgOH+1,6.59221e-3,6.59276e-3,
OH-1,6.40637e-3,6.40691e-3,
MgSO4,6.31922e-3,6.31974e-3,0.0
CaOH+1,5.16387e-3,5.1643e-3,
H3O+1,4.93146e-3,4.93187e-3,
FeCl+1,3.52375e-3,3.52404e-3,
HSO4-1,1.81793e-3,1.81808e-3,
Fe2O3 (Hematite),1.13919e-3,,1.13928e-3
FeSO4,3.47041e-4,3.47069e-4,0.0
BaCO3 (Witherite),1.23704e-4,1.23714e-4,0.0
HS-1,2.8611e-5,2.86133e-5,
H2S,2.59042e-5,2.59063e-5,
FeS (Pyrrhotite),1.31586e-5,1.31597e-5,0.0
FeO,1.18031e-6,1.18041e-6,
HFeO2,9.50128e-7,9.50207e-7,
BaOH+1,7.10084e-7,7.10143e-7,
Na2SO4.NaHSO4,6.60785e-7,6.60839e-7,0.0
FeHS+1,3.75362e-7,3.75393e-7,
FeO+1,1.68365e-7,1.68379e-7,
H2,4.84167e-8,4.84207e-8,
NaOH.Na2SO4,3.94196e-8,3.94229e-8,
NaOH,3.68142e-8,3.68172e-8,0.0
NaOHCO3-2,6.26217e-9,6.26269e-9,
FeO2-1,3.9859e-9,3.98623e-9,
S2O3-2,2.49987e-9,2.50007e-9,
HCl,1.70673e-9,1.70687e-9,
SO3-2,1.60031e-9,1.60044e-9,
HSO3-1,1.25219e-9,1.25229e-9,
FeOH+2,1.28921e-10,1.28931e-10,
HFeO2-1,4.5211e-11,4.52147e-11,

S-2,3.61767e-12,3.61797e-12,
FeCl+2,1.00888e-13,1.00896e-13,
MgCl2,3.23337e-14,3.23363e-14,0.0
SO2,2.02435e-14,2.02452e-14,
HS2O3-1,7.35466e-15,7.35527e-15,
S2-2,4.85777e-15,4.85817e-15,
Fe+3,3.62253e-15,3.62283e-15,
H2SO4,2.65019e-15,2.65041e-15,
FeCl2+1,4.57854e-17,4.57892e-17,
CO2S,2.32027e-18,2.32046e-18,
S3-2,6.43977e-20,6.4403e-20,
FeHSO4+2,1.71819e-20,1.71834e-20,
H2S2O3,8.3134e-21,8.31409e-21,
S2O5-2,1.29063e-23,1.29073e-23,
S4-2,4.74186e-25,4.74225e-25,
Fe2(OH)2+4,5.03851e-27,5.03893e-27,
S2O4-2,1.24552e-27,1.24563e-27,
SO3,3.50337e-28,3.50366e-28,
S2O6-2,9.5285e-30,9.52929e-30,
S5-2,2.05135e-30,2.05152e-30,
HClO,1.82476e-41,1.82491e-41,
ClO-1,4.77546e-42,4.77586e-42,
Cl2,8.40725e-45,8.40795e-45,
S5O6-2,4.23815e-49,4.2385e-49,
S8 (Sulfur),1.0973e-49,1.0974e-49,0.0
FeO4-2,1.34274e-50,1.34285e-50,
HSO5-1,6.16904e-53,6.16955e-53,
O2,3.13081e-60,3.13107e-60,
S2O8-2,8.44811e-67,8.44881e-67,
ClO2-1,3.31852e-81,3.3188e-81,
HClO2,8.25411e-86,8.25479e-86,
ClO2,3.10449e-101,3.10475e-101,
ClO3-1,1.35487e-107,1.35498e-107,
Total (by phase),1.04394e6,1.04374e6,281.735

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid
,mg/L,mg/L,mg/L
H(+1),1.09157e5,1.09166e5,0.0
Na(+1),24791.9,24793.9,0.0
Ba(+2),81.9932,0.955532,81.0444
Ca(+2),1362.89,1308.85,54.1496
Fe(+2),7.99854,3.7721,4.2271
Mg(+2),341.972,342.0,0.0
Fe(+3),7.97517e-4,7.30747e-7,7.96853e-4
O(-2),8.66868e5,8.66834e5,106.252
Cl(-1),41089.6,41093.0,0.0
C(+4),70.224,53.0924,17.1374
S(+4),1.13621e-9,1.1363e-9,0.0
S(+6),166.886,147.976,18.9236

S(-2),5.70459e-5,5.70506e-5,0.0
S(+2),1.42978e-9,1.4299e-9,0.0
H(0),4.84182e-8,4.84222e-8,0.0
O(0),3.13081e-60,3.13107e-60,0.0
S(+8),1.74949e-53,1.74963e-53,0.0
Cl(+1),1.56265e-41,1.56278e-41,0.0
Cl(+5),5.75595e-108,5.75643e-108,0.0
S(+3),6.23416e-28,6.23467e-28,0.0
S(+5),3.8162e-30,3.81651e-30,0.0
S(+7),2.81998e-67,2.82021e-67,0.0
Cl(+3),1.74427e-81,1.74442e-81,0.0
Cl(+4),1.63174e-101,1.63187e-101,0.0
Fe(+6),6.2571e-51,6.25762e-51,0.0
S(0),2.4299e-15,2.43011e-15,0.0

Element Distribution

 ,Total,Total,Liquid-1,Solid
,mol,mole %,% of Total,% of Total
H(+1),108.3,65.7227,100.0,0.0
Na(+1),1.07847,0.654476,100.0,0.0
Ba(+2),5.97102e-4,3.62356e-4,1.16528,98.8347
Ca(+2),0.0340087,0.0206384,96.0272,3.97282
Fe(+2),1.43234e-4,8.69228e-5,47.156,52.844
Mg(+2),0.0140712,8.53921e-3,100.0,0.0
Fe(+3),1.42816e-8,8.66689e-9,0.0916201,99.9084
O(-2),54.1858,32.8831,99.9877,0.0122559
Cl(-1),1.15908,0.703399,100.0,0.0
C(+4),5.84708e-3,3.54835e-3,75.5981,24.4019
S(+4),3.54364e-14,2.15049e-14,100.0,0.0
S(+6),5.20488e-3,3.15862e-3,88.6617,11.3383
S(-2),1.77916e-9,1.0797e-9,100.0,0.0
S(+2),4.45925e-14,2.70613e-14,100.0,0.0
H(0),4.80379e-11,2.91522e-11,100.0,0.0
O(0),1.95699e-64,1.18762e-64,100.0,0.0
S(+8),5.45635e-58,3.31123e-58,100.0,0.0
Cl(+1),4.40803e-46,2.67505e-46,100.0,0.0
Cl(+5),1.62368e-112,9.85343e-113,100.0,0.0
S(+3),1.94433e-32,1.17993e-32,100.0,0.0
S(+5),1.19021e-34,7.22286e-35,100.0,0.0
S(+7),8.79501e-72,5.33732e-72,100.0,0.0
Cl(+3),4.92037e-86,2.98597e-86,100.0,0.0
Cl(+4),4.60292e-106,2.79332e-106,100.0,0.0
Fe(+6),1.12049e-55,6.7998e-56,100.0,0.0
S(0),7.57845e-20,4.59904e-20,100.0,0.0

Calculation Summary
06-0-6 25Cr Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE-SRK (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE-SRK (H3O+ ion)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

MSE-SRK was not designed to work with these components. The results may be in error.
,> FeS2

,> CO2S

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2507

Flow Type: Complete Agitation
Scales included - passivating films included.

The Corrosion databank is not selected and is usually required.
Please add the Corrosion databank unless you know it's not needed.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mg/L,mg/L
H2O,9.74892e5,9.75449e5
BaCl2,1.42242,1.42242
CaCl2,2903.43,2903.43
CaO,363.788,363.788
CO2,194.219,194.219
FeCl2,8.55693,8.55693
MgCl2,1339.62,1339.62
NaCl,63023.6,63023.6

SO3,369.435,369.435
BaSO4,137.754,137.754
CaCO3,135.897,135.897
FeCO3,8.77356,8.77356

Calculated Rates

Corrosion Rate,2.43893e-4,mm/yr
Corrosion Potential,-0.424994,V (SHE)
Repassivation Potential*,0.117996,V (SHE)
Corrosion Current Density,2.37714e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
,CaCO3 (Calcite),1.0
,FeCO3 (Siderite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaCO3 (Aragonite),0.772189
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,1.00008,L
Temperature,50.0000,°C
Pressure,3398.00,psia

Liquid 1 Properties
pH,6.56158,
Ionic Strength (x-based),0.0216280,mol/mol
Ionic Strength (m-based),1.25136,mol/kg
Dielectric Constant,56.3345,
ORP,-0.169570,V (SHE)
Osmotic Pressure,871.861,psia
Specific Electrical Conductivity,1.45176e5,µmho/cm
"Viscosity, absolute",0.632398,cP
Thermal Conductivity,554.991,cal/hr m °C
Surface Tension,0.0710685,N/m
Standard Liquid Volume,1.01839,L
"Volume, Std. Conditions",0.998916,L
"Total Dissolved Solids, Estimated",68213.3,mg/L
Hardness,4676.55,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,7.16797e-5,L

Thermodynamic Properties

,Unit,Total,Liquid-1,Solid
Density,g/ml,1.04394,1.04374,3.40023
Enthalpy,J,-1.58427e7,-1.58402e7,-2553.31

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
Mole (True),56.4426,56.4405,2.01695e-3
Mole (App),55.2863,55.2843,2.01695e-3
,g,g,g
Mass,1044.03,1043.74,0.281735
,L,L,cm3
Volume,1.00008,1.00000,0.0828575

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
FeCO3 (Siderite),1.00000,7.64936e-3
CaCO3 (Calcite),1.00000,0.0108418
BaSO4 (Barite),1.00000,147.046
Fe2O3 (Hematite),1.00000,1.25460e-7
CaCO3 (Aragonite),0.772189,8.37191e-3
H2O,0.592637,0.592466
FeS2 (Pyrite),0.273409,3.10519e9
FeS2(marcasite) (Marcasite),0.0788064,8.95028e8
FeO(OH) (Goethite),0.0782743,2.77144e-5
CaSO4 (Anhydrite),0.0752298,0.133100
CaSO4.2H2O (Gypsum),0.0668603,0.118224
CaSO4.0.5H2O (Bassanite),0.0215167,0.0380629
CaSO4.0.5H2O (Bassanite),0.0169798,0.0300372
NaCl (Halite),0.0127226,0.0127665
Fe3O4 (Magnetite),9.66591e-3,1.33749e-12
NaCl.2H2O (hydrohalite),8.19690e-3,8.22044e-3
Fe(OH)3 (Bernalite),5.22680e-3,1.85011e-6
FeS (Pyrrhotite),2.06594e-3,22.7662
NaHCO3 (Nahcolite),1.97075e-3,5.31798e-4
MgCO3,5.53372e-4,5.72547e-6
Na2SO4 (Thenardite),2.70960e-4,4.64156e-4
BaCO3 (Witherite),1.57714e-4,1.42114e-4
Na2SO4.10H2O (Mirabilite),1.11666e-4,1.90733e-4
Na2SO4.CaSO4 (Glauberite),5.81173e-5,1.76138e-4
FeS (Mackinawite),4.72230e-5,0.520386
FeS(amorphous) (FeS amorphous),1.75500e-6,0.0193397
Fe3S4 (Greigite),3.67086e-20,0.0506277

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mg/L,mg/L,mg/L
H2O,9.75416e5,9.75497e5,0.0
Cl-1,41089.5,41092.9,
Na+1,24785.6,24787.7,
Ca+2,1291.28,1291.38,
SO4-2,378.73,378.761,
Mg+2,335.309,335.336,
HCO3-1,223.805,223.823,
CaCO3 (Calcite),138.697,3.48028,135.228
BaSO4 (Barite),137.724,,137.736
CaSO4 (Anhydrite),54.4281,54.4326,0.0
NaMgSO4+1,38.9934,38.9967,
CO2,30.1471,30.1496,
FeCO3 (Siderite),8.76852,,8.76925
Fe+2,2.56854,2.56876,
FeCO2+2,2.1263,2.12647,
Ba+2,0.955366,0.955445,
CO3-2,0.52952,0.529563,
MgCO3,0.162486,0.162499,0.0
CaCl2 (Hydrophilite),0.124752,0.124763,0.0
FeH(CO3)2-1,0.01794,0.0179415,
FeOH+1,7.97431e-3,7.97497e-3,
MgOH+1,6.59221e-3,6.59276e-3,
OH-1,6.40637e-3,6.40691e-3,
MgSO4,6.31922e-3,6.31974e-3,0.0
CaOH+1,5.16387e-3,5.1643e-3,
H3O+1,4.93146e-3,4.93187e-3,
FeCl+1,3.52375e-3,3.52404e-3,
HSO4-1,1.81793e-3,1.81808e-3,
Fe2O3 (Hematite),1.13919e-3,,1.13928e-3
FeSO4,3.47041e-4,3.47069e-4,0.0
BaCO3 (Witherite),1.23704e-4,1.23714e-4,0.0
HS-1,2.8611e-5,2.86133e-5,
H2S,2.59042e-5,2.59063e-5,
FeS (Pyrrhotite),1.31586e-5,1.31597e-5,0.0
FeO,1.18031e-6,1.18041e-6,
HFeO2,9.50128e-7,9.50207e-7,
BaOH+1,7.10084e-7,7.10143e-7,
Na2SO4.NaHSO4,6.60785e-7,6.60839e-7,0.0
FeHS+1,3.75362e-7,3.75393e-7,
FeO+1,1.68365e-7,1.68379e-7,
H2,4.84167e-8,4.84207e-8,
NaOH.Na2SO4,3.94196e-8,3.94229e-8,
NaOH,3.68142e-8,3.68172e-8,0.0
NaOHCO3-2,6.26217e-9,6.26269e-9,
FeO2-1,3.9859e-9,3.98623e-9,
S2O3-2,2.49987e-9,2.50007e-9,
HCl,1.70673e-9,1.70687e-9,
SO3-2,1.60031e-9,1.60044e-9,
HSO3-1,1.25219e-9,1.25229e-9,
FeOH+2,1.28921e-10,1.28931e-10,
HFeO2-1,4.5211e-11,4.52147e-11,

S-2,3.61767e-12,3.61797e-12,
FeCl+2,1.00888e-13,1.00896e-13,
MgCl2,3.23337e-14,3.23363e-14,0.0
SO2,2.02435e-14,2.02452e-14,
HS2O3-1,7.35466e-15,7.35527e-15,
S2-2,4.85777e-15,4.85817e-15,
Fe+3,3.62253e-15,3.62283e-15,
H2SO4,2.65019e-15,2.65041e-15,
FeCl2+1,4.57854e-17,4.57892e-17,
CO2S,2.32027e-18,2.32046e-18,
S3-2,6.43977e-20,6.4403e-20,
FeHSO4+2,1.71819e-20,1.71834e-20,
H2S2O3,8.3134e-21,8.31409e-21,
S2O5-2,1.29063e-23,1.29073e-23,
S4-2,4.74186e-25,4.74225e-25,
Fe2(OH)2+4,5.03851e-27,5.03893e-27,
S2O4-2,1.24552e-27,1.24563e-27,
SO3,3.50337e-28,3.50366e-28,
S2O6-2,9.5285e-30,9.52929e-30,
S5-2,2.05135e-30,2.05152e-30,
HClO,1.82476e-41,1.82491e-41,
ClO-1,4.77546e-42,4.77586e-42,
Cl2,8.40725e-45,8.40795e-45,
S5O6-2,4.23815e-49,4.2385e-49,
S8 (Sulfur),1.0973e-49,1.0974e-49,0.0
FeO4-2,1.34274e-50,1.34285e-50,
HSO5-1,6.16904e-53,6.16955e-53,
O2,3.13081e-60,3.13107e-60,
S2O8-2,8.44811e-67,8.44881e-67,
ClO2-1,3.31852e-81,3.3188e-81,
HClO2,8.25411e-86,8.25479e-86,
ClO2,3.10449e-101,3.10475e-101,
ClO3-1,1.35487e-107,1.35498e-107,
Total (by phase),1.04394e6,1.04374e6,281.735

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid
,mg/L,mg/L,mg/L
H(+1),1.09157e5,1.09166e5,0.0
Na(+1),24791.9,24793.9,0.0
Ba(+2),81.9932,0.955532,81.0444
Ca(+2),1362.89,1308.85,54.1496
Fe(+2),7.99854,3.7721,4.2271
Mg(+2),341.972,342.0,0.0
Fe(+3),7.97517e-4,7.30747e-7,7.96853e-4
O(-2),8.66868e5,8.66834e5,106.252
Cl(-1),41089.6,41093.0,0.0
C(+4),70.224,53.0924,17.1374
S(+4),1.13621e-9,1.1363e-9,0.0
S(+6),166.886,147.976,18.9236

S(-2),5.70459e-5,5.70506e-5,0.0
S(+2),1.42978e-9,1.4299e-9,0.0
H(0),4.84182e-8,4.84222e-8,0.0
O(0),3.13081e-60,3.13107e-60,0.0
S(+8),1.74949e-53,1.74963e-53,0.0
Cl(+1),1.56265e-41,1.56278e-41,0.0
Cl(+5),5.75595e-108,5.75643e-108,0.0
S(+3),6.23416e-28,6.23467e-28,0.0
S(+5),3.8162e-30,3.81651e-30,0.0
S(+7),2.81998e-67,2.82021e-67,0.0
Cl(+3),1.74427e-81,1.74442e-81,0.0
Cl(+4),1.63174e-101,1.63187e-101,0.0
Fe(+6),6.2571e-51,6.25762e-51,0.0
S(0),2.4299e-15,2.43011e-15,0.0

Element Distribution

 ,Total,Total,Liquid-1,Solid
,mol,mole %,% of Total,% of Total
H(+1),108.3,65.7227,100.0,0.0
Na(+1),1.07847,0.654476,100.0,0.0
Ba(+2),5.97102e-4,3.62356e-4,1.16528,98.8347
Ca(+2),0.0340087,0.0206384,96.0272,3.97282
Fe(+2),1.43234e-4,8.69228e-5,47.156,52.844
Mg(+2),0.0140712,8.53921e-3,100.0,0.0
Fe(+3),1.42816e-8,8.66689e-9,0.0916201,99.9084
O(-2),54.1858,32.8831,99.9877,0.0122559
Cl(-1),1.15908,0.703399,100.0,0.0
C(+4),5.84708e-3,3.54835e-3,75.5981,24.4019
S(+4),3.54364e-14,2.15049e-14,100.0,0.0
S(+6),5.20488e-3,3.15862e-3,88.6617,11.3383
S(-2),1.77916e-9,1.0797e-9,100.0,0.0
S(+2),4.45925e-14,2.70613e-14,100.0,0.0
H(0),4.80379e-11,2.91522e-11,100.0,0.0
O(0),1.95699e-64,1.18762e-64,100.0,0.0
S(+8),5.45635e-58,3.31123e-58,100.0,0.0
Cl(+1),4.40803e-46,2.67505e-46,100.0,0.0
Cl(+5),1.62368e-112,9.85343e-113,100.0,0.0
S(+3),1.94433e-32,1.17993e-32,100.0,0.0
S(+5),1.19021e-34,7.22286e-35,100.0,0.0
S(+7),8.79501e-72,5.33732e-72,100.0,0.0
Cl(+3),4.92037e-86,2.98597e-86,100.0,0.0
Cl(+4),4.60292e-106,2.79332e-106,100.0,0.0
Fe(+6),1.12049e-55,6.7998e-56,100.0,0.0
S(0),7.57845e-20,4.59904e-20,100.0,0.0

Calculation Summary
06-1 Alloy-1 Calculation

Unit Set: Custom

Automatic Chemistry Model
,Aqueous (H+ ion) Databanks:
,,Corrosion (AQ)
,,Aqueous (H+ ion)
,Second Liquid phase
,Redox selected
,Using K-fit Polynomials
,,T-span: 25.0 - 225.0
,,P-span: 1.0 - 1500.0

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Super13Cr stainless steel

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3.1H2O

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,5.35989,5.35989
CO2,0.117452,0.117452
N2,9.42087e-4,9.42087e-4
CO,6.05939e-5,6.05939e-5
O2,2.79025e-6,2.79025e-6
NH3,1.47447e-3,1.47447e-3
CH3OH,6.04056e-4,6.04056e-4
H2S,1.24254e-5,1.24254e-5
SO2,1.78309e-3,1.78309e-3

NO2,1.95370e-5,1.95370e-5
BaCl2,1.85435e-7,1.85435e-7
CaCl2,2.60922e-3,2.60922e-3
CaO,7.91645e-4,7.91645e-4
FeCl2,1.43249e-5,1.43249e-5
MgCl2,1.40712e-3,1.40712e-3
NaCl,0.107847,0.107847
SO3,4.60964e-4,4.60964e-4
BaSO4,5.95248e-5,5.95248e-5
C6H14O4,1.84742e-5,1.84742e-5

Calculated Rates

Corrosion Rate,7.27738e-4,mm/yr
Corrosion Potential,-0.174273,V (SHE)
Repassivation Potential*,-0.240675,V (SHE)
Corrosion Current Density,6.70597e-4,A/sq-m
Maximum Pit Current Density,0.0749974,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.2H2O (Gypsum),0.258695
,CaSO4 (Anhydrite),0.218516
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,5.59545,mol
Temperature,83.6413,°F
Pressure,3398.00,psia

Aqueous Properties
pH,2.53521,
Ionic Strength (x-based),0.0218773,mol/mol
Ionic Strength (m-based),1.29351,mol/kg
ORP,0.121530,V (SHE)
Osmotic Pressure,1310.98,psia
Specific Electrical Conductivity,1.03816e5,µmho/cm
"Electrical Conductivity, molar",4.49829e-3,m2/ohm-mol
"Viscosity, absolute",0.940026,cP
"Viscosity, relative",1.14526,
Standard Liquid Volume,0.105271,L
"Volume, Std. Conditions",0.102796,L
"Total Dissolved Solids, Estimated",68517.9,mg/L
Hardness,4714.35,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,1.43844e-6,L

Second Liquid Properties
Standard Liquid Volume,6.57109e-5,L
"Volume, Std. Conditions",9.61711e-5,L

Thermodynamic Properties
,Unit,Total,Aqueous,Solid,2nd Liquid
Density,g/ml,1.06393,1.06443,3.11397,0.566690
Enthalpy,J,-1.62598e6,-1.62519e6,-90.3511,-699.262

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid,2nd Liquid
,mol,mol,mol,mol
Mole (True),5.70876,5.70688,1.06387e-4,1.77644e-3
Mole (App),5.59460,5.59271,1.06387e-4,1.77644e-3
,g,g,g,g
Mass,108.744,108.643,0.0239560,0.0769431
,L,L,cm3,L
Volume,0.102210,0.102066,7.69306e-3,1.35776e-4

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
S8 (Sulfur),1.00000,7431.32
BaSO4 (Barite),1.00000,1241.45
FeS2 (Pyrite),1.00000,29823.7
FeS2(marcasite) (Marcasite),0.261913,7811.20
CaSO4.2H2O (Gypsum),0.258695,0.297790
CaSO4 (Anhydrite),0.218516,0.251724
CaSO4.0.5H2O (Bassanite),0.0599063,0.0689974
NaCl (Halite),0.0152568,0.0152351
Na2SO4.10H2O (Mirabilite),5.28614e-3,6.09847e-3
Na2SO4 (Thenardite),1.68122e-3,1.94672e-3
NaHCO3 (Nahcolite),7.24745e-4,7.46780e-4
NH4Cl (Sal ammoniac),5.04220e-4,6.34732e-4
MgSO4.7H2O (Epsomite),3.04613e-4,3.49668e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid,2nd Liquid
,mol,mol,mol,mol
H2O,5.35774,5.35771,,2.55726e-5
CO2,0.117369,0.115661,,1.70752e-3

Cl-1,0.115908,0.115908,,
Na+1,0.107149,0.107149,,
Ca+2,3.36445e-3,3.36445e-3,,
NH4+1,2.03515e-3,2.03515e-3,,
Mg+2,1.3661e-3,1.3661e-3,,
SO4-2,1.13139e-3,1.13139e-3,,
NaSO4-1,6.76892e-4,6.76892e-4,,
N2,6.53652e-4,6.1346e-4,,4.0192e-5
CH3OH,6.04056e-4,6.03974e-4,,8.27116e-8
H+1,3.38688e-4,3.38688e-4,,
CO,6.05939e-5,5.85179e-5,,2.07597e-6
BaSO4 (Barite),5.96545e-5,,5.96545e-5,
HCO3-1,5.7221e-5,5.7221e-5,,
HSO4-1,4.83588e-5,4.83588e-5,,
CaSO4 (Anhydrite),3.64096e-5,3.64096e-5,0.0,
MgSO4,3.57859e-5,3.57859e-5,0.0,
NH4SO4-1,3.57247e-5,3.57247e-5,,
S8 (Sulfur),3.2414e-5,,3.2414e-5,
NaHCO3 (Nahcolite),2.07317e-5,2.07317e-5,0.0,
C6H14O4,1.84742e-5,1.74941e-5,,9.80147e-7
FeS2 (Pyrite),1.43183e-5,,1.43183e-5,
MgHCO3+1,5.22877e-6,5.22877e-6,,
H2S,3.84054e-6,3.81534e-6,,2.51976e-8
Ba+2,4.12951e-8,4.12951e-8,,
BaCl(+1),1.43677e-8,1.43677e-8,,
CaHCO3+1,7.29764e-9,7.29764e-9,,
Fe+2,6.51939e-9,6.51939e-9,,
CaCl+1,5.74034e-9,5.74034e-9,,
S2O3-2,4.22497e-10,4.22497e-10,,
HS-1,3.2328e-10,3.2328e-10,,
NH3,2.19442e-10,2.19437e-10,,5.56751e-15
NaS2O3-1,2.16847e-10,2.16847e-10,,
HCl,1.3499e-10,1.34923e-10,,6.69607e-14
BaHCO3+1,4.91699e-11,4.91699e-11,,
CaCO3 (Calcite),3.99438e-11,3.99438e-11,0.0,
CO3-2,8.50388e-12,8.50388e-12,,
FeCl+1,3.41377e-12,3.41377e-12,,
NaCO3-1,2.64969e-12,2.64969e-12,,
MgCO3 (Magnesite),2.36423e-12,2.36423e-12,0.0,
HSO3-1,1.42929e-12,1.42929e-12,,
OH-1,6.82105e-13,6.82105e-13,,
MgOH+1,4.94218e-13,4.94218e-13,,
NH2CO2-1,3.29121e-13,3.29121e-13,,
SO2,1.87688e-13,1.87271e-13,,4.16899e-16
FeHS+1,1.5802e-13,1.5802e-13,,
FeHCO3+1,1.07626e-13,1.07626e-13,,
CaOH+1,7.13362e-14,7.13362e-14,,
H2,4.23123e-14,4.16164e-14,,6.9595e-16
FeCl2 (Lawrencite),5.16638e-15,5.16638e-15,0.0,
FeCO3 (Siderite),9.28201e-16,9.28201e-16,0.0,
S5-2,6.52368e-16,6.52368e-16,,
FeOH+1,5.80723e-16,5.80723e-16,,
Fe(NH3)+2,2.63388e-16,2.63388e-16,,
SO3-2,2.54945e-16,2.54945e-16,,

S4-2,1.52611e-16,1.52611e-16,,
S3-2,2.16502e-17,2.16502e-17,,
BaCO3 (Witherite),1.74807e-17,1.74807e-17,0.0,
H2SO4,4.17512e-18,2.84908e-18,,1.32604e-18
Fe+3,2.38374e-18,2.38374e-18,,
S2-2,1.86312e-18,1.86312e-18,,
FeOH+2,1.86432e-19,1.86432e-19,,
S-2,7.9195e-20,7.9195e-20,,
FeCl2+1,2.95877e-20,2.95877e-20,,
BaOH+1,2.30623e-20,2.30623e-20,,
FeCl+2,1.13928e-20,1.13928e-20,,
FeSO4+1,2.04113e-21,2.04113e-21,,
CaCl2 (Hydrophilite),1.47673e-21,1.47673e-21,0.0,
FeCl3 (Molysite),6.51023e-22,6.51023e-22,0.0,
Fe(OH)2+1,5.13096e-22,5.13096e-22,,
SO3,3.4193e-22,3.4193e-22,,5.58923e-31
Fe(NH3)2+2,5.79898e-23,5.79898e-23,,
FeCl4-1,1.20605e-23,1.20605e-23,,
FeS(HS)-1,3.39343e-24,3.39343e-24,,
Fe(CO3)2-2,2.66766e-24,2.66766e-24,,
Fe(OH)3 (Bernalite),9.44943e-25,9.44943e-25,0.0,
S2O5-2,1.87193e-27,1.87193e-27,,
S2O4-2,2.00568e-28,2.00568e-28,,
S2O6-2,6.54647e-29,6.54647e-29,,
Na2S2O4,9.40063e-30,9.40063e-30,0.0,
Fe(NH3)3+2,3.17552e-30,3.17552e-30,,
S5O6-2,3.08411e-30,3.08411e-30,,
Fe(OH)4-1,1.97724e-31,1.97724e-31,,
HFeO2-1,1.93865e-33,1.93865e-33,,
N2H5+1,2.25623e-35,2.25623e-35,,
Fe2(OH)2+4,1.33795e-39,1.33795e-39,,
Fe(NH3)4+2,2.13823e-40,2.13823e-40,,
N2H4,4.63101e-41,4.63101e-41,,5.65523e-48
NH2OH,1.64867e-42,1.64866e-42,,6.83987e-48
Fe(NH3)5+2,1.43984e-50,1.43984e-50,,
NO,9.19182e-51,9.013e-51,,1.78814e-52
N2O,4.04272e-52,3.97158e-52,,7.11346e-54
HSO5-1,2.55471e-57,2.55471e-57,,
Fe(NH3)6+2,9.69506e-61,9.69506e-61,,
HNO2,6.1951e-61,6.09905e-61,,9.60429e-63
NO2-1,3.0484e-61,3.0484e-61,,
S2O8-2,4.22719e-67,4.22719e-67,,
O2,1.4425e-68,1.36409e-68,,7.84148e-70
NO2,4.97741e-74,4.95864e-74,,1.87683e-76
FeO4-2,2.66028e-79,2.66028e-79,,
NO3-1,1.56011e-79,1.56011e-79,,
NH4NO3 (Gwihabaite),9.34053e-81,9.34053e-81,0.0,
NaNO3 (Nitratine),6.97754e-81,6.97754e-81,0.0,
Ca(NO3)+1,3.62436e-81,3.62436e-81,,
HNO3,2.99429e-87,2.98892e-87,,5.36315e-90
FeNO3+2,1.69307e-98,1.69307e-98,,
Total (by phase),5.70876,5.70688,1.06387e-4,1.77644e-3

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid,2nd Liquid
,mol,mol,mol,mol
H(+1),10.7242,10.7242,0.0,5.11957e-5
Na(+1),0.107847,0.107847,0.0,0.0
N(-3),2.07088e-3,2.07088e-3,0.0,5.56751e-15
Ba(+2),5.97102e-5,5.5712e-8,5.96545e-5,0.0
Ca(+2),3.40087e-3,3.40087e-3,0.0,0.0
Fe(+2),1.43249e-5,6.52307e-9,1.43183e-5,0.0
Mg(+2),1.40712e-3,1.40712e-3,0.0,0.0
Fe(+3),2.61437e-18,2.61437e-18,0.0,0.0
O(-2),5.60088,5.5972,2.38618e-4,3.44268e-3
Cl(-1),0.115908,0.115908,0.0,6.69607e-14
C(+4),0.117452,0.115745,0.0,1.70752e-3
S(+4),1.61724e-12,1.61682e-12,0.0,4.16899e-16
S(+6),2.02422e-3,1.96456e-3,5.96545e-5,1.32604e-18
S(-2),1.81592e-5,3.81567e-6,1.43183e-5,2.51976e-8
S(+2),1.27869e-9,1.27869e-9,0.0,0.0
N(+3),9.2435e-61,9.14746e-61,0.0,9.60429e-63
N(+5),1.75953e-79,1.75953e-79,0.0,5.36315e-90
N(0),1.3073e-3,1.22692e-3,0.0,8.0384e-5
H(0),8.46246e-14,8.32327e-14,0.0,1.3919e-15
O(0),2.885e-68,2.72818e-68,0.0,1.5683e-69
S(+8),2.55471e-57,2.55471e-57,0.0,0.0
S(+3),4.19938e-28,4.19938e-28,0.0,0.0
S(+5),1.30929e-28,1.30929e-28,0.0,0.0
S(+7),8.45437e-67,8.45437e-67,0.0,0.0
N(+2),9.19182e-51,9.013e-51,0.0,1.78814e-52
N(+4),4.97741e-74,4.95864e-74,0.0,1.87683e-76
N(+1),8.08544e-52,7.94317e-52,0.0,1.42269e-53
N(-2),4.51246e-35,4.51246e-35,0.0,1.13105e-47
C(+2),6.05939e-5,5.85179e-5,0.0,2.07597e-6
Fe(+6),2.66028e-79,2.66028e-79,0.0,0.0
S(0),2.7363e-4,3.11247e-15,2.7363e-4,0.0
N(-1),1.64867e-42,1.64866e-42,0.0,6.83987e-48
METHANOL,6.04056e-4,6.03974e-4,0.0,8.27116e-8
TRIETLNGLY,1.84742e-5,1.74941e-5,0.0,9.80147e-7

Element Distribution

,Total,Total,Aqueous,Solid,2nd Liquid
,mol,mole %,% of Total,% of Total,% of Total
H(+1),10.7242,64.3033,99.9995,0.0,4.77383e-4
Na(+1),0.107847,0.646656,100.0,0.0,0.0
N(-3),2.07088e-3,0.0124171,100.0,0.0,2.68848e-10
Ba(+2),5.97102e-5,3.58027e-4,0.0933039,99.9067,0.0
Ca(+2),3.40087e-3,0.0203918,100.0,0.0,0.0
Fe(+2),1.43249e-5,8.58928e-5,0.0455368,99.9545,0.0
Mg(+2),1.40712e-3,8.43718e-3,100.0,0.0,0.0
Fe(+3),2.61437e-18,1.56759e-17,100.0,0.0,0.0

O(-2),5.60088,33.5833,99.9343,4.26036e-3,0.0614667
Cl(-1),0.115908,0.694995,100.0,0.0,5.77704e-11
C(+4),0.117452,0.704251,98.5462,0.0,1.4538
S(+4),1.61724e-12,9.69707e-12,99.9742,0.0,0.0257785
S(+6),2.02422e-3,0.0121374,97.053,2.94704,6.55086e-14
S(-2),1.81592e-5,1.08884e-4,21.0123,78.8489,0.13876
S(+2),1.27869e-9,7.6671e-9,100.0,0.0,0.0
N(+3),9.2435e-61,5.54247e-60,98.961,0.0,1.03903
N(+5),1.75953e-79,1.05503e-78,100.0,0.0,3.04805e-9
N(0),1.3073e-3,7.83868e-3,93.8512,0.0,6.14884
H(0),8.46246e-14,5.07415e-13,98.3552,0.0,1.64479
O(0),2.885e-68,1.72987e-67,94.564,0.0,5.43603
S(+8),2.55471e-57,1.53182e-56,100.0,0.0,0.0
S(+3),4.19938e-28,2.51798e-27,100.0,0.0,0.0
S(+5),1.30929e-28,7.85062e-28,100.0,0.0,0.0
S(+7),8.45437e-67,5.0693e-66,100.0,0.0,0.0
N(+2),9.19182e-51,5.51148e-50,98.0546,0.0,1.94536
N(+4),4.97741e-74,2.98449e-73,99.6229,0.0,0.377071
N(+1),8.08544e-52,4.84808e-51,98.2404,0.0,1.75957
N(-2),4.51246e-35,2.7057e-34,100.0,0.0,2.50649e-11
C(+2),6.05939e-5,3.63325e-4,96.574,0.0,3.42604
Fe(+6),2.66028e-79,1.59512e-78,100.0,0.0,0.0
S(0),2.7363e-4,1.64071e-3,1.13747e-9,100.0,0.0
N(-1),1.64867e-42,9.88552e-42,99.9996,0.0,4.14873e-4
METHANOL,6.04056e-4,3.62196e-3,99.9863,0.0,0.0136927
TRIETLNGLY,1.84742e-5,1.10773e-4,94.6945,0.0,5.30549

Calculation Summary
06-1 Alloy-4 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2205

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3.1H2O

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,5.35989,5.35989
CO2,0.117452,0.117452
N2,9.42087e-4,9.42087e-4
CO,6.05939e-5,6.05939e-5
O2,2.79025e-6,2.79025e-6
NH3,1.47447e-3,1.47447e-3
CH3OH,6.04056e-4,6.04056e-4
H2S,1.24254e-5,1.24254e-5
SO2,1.78309e-3,1.78309e-3
NO2,1.95370e-5,1.95370e-5
BaCl2,1.85435e-7,1.85435e-7

CaCl2,2.60922e-3,2.60922e-3
CaO,7.91645e-4,7.91645e-4
FeCl2,1.43249e-5,1.43249e-5
MgCl2,1.40712e-3,1.40712e-3
NaCl,0.107847,0.107847
SO3,4.60964e-4,4.60964e-4
BaSO4,5.95248e-5,5.95248e-5
C6H14O4,1.84742e-5,1.84742e-5

Calculated Rates

Corrosion Rate,1.93592e-4,mm/yr
Corrosion Potential,-0.113883,V (SHE)
Repassivation Potential*,-0.0730874,V (SHE)
Corrosion Current Density,1.83346e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.2H2O (Gypsum),0.330843
,CaSO4 (Anhydrite),0.266135
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,5.59545,mol
Temperature,83.6413,°F
Pressure,3398.00,psia

Liquid 1 Properties
pH,2.24050,
Ionic Strength (x-based),0.0218055,mol/mol
Ionic Strength (m-based),1.28624,mol/kg
Dielectric Constant,58.4911,
ORP,0.143810,V (SHE)
Osmotic Pressure,1328.28,psia
Specific Electrical Conductivity,1.02303e5,µmho/cm
"Viscosity, absolute",0.943026,cP
Thermal Conductivity,531.258,cal/hr m °C
Surface Tension,0.0740070,N/m
Interfacial Tension LLE,1.30535e-4,N/m
Standard Liquid Volume,0.104790,L
"Volume, Std. Conditions",0.102664,L
"Total Dissolved Solids, Estimated",68236.4,mg/L
Hardness,4679.53,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,2.22068e-6,L

Liquid 2 Properties
pH,0.944221,
Ionic Strength (x-based),5.49331e-3,mol/mol
Ionic Strength (m-based),75.9611,mol/kg
Dielectric Constant,4.76273,
Specific Electrical Conductivity,9087.68,µmho/cm
"Viscosity, absolute",0.905541,cP
Surface Tension,0.0440035,N/m
Thermal Conductivity,529.215,cal/hr m °C
Standard Liquid Volume,5.50080e-4,L
"Volume, Std. Conditions",1.00377e-3,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid,Liquid-2
Density,g/ml,1.05858,1.05957,2.75086,0.894627
Enthalpy,J,-1.62627e6,-1.62029e6,-87.8158,-5899.09

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
Mole (True),5.70910,5.69412,1.24375e-4,0.0148524
Mole (App),5.59483,5.57977,1.24375e-4,0.0149418
,g,g,g,g
Mass,108.744,108.063,0.0305257,0.650728
,L,L,cm3,L
Volume,0.102726,0.101988,0.0110968,7.27374e-4

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,1201.43
S8 (Sulfur),1.00000,1763.00
S8 (Sulfur monoclinic),0.754401,1330.01
H2O,0.700000,0.697565
CaSO4.2H2O (Gypsum),0.330843,0.431193
CaSO4 (Anhydrite),0.266135,0.349284
CaSO4.0.5H2O (Bassanite),0.0689498,0.0903343
CaSO4.0.5H2O (Bassanite),0.0547689,0.0717552
NaCl (Halite),0.0168136,0.0172518
NaCl.2H2O (hydrohalite),0.0153163,0.0156063
Na2SO4.10H2O (Mirabilite),3.97154e-3,5.10582e-3
FeS2 (Pyrite),3.90707e-3,1193.24
Na2SO4 (Thenardite),1.24565e-3,1.65820e-3
FeS2(marcasite) (Marcasite),1.02324e-3,312.501
Na2SO4.CaSO4 (Glauberite),7.84408e-4,1.37044e-3
NH4Cl (Sal ammoniac),3.46634e-4,5.05488e-4

NaHCO3 (Nahcolite),2.55754e-4,4.03851e-4
NH4Cl,2.01379e-4,2.93665e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H2O,5.35836,5.3583,0.0,5.96207e-5
CO2,0.117362,0.103093,,0.0142687
Cl-1,0.115908,0.115905,,3.45528e-6
Na+1,0.107626,0.107626,,1.93172e-12
Ca+2,3.2098e-3,3.2098e-3,,1.28495e-20
NH4+1,1.55544e-3,1.5554e-3,,4.09795e-8
SO4-2,1.25662e-3,1.25662e-3,,5.67246e-12
Mg+2,1.18674e-3,1.18674e-3,,1.77897e-21
N2,8.79466e-4,4.77088e-4,,4.02378e-4
CH3OH,6.04022e-4,6.03556e-4,,4.65596e-7
H3O+1,3.53467e-4,3.53467e-4,,3.60712e-16
NaMgSO4+1,2.20367e-4,1.81796e-4,,3.85716e-5
CaSO4 (Anhydrite),1.90983e-4,1.90361e-4,0.0,6.22342e-7
HSO4-1,6.58935e-5,6.58935e-5,,5.68981e-11
S8 (Sulfur),6.48398e-5,1.16098e-8,6.47312e-5,9.70352e-8
NH2CO2-1,6.38089e-5,9.71697e-14,,6.38089e-5
CO,6.05939e-5,6.04642e-5,,1.29623e-7
BaSO4 (Barite),5.96434e-5,,5.96434e-5,
HCO3-1,2.61949e-5,2.61941e-5,,8.23558e-10
C6H14O4,1.84742e-5,1.8474e-5,,1.70842e-10
Fe+2,1.4324e-5,2.77517e-10,,1.43237e-5
H2S,3.70225e-6,3.53031e-6,,1.71944e-7
Ba+2,6.68303e-8,6.68303e-8,,3.68704e-25
CaCl2 (Hydrophilite),5.21327e-8,5.21327e-8,0.0,1.04294e-24
Na2SO4.NaHSO4,3.85266e-8,3.85266e-8,0.0,2.93577e-17
CaClCH3OH+1,3.43854e-8,2.93506e-8,,5.03472e-9
MgSO4,6.50421e-9,6.48229e-9,0.0,2.19176e-11
FeCO2+2,8.62104e-10,8.62104e-10,,3.16243e-110
S2O3-2,2.18939e-10,2.18938e-10,,5.45621e-16
HS-1,1.03067e-10,1.03054e-10,,1.28988e-14
CH5O+1,7.41252e-11,5.51185e-11,,1.90067e-11
NH4OH,7.39765e-11,7.39548e-11,,2.16483e-14
NH3,2.0788e-11,2.07833e-11,,4.69368e-15
CH3OH.HCl,1.84974e-11,1.84579e-11,,3.95512e-14
C6H15O4+1,1.82835e-11,1.69533e-11,,1.33024e-12
HCl,1.41602e-11,1.32922e-11,,8.67937e-13
HS2O3-1,9.75099e-12,9.74992e-12,,1.07565e-15
CaCO3 (Calcite),8.97428e-12,8.96494e-12,0.0,9.33713e-15
MgClCH3OH+1,4.69057e-12,1.31111e-12,,3.37945e-12
CO3-2,2.2379e-12,2.2379e-12,,3.0364e-18
HO(CH2CH2O)3CO2(-1),1.59025e-12,1.59012e-12,,1.31128e-16
HSO3-1,1.31982e-12,1.31968e-12,,1.37571e-16
MgCO3,6.73623e-13,6.72182e-13,0.0,1.44102e-15
OH-1,5.02033e-13,5.02014e-13,,1.93611e-17

H2SO4,3.88821e-13,3.88821e-13,,1.65658e-21
SO2,3.08638e-13,3.0286e-13,,5.77798e-15
MgOH+1,2.8714e-13,2.75257e-13,,1.18839e-14
CaOH+1,1.70414e-13,1.66654e-13,,3.76023e-15
H2S2O3,1.52817e-13,1.5249e-13,,3.26907e-16
FeCl+1,5.28325e-14,5.04664e-14,,2.36609e-15
H2,3.47659e-14,3.46704e-14,,9.54829e-17
FeSO4,2.44057e-14,2.43534e-14,0.0,5.22432e-17
CO2S,6.91062e-16,6.89584e-16,,1.47832e-18
S1,3.62315e-16,3.6154e-16,,7.75067e-19
S2,3.57759e-16,3.56994e-16,,7.65319e-19
S3,3.53234e-16,3.52478e-16,,7.55639e-19
S4,3.48817e-16,3.48071e-16,,7.46191e-19
S5,3.44472e-16,3.43735e-16,,7.36897e-19
S6,3.40198e-16,3.39471e-16,,7.27754e-19
S7,3.35821e-16,3.35103e-16,,7.18391e-19
CH3O-1,1.26468e-16,1.26454e-16,,1.39701e-20
SO3-2,1.10067e-16,1.10066e-16,,2.90349e-22
FeHS+1,6.64996e-17,6.37473e-17,,2.75222e-18
S5-2,4.30057e-17,4.30054e-17,,2.12944e-22
BaCO3 (Witherite),1.90592e-17,1.90184e-17,0.0,4.07715e-20
S4-2,1.05691e-17,1.05691e-17,,5.23335e-23
FeOH+1,7.53281e-18,7.22105e-18,,3.11761e-19
Fe(NH3)+2,6.67214e-18,2.99292e-18,,3.67922e-18
C6H13O4-1,3.96029e-18,3.95986e-18,,4.28655e-22
NaOH.Na2SO4,2.66744e-18,2.66744e-18,,3.4721e-34
S3-2,1.57519e-18,1.57518e-18,,7.7996e-24
BaOH+1,6.81193e-19,6.56633e-19,,2.45599e-20
Fe+3,6.07055e-19,1.43112e-20,,5.92744e-19
FeCl+2,2.74741e-19,1.46723e-19,,1.28019e-19
NaOH,2.33436e-19,2.33421e-19,0.0,1.56089e-23
S2-2,1.4241e-19,1.42409e-19,,7.05147e-25
FeH(CO3)2-1,9.668e-20,9.66694e-20,,1.0665e-23
FeS (Pyrrhotite),1.52978e-20,1.52651e-20,0.0,3.27251e-23
FeOH+2,1.52596e-20,8.67685e-21,,6.58271e-21
MgCl2,3.31053e-21,3.28005e-21,0.0,3.04806e-23
FeHSO4+2,1.34215e-21,7.53619e-22,,5.88533e-22
FeO+1,2.41001e-22,2.31027e-22,,9.97432e-24
S-2,1.25605e-22,1.25599e-22,,5.63275e-27
FeCl2+1,2.94758e-23,2.88583e-23,,6.17513e-25
S2O5-2,5.76278e-24,5.76275e-24,,2.84418e-29
Fe(NH3)2+2,6.78895e-25,3.04532e-25,,3.74363e-25
NaOHCO3-2,2.4814e-25,2.48139e-25,,1.22868e-30
HFeO2,1.18096e-26,1.17843e-26,,2.52631e-29
FeO,1.02006e-26,1.01787e-26,,2.18211e-29
SO3,6.08685e-27,6.08684e-27,,2.78581e-33
S2O4-2,5.41837e-29,5.41834e-29,,2.68293e-34
S2O6-2,3.54169e-29,3.54167e-29,,1.75368e-34
S5O6-2,1.75537e-30,1.75536e-30,,8.69179e-36
Fe(NH3)3+2,1.71808e-32,7.70679e-33,,9.47401e-33
FeO2-1,1.11551e-33,1.11539e-33,,1.23054e-37
N2H5+1,1.01838e-35,9.76256e-36,,4.21268e-37
HFeO2-1,5.01179e-36,5.01124e-36,,5.52861e-40
NH2OH2+1,6.35633e-38,6.09385e-38,,2.62472e-39

N2H6+2,3.27152e-38,1.86103e-38,,1.41049e-38
Fe2(OH)2+4,2.07787e-39,1.32983e-41,,2.06457e-39
N2H4,9.77428e-42,9.774e-42,,2.82854e-46
NH2OH,8.07545e-42,8.06596e-42,0.0,9.49403e-45
Fe(NH3)4+2,5.34631e-43,2.39819e-43,,2.94812e-43
Cl2,1.08301e-43,1.08069e-43,,2.31678e-46
HClO,8.8214e-45,8.80252e-45,,1.88708e-47
NH2Cl,2.5851e-45,2.57957e-45,,5.53007e-48
ClO-1,8.61343e-50,8.61248e-50,,9.50165e-54
NO,2.39821e-50,2.05878e-50,,3.39435e-51
N2O,7.2641e-52,6.66513e-52,,5.98974e-53
Fe(NH3)5+2,1.66376e-53,7.46314e-54,,9.17449e-54
NH3Cl+1,1.13974e-53,1.09257e-53,,4.71705e-55
HSO5-1,4.10121e-57,4.10075e-57,,4.52412e-61
HNO2,1.29541e-60,1.29264e-60,,2.77115e-63
NO2-1,1.92377e-61,1.92357e-61,,1.91749e-65
Fe(NH3)6+2,5.17729e-64,2.32237e-64,,2.85491e-64
S2O8-2,4.56198e-67,4.56196e-67,,2.25888e-72
O2,3.34813e-68,2.91871e-68,,4.29421e-69
NO2,4.98343e-74,4.7258e-74,,2.57624e-75
NO3-1,1.67564e-79,1.67564e-79,,3.5748e-85
FeO4-2,3.3925e-82,3.39249e-82,,1.67981e-87
NHCl2,1.2483e-82,1.24563e-82,,2.67038e-85
HNO3,2.99142e-83,2.99141e-83,,2.07016e-89
NH2Cl2+1,4.70675e-88,4.51195e-88,,1.94798e-89
NH4NO3.(NH4)2SO4,8.64285e-90,8.62436e-90,0.0,1.84888e-92
ClO2-1,6.49217e-91,6.49145e-91,,7.16164e-95
HClO2,2.10054e-91,2.09604e-91,,4.49347e-94
ClO2,3.36142e-107,3.35423e-107,,7.19077e-110
ClO3-1,2.40491e-118,2.40464e-118,,2.65291e-122
NCl3,2.94329e-120,4.50915e-121,,2.49237e-120
N2O3,2.00868e-121,2.78342e-125,,2.0084e-121
NHCl3+1,1.39858e-123,1.3407e-123,,5.78832e-125
Total (by phase),5.7091,5.69412,1.24375e-4,0.0148524

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H(+1),10.7249,10.7246,0.0,2.47839e-4
Na(+1),0.107847,0.107808,0.0,3.85716e-5
N(-3),1.61925e-3,1.5554e-3,0.0,6.38499e-5
Ba(+2),5.97102e-5,6.68303e-8,5.96434e-5,6.53318e-20
Ca(+2),3.40087e-3,3.40024e-3,0.0,6.27377e-7
Fe(+2),1.43249e-5,1.1397e-9,0.0,1.43237e-5
Mg(+2),1.40712e-3,1.36855e-3,0.0,3.85716e-5
Fe(+3),8.98668e-19,1.70724e-19,0.0,7.27944e-19
O(-2),5.60088,5.57176,2.38573e-4,0.0288816
Cl(-1),0.115908,0.115905,0.0,3.46031e-6
C(+4),0.117452,0.10312,0.0,0.0143325
S(+4),1.62856e-12,1.62265e-12,0.0,5.91555e-15

S(+6),1.79359e-3,1.69475e-3,5.96434e-5,3.9194e-5
S(-2),3.70235e-6,3.53041e-6,0.0,1.71944e-7
S(+2),4.57685e-10,4.57681e-10,0.0,3.89636e-15
N(+3),1.48779e-60,1.485e-60,0.0,2.79033e-63
N(+5),1.67594e-79,1.67594e-79,0.0,3.57501e-85
N(0),1.75893e-3,9.54176e-4,0.0,8.04756e-4
H(0),6.95318e-14,6.93409e-14,0.0,1.90966e-16
O(0),6.69627e-68,5.83743e-68,0.0,8.58841e-69
S(+8),4.10121e-57,4.10075e-57,0.0,4.52412e-61
Cl(+1),1.19707e-43,1.19451e-43,0.0,2.56078e-46
Cl(+5),2.40491e-118,2.40464e-118,0.0,2.65291e-122
S(+3),1.08367e-28,1.08367e-28,0.0,5.36585e-34
S(+5),7.08337e-29,7.08334e-29,0.0,3.50736e-34
S(+7),9.12397e-67,9.12392e-67,0.0,4.51777e-72
N(+2),2.39821e-50,2.05878e-50,0.0,3.39435e-51
N(+4),4.98343e-74,4.7258e-74,0.0,2.57624e-75
Cl(+3),8.5927e-91,8.58749e-91,0.0,5.20964e-94
Cl(+4),3.36142e-107,3.35423e-107,0.0,7.19077e-110
N(+1),1.45282e-51,1.33303e-51,0.0,1.19795e-52
N(-2),2.04331e-35,1.95624e-35,0.0,8.70746e-37
C(+2),6.05939e-5,6.04642e-5,0.0,1.29623e-7
Fe(+6),3.3925e-82,3.39249e-82,0.0,1.67981e-87
S(0),5.18719e-4,9.28781e-8,5.17849e-4,7.76281e-7
MeO(-1),6.04056e-4,6.03586e-4,0.0,4.70654e-7
N(-1),6.35713e-38,6.09466e-38,0.0,2.62473e-39
TEGION,1.84742e-5,1.8474e-5,0.0,1.72173e-10

Element Distribution

,Total,Total,Liquid-1,Solid,Liquid-2
,mol,mole %,% of Total,% of Total,% of Total
H(+1),10.7249,64.3046,99.9977,0.0,2.31088e-3
Na(+1),0.107847,0.646632,99.9642,0.0,0.0357652
N(-3),1.61925e-3,9.70876e-3,96.0568,0.0,3.94318
Ba(+2),5.97102e-5,3.58013e-4,0.111924,99.8881,1.09415e-13
Ca(+2),3.40087e-3,0.0203911,99.9816,0.0,0.0184475
Fe(+2),1.43249e-5,8.58896e-5,7.95608e-3,0.0,99.992
Mg(+2),1.40712e-3,8.43686e-3,97.2588,0.0,2.74118
Fe(+3),8.98668e-19,5.38828e-18,18.9975,0.0,81.0025
O(-2),5.60088,33.582,99.4801,4.25957e-3,0.515661
Cl(-1),0.115908,0.694969,99.997,0.0,2.98539e-3
C(+4),0.117452,0.704225,87.7971,0.0,12.2029
S(+4),1.62856e-12,9.76462e-12,99.6368,0.0,0.363237
S(+6),1.79359e-3,0.0107541,94.4894,3.32537,2.18523
S(-2),3.70235e-6,2.21987e-5,95.3558,0.0,4.64417
S(+2),4.57685e-10,2.74421e-9,99.9991,0.0,8.51319e-4
N(+3),1.48779e-60,8.92056e-60,99.8125,0.0,0.187549
N(+5),1.67594e-79,1.00487e-78,99.9998,0.0,2.13313e-4
N(0),1.75893e-3,0.0105463,54.2475,0.0,45.7525
H(0),6.95318e-14,4.16902e-13,99.7254,0.0,0.274645
O(0),6.69627e-68,4.01498e-67,87.1743,0.0,12.8257
S(+8),4.10121e-57,2.45902e-56,99.989,0.0,0.0110312
Cl(+1),1.19707e-43,7.17747e-43,99.7861,0.0,0.21392

Cl(+5),2.40491e-118,1.44195e-117,99.989,0.0,0.0110312
S(+3),1.08367e-28,6.49754e-28,99.9995,0.0,4.95154e-4
S(+5),7.08337e-29,4.24708e-28,99.9995,0.0,4.95154e-4
S(+7),9.12397e-67,5.47059e-66,99.9995,0.0,4.95154e-4
N(+2),2.39821e-50,1.43793e-49,85.8463,0.0,14.1537
N(+4),4.98343e-74,2.98799e-73,94.8304,0.0,5.16962
Cl(+3),8.5927e-91,5.15205e-90,99.9394,0.0,0.0606286
Cl(+4),3.36142e-107,2.01546e-106,99.7861,0.0,0.21392
N(+1),1.45282e-51,8.71089e-51,91.7543,0.0,8.24567
N(-2),2.04331e-35,1.22514e-34,95.7386,0.0,4.26144
C(+2),6.05939e-5,3.63312e-4,99.7861,0.0,0.21392
Fe(+6),3.3925e-82,2.03409e-81,99.9995,0.0,4.95154e-4
S(0),5.18719e-4,3.11016e-3,0.0179053,99.8324,0.149654
MeO(-1),6.04056e-4,3.62183e-3,99.9221,0.0,0.0779155
N(-1),6.35713e-38,3.81164e-37,95.8712,0.0,4.1288
TEGION,1.84742e-5,1.10769e-4,99.9991,0.0,9.31963e-4

Calculation Summary
06-1 Alloy-5 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2507

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3.1H2O

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,5.35989,5.35989
CO2,0.117452,0.117452
N2,9.42087e-4,9.42087e-4
CO,6.05939e-5,6.05939e-5
O2,2.79025e-6,2.79025e-6
NH3,1.47447e-3,1.47447e-3
CH3OH,6.04056e-4,6.04056e-4
H2S,1.24254e-5,1.24254e-5
SO2,1.78309e-3,1.78309e-3
NO2,1.95370e-5,1.95370e-5
BaCl2,1.85435e-7,1.85435e-7

CaCl2,2.60922e-3,2.60922e-3
CaO,7.91645e-4,7.91645e-4
FeCl2,1.43249e-5,1.43249e-5
MgCl2,1.40712e-3,1.40712e-3
NaCl,0.107847,0.107847
SO3,4.60964e-4,4.60964e-4
BaSO4,5.95248e-5,5.95248e-5
C6H14O4,1.84742e-5,1.84742e-5

Calculated Rates

Corrosion Rate,1.84392e-4,mm/yr
Corrosion Potential,-0.121187,V (SHE)
Repassivation Potential*,-7.77983e-3,V (SHE)
Corrosion Current Density,1.79720e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.2H2O (Gypsum),0.330843
,CaSO4 (Anhydrite),0.266135
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,5.59545,mol
Temperature,83.6413,°F
Pressure,3398.00,psia

Liquid 1 Properties
pH,2.24050,
Ionic Strength (x-based),0.0218055,mol/mol
Ionic Strength (m-based),1.28624,mol/kg
Dielectric Constant,58.4911,
ORP,0.143810,V (SHE)
Osmotic Pressure,1328.28,psia
Specific Electrical Conductivity,1.02303e5,µmho/cm
"Viscosity, absolute",0.943026,cP
Thermal Conductivity,531.258,cal/hr m °C
Surface Tension,0.0740070,N/m
Interfacial Tension LLE,1.30535e-4,N/m
Standard Liquid Volume,0.104790,L
"Volume, Std. Conditions",0.102664,L
"Total Dissolved Solids, Estimated",68236.4,mg/L
Hardness,4679.53,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,2.22068e-6,L

Liquid 2 Properties
pH,0.944221,
Ionic Strength (x-based),5.49331e-3,mol/mol
Ionic Strength (m-based),75.9611,mol/kg
Dielectric Constant,4.76273,
Specific Electrical Conductivity,9087.68,µmho/cm
"Viscosity, absolute",0.905541,cP
Surface Tension,0.0440035,N/m
Thermal Conductivity,529.215,cal/hr m °C
Standard Liquid Volume,5.50080e-4,L
"Volume, Std. Conditions",1.00377e-3,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid,Liquid-2
Density,g/ml,1.05858,1.05957,2.75086,0.894627
Enthalpy,J,-1.62627e6,-1.62029e6,-87.8158,-5899.09

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
Mole (True),5.70910,5.69412,1.24375e-4,0.0148524
Mole (App),5.59483,5.57977,1.24375e-4,0.0149418
,g,g,g,g
Mass,108.744,108.063,0.0305257,0.650728
,L,L,cm3,L
Volume,0.102726,0.101988,0.0110968,7.27374e-4

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,1201.43
S8 (Sulfur),1.00000,1763.00
S8 (Sulfur monoclinic),0.754401,1330.01
H2O,0.700000,0.697565
CaSO4.2H2O (Gypsum),0.330843,0.431193
CaSO4 (Anhydrite),0.266135,0.349284
CaSO4.0.5H2O (Bassanite),0.0689498,0.0903343
CaSO4.0.5H2O (Bassanite),0.0547689,0.0717552
NaCl (Halite),0.0168136,0.0172518
NaCl.2H2O (hydrohalite),0.0153163,0.0156063
Na2SO4.10H2O (Mirabilite),3.97154e-3,5.10582e-3
FeS2 (Pyrite),3.90707e-3,1193.24
Na2SO4 (Thenardite),1.24565e-3,1.65820e-3
FeS2(marcasite) (Marcasite),1.02324e-3,312.501
Na2SO4.CaSO4 (Glauberite),7.84408e-4,1.37044e-3
NH4Cl (Sal ammoniac),3.46634e-4,5.05488e-4

NaHCO3 (Nahcolite),2.55754e-4,4.03851e-4
NH4Cl,2.01379e-4,2.93665e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H2O,5.35836,5.3583,0.0,5.96207e-5
CO2,0.117362,0.103093,,0.0142687
Cl-1,0.115908,0.115905,,3.45528e-6
Na+1,0.107626,0.107626,,1.93172e-12
Ca+2,3.2098e-3,3.2098e-3,,1.28495e-20
NH4+1,1.55544e-3,1.5554e-3,,4.09795e-8
SO4-2,1.25662e-3,1.25662e-3,,5.67246e-12
Mg+2,1.18674e-3,1.18674e-3,,1.77897e-21
N2,8.79466e-4,4.77088e-4,,4.02378e-4
CH3OH,6.04022e-4,6.03556e-4,,4.65596e-7
H3O+1,3.53467e-4,3.53467e-4,,3.60712e-16
NaMgSO4+1,2.20367e-4,1.81796e-4,,3.85716e-5
CaSO4 (Anhydrite),1.90983e-4,1.90361e-4,0.0,6.22342e-7
HSO4-1,6.58935e-5,6.58935e-5,,5.68981e-11
S8 (Sulfur),6.48398e-5,1.16098e-8,6.47312e-5,9.70352e-8
NH2CO2-1,6.38089e-5,9.71697e-14,,6.38089e-5
CO,6.05939e-5,6.04642e-5,,1.29623e-7
BaSO4 (Barite),5.96434e-5,,5.96434e-5,
HCO3-1,2.61949e-5,2.61941e-5,,8.23558e-10
C6H14O4,1.84742e-5,1.8474e-5,,1.70842e-10
Fe+2,1.4324e-5,2.77517e-10,,1.43237e-5
H2S,3.70225e-6,3.53031e-6,,1.71944e-7
Ba+2,6.68303e-8,6.68303e-8,,3.68704e-25
CaCl2 (Hydrophilite),5.21327e-8,5.21327e-8,0.0,1.04294e-24
Na2SO4.NaHSO4,3.85266e-8,3.85266e-8,0.0,2.93577e-17
CaClCH3OH+1,3.43854e-8,2.93506e-8,,5.03472e-9
MgSO4,6.50421e-9,6.48229e-9,0.0,2.19176e-11
FeCO2+2,8.62104e-10,8.62104e-10,,3.16243e-110
S2O3-2,2.18939e-10,2.18938e-10,,5.45621e-16
HS-1,1.03067e-10,1.03054e-10,,1.28988e-14
CH5O+1,7.41252e-11,5.51185e-11,,1.90067e-11
NH4OH,7.39765e-11,7.39548e-11,,2.16483e-14
NH3,2.0788e-11,2.07833e-11,,4.69368e-15
CH3OH.HCl,1.84974e-11,1.84579e-11,,3.95512e-14
C6H15O4+1,1.82835e-11,1.69533e-11,,1.33024e-12
HCl,1.41602e-11,1.32922e-11,,8.67937e-13
HS2O3-1,9.75099e-12,9.74992e-12,,1.07565e-15
CaCO3 (Calcite),8.97428e-12,8.96494e-12,0.0,9.33713e-15
MgClCH3OH+1,4.69057e-12,1.31111e-12,,3.37945e-12
CO3-2,2.2379e-12,2.2379e-12,,3.0364e-18
HO(CH2CH2O)3CO2(-1),1.59025e-12,1.59012e-12,,1.31128e-16
HSO3-1,1.31982e-12,1.31968e-12,,1.37571e-16
MgCO3,6.73623e-13,6.72182e-13,0.0,1.44102e-15
OH-1,5.02033e-13,5.02014e-13,,1.93611e-17

H2SO4,3.88821e-13,3.88821e-13,,1.65658e-21
SO2,3.08638e-13,3.0286e-13,,5.77798e-15
MgOH+1,2.8714e-13,2.75257e-13,,1.18839e-14
CaOH+1,1.70414e-13,1.66654e-13,,3.76023e-15
H2S2O3,1.52817e-13,1.5249e-13,,3.26907e-16
FeCl+1,5.28325e-14,5.04664e-14,,2.36609e-15
H2,3.47659e-14,3.46704e-14,,9.54829e-17
FeSO4,2.44057e-14,2.43534e-14,0.0,5.22432e-17
CO2S,6.91062e-16,6.89584e-16,,1.47832e-18
S1,3.62315e-16,3.6154e-16,,7.75067e-19
S2,3.57759e-16,3.56994e-16,,7.65319e-19
S3,3.53234e-16,3.52478e-16,,7.55639e-19
S4,3.48817e-16,3.48071e-16,,7.46191e-19
S5,3.44472e-16,3.43735e-16,,7.36897e-19
S6,3.40198e-16,3.39471e-16,,7.27754e-19
S7,3.35821e-16,3.35103e-16,,7.18391e-19
CH3O-1,1.26468e-16,1.26454e-16,,1.39701e-20
SO3-2,1.10067e-16,1.10066e-16,,2.90349e-22
FeHS+1,6.64996e-17,6.37473e-17,,2.75222e-18
S5-2,4.30057e-17,4.30054e-17,,2.12944e-22
BaCO3 (Witherite),1.90592e-17,1.90184e-17,0.0,4.07715e-20
S4-2,1.05691e-17,1.05691e-17,,5.23335e-23
FeOH+1,7.53281e-18,7.22105e-18,,3.11761e-19
Fe(NH3)+2,6.67214e-18,2.99292e-18,,3.67922e-18
C6H13O4-1,3.96029e-18,3.95986e-18,,4.28655e-22
NaOH.Na2SO4,2.66744e-18,2.66744e-18,,3.4721e-34
S3-2,1.57519e-18,1.57518e-18,,7.7996e-24
BaOH+1,6.81193e-19,6.56633e-19,,2.45599e-20
Fe+3,6.07055e-19,1.43112e-20,,5.92744e-19
FeCl+2,2.74741e-19,1.46723e-19,,1.28019e-19
NaOH,2.33436e-19,2.33421e-19,0.0,1.56089e-23
S2-2,1.4241e-19,1.42409e-19,,7.05147e-25
FeH(CO3)2-1,9.668e-20,9.66694e-20,,1.0665e-23
FeS (Pyrrhotite),1.52978e-20,1.52651e-20,0.0,3.27251e-23
FeOH+2,1.52596e-20,8.67685e-21,,6.58271e-21
MgCl2,3.31053e-21,3.28005e-21,0.0,3.04806e-23
FeHSO4+2,1.34215e-21,7.53619e-22,,5.88533e-22
FeO+1,2.41001e-22,2.31027e-22,,9.97432e-24
S-2,1.25605e-22,1.25599e-22,,5.63275e-27
FeCl2+1,2.94758e-23,2.88583e-23,,6.17513e-25
S2O5-2,5.76278e-24,5.76275e-24,,2.84418e-29
Fe(NH3)2+2,6.78895e-25,3.04532e-25,,3.74363e-25
NaOHCO3-2,2.4814e-25,2.48139e-25,,1.22868e-30
HFeO2,1.18096e-26,1.17843e-26,,2.52631e-29
FeO,1.02006e-26,1.01787e-26,,2.18211e-29
SO3,6.08685e-27,6.08684e-27,,2.78581e-33
S2O4-2,5.41837e-29,5.41834e-29,,2.68293e-34
S2O6-2,3.54169e-29,3.54167e-29,,1.75368e-34
S5O6-2,1.75537e-30,1.75536e-30,,8.69179e-36
Fe(NH3)3+2,1.71808e-32,7.70679e-33,,9.47401e-33
FeO2-1,1.11551e-33,1.11539e-33,,1.23054e-37
N2H5+1,1.01838e-35,9.76256e-36,,4.21268e-37
HFeO2-1,5.01179e-36,5.01124e-36,,5.52861e-40
NH2OH2+1,6.35633e-38,6.09385e-38,,2.62472e-39

N2H6+2,3.27152e-38,1.86103e-38,,1.41049e-38
Fe2(OH)2+4,2.07787e-39,1.32983e-41,,2.06457e-39
N2H4,9.77428e-42,9.774e-42,,2.82854e-46
NH2OH,8.07545e-42,8.06596e-42,0.0,9.49403e-45
Fe(NH3)4+2,5.34631e-43,2.39819e-43,,2.94812e-43
Cl2,1.08301e-43,1.08069e-43,,2.31678e-46
HClO,8.8214e-45,8.80252e-45,,1.88708e-47
NH2Cl,2.5851e-45,2.57957e-45,,5.53007e-48
ClO-1,8.61343e-50,8.61248e-50,,9.50165e-54
NO,2.39821e-50,2.05878e-50,,3.39435e-51
N2O,7.2641e-52,6.66513e-52,,5.98974e-53
Fe(NH3)5+2,1.66376e-53,7.46314e-54,,9.17449e-54
NH3Cl+1,1.13974e-53,1.09257e-53,,4.71705e-55
HSO5-1,4.10121e-57,4.10075e-57,,4.52412e-61
HNO2,1.29541e-60,1.29264e-60,,2.77115e-63
NO2-1,1.92377e-61,1.92357e-61,,1.91749e-65
Fe(NH3)6+2,5.17729e-64,2.32237e-64,,2.85491e-64
S2O8-2,4.56198e-67,4.56196e-67,,2.25888e-72
O2,3.34813e-68,2.91871e-68,,4.29421e-69
NO2,4.98343e-74,4.7258e-74,,2.57624e-75
NO3-1,1.67564e-79,1.67564e-79,,3.5748e-85
FeO4-2,3.3925e-82,3.39249e-82,,1.67981e-87
NHCl2,1.2483e-82,1.24563e-82,,2.67038e-85
HNO3,2.99142e-83,2.99141e-83,,2.07016e-89
NH2Cl2+1,4.70675e-88,4.51195e-88,,1.94798e-89
NH4NO3.(NH4)2SO4,8.64285e-90,8.62436e-90,0.0,1.84888e-92
ClO2-1,6.49217e-91,6.49145e-91,,7.16164e-95
HClO2,2.10054e-91,2.09604e-91,,4.49347e-94
ClO2,3.36142e-107,3.35423e-107,,7.19077e-110
ClO3-1,2.40491e-118,2.40464e-118,,2.65291e-122
NCl3,2.94329e-120,4.50915e-121,,2.49237e-120
N2O3,2.00868e-121,2.78342e-125,,2.0084e-121
NHCl3+1,1.39858e-123,1.3407e-123,,5.78832e-125
Total (by phase),5.7091,5.69412,1.24375e-4,0.0148524

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H(+1),10.7249,10.7246,0.0,2.47839e-4
Na(+1),0.107847,0.107808,0.0,3.85716e-5
N(-3),1.61925e-3,1.5554e-3,0.0,6.38499e-5
Ba(+2),5.97102e-5,6.68303e-8,5.96434e-5,6.53318e-20
Ca(+2),3.40087e-3,3.40024e-3,0.0,6.27377e-7
Fe(+2),1.43249e-5,1.1397e-9,0.0,1.43237e-5
Mg(+2),1.40712e-3,1.36855e-3,0.0,3.85716e-5
Fe(+3),8.98668e-19,1.70724e-19,0.0,7.27944e-19
O(-2),5.60088,5.57176,2.38573e-4,0.0288816
Cl(-1),0.115908,0.115905,0.0,3.46031e-6
C(+4),0.117452,0.10312,0.0,0.0143325
S(+4),1.62856e-12,1.62265e-12,0.0,5.91555e-15

S(+6),1.79359e-3,1.69475e-3,5.96434e-5,3.9194e-5
S(-2),3.70235e-6,3.53041e-6,0.0,1.71944e-7
S(+2),4.57685e-10,4.57681e-10,0.0,3.89636e-15
N(+3),1.48779e-60,1.485e-60,0.0,2.79033e-63
N(+5),1.67594e-79,1.67594e-79,0.0,3.57501e-85
N(0),1.75893e-3,9.54176e-4,0.0,8.04756e-4
H(0),6.95318e-14,6.93409e-14,0.0,1.90966e-16
O(0),6.69627e-68,5.83743e-68,0.0,8.58841e-69
S(+8),4.10121e-57,4.10075e-57,0.0,4.52412e-61
Cl(+1),1.19707e-43,1.19451e-43,0.0,2.56078e-46
Cl(+5),2.40491e-118,2.40464e-118,0.0,2.65291e-122
S(+3),1.08367e-28,1.08367e-28,0.0,5.36585e-34
S(+5),7.08337e-29,7.08334e-29,0.0,3.50736e-34
S(+7),9.12397e-67,9.12392e-67,0.0,4.51777e-72
N(+2),2.39821e-50,2.05878e-50,0.0,3.39435e-51
N(+4),4.98343e-74,4.7258e-74,0.0,2.57624e-75
Cl(+3),8.5927e-91,8.58749e-91,0.0,5.20964e-94
Cl(+4),3.36142e-107,3.35423e-107,0.0,7.19077e-110
N(+1),1.45282e-51,1.33303e-51,0.0,1.19795e-52
N(-2),2.04331e-35,1.95624e-35,0.0,8.70746e-37
C(+2),6.05939e-5,6.04642e-5,0.0,1.29623e-7
Fe(+6),3.3925e-82,3.39249e-82,0.0,1.67981e-87
S(0),5.18719e-4,9.28781e-8,5.17849e-4,7.76281e-7
MeO(-1),6.04056e-4,6.03586e-4,0.0,4.70654e-7
N(-1),6.35713e-38,6.09466e-38,0.0,2.62473e-39
TEGION,1.84742e-5,1.8474e-5,0.0,1.72173e-10

Element Distribution

,Total,Total,Liquid-1,Solid,Liquid-2
,mol,mole %,% of Total,% of Total,% of Total
H(+1),10.7249,64.3046,99.9977,0.0,2.31088e-3
Na(+1),0.107847,0.646632,99.9642,0.0,0.0357652
N(-3),1.61925e-3,9.70876e-3,96.0568,0.0,3.94318
Ba(+2),5.97102e-5,3.58013e-4,0.111924,99.8881,1.09415e-13
Ca(+2),3.40087e-3,0.0203911,99.9816,0.0,0.0184475
Fe(+2),1.43249e-5,8.58896e-5,7.95608e-3,0.0,99.992
Mg(+2),1.40712e-3,8.43686e-3,97.2588,0.0,2.74118
Fe(+3),8.98668e-19,5.38828e-18,18.9975,0.0,81.0025
O(-2),5.60088,33.582,99.4801,4.25957e-3,0.515661
Cl(-1),0.115908,0.694969,99.997,0.0,2.98539e-3
C(+4),0.117452,0.704225,87.7971,0.0,12.2029
S(+4),1.62856e-12,9.76462e-12,99.6368,0.0,0.363237
S(+6),1.79359e-3,0.0107541,94.4894,3.32537,2.18523
S(-2),3.70235e-6,2.21987e-5,95.3558,0.0,4.64417
S(+2),4.57685e-10,2.74421e-9,99.9991,0.0,8.51319e-4
N(+3),1.48779e-60,8.92056e-60,99.8125,0.0,0.187549
N(+5),1.67594e-79,1.00487e-78,99.9998,0.0,2.13313e-4
N(0),1.75893e-3,0.0105463,54.2475,0.0,45.7525
H(0),6.95318e-14,4.16902e-13,99.7254,0.0,0.274645
O(0),6.69627e-68,4.01498e-67,87.1743,0.0,12.8257
S(+8),4.10121e-57,2.45902e-56,99.989,0.0,0.0110312
Cl(+1),1.19707e-43,7.17747e-43,99.7861,0.0,0.21392

Cl(+5),2.40491e-118,1.44195e-117,99.989,0.0,0.0110312
S(+3),1.08367e-28,6.49754e-28,99.9995,0.0,4.95154e-4
S(+5),7.08337e-29,4.24708e-28,99.9995,0.0,4.95154e-4
S(+7),9.12397e-67,5.47059e-66,99.9995,0.0,4.95154e-4
N(+2),2.39821e-50,1.43793e-49,85.8463,0.0,14.1537
N(+4),4.98343e-74,2.98799e-73,94.8304,0.0,5.16962
Cl(+3),8.5927e-91,5.15205e-90,99.9394,0.0,0.0606286
Cl(+4),3.36142e-107,2.01546e-106,99.7861,0.0,0.21392
N(+1),1.45282e-51,8.71089e-51,91.7543,0.0,8.24567
N(-2),2.04331e-35,1.22514e-34,95.7386,0.0,4.26144
C(+2),6.05939e-5,3.63312e-4,99.7861,0.0,0.21392
Fe(+6),3.3925e-82,2.03409e-81,99.9995,0.0,4.95154e-4
S(0),5.18719e-4,3.11016e-3,0.0179053,99.8324,0.149654
MeO(-1),6.04056e-4,3.62183e-3,99.9221,0.0,0.0779155
N(-1),6.35713e-38,3.81164e-37,95.8712,0.0,4.1288
TEGION,1.84742e-5,1.10769e-4,99.9991,0.0,9.31963e-4

Calculation Summary
06-2 Alloy-1 Calculation

Unit Set: Custom

Automatic Chemistry Model
,Aqueous (H+ ion) Databanks:
,,Corrosion (AQ)
,,Aqueous (H+ ion)
,Second Liquid phase
,Redox selected
,Using K-fit Polynomials
,,T-span: 25.0 - 225.0
,,P-span: 1.0 - 1500.0

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Super13Cr stainless steel

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,(NH4)2SO3
,C6H14O4

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,27.0272,27.0272
CO2,0.500189,0.500189
N2,3.52818e-3,3.52818e-3
CO,2.12661e-4,2.12661e-4
O2,1.11890e-5,1.11890e-5
NH3,6.74808e-4,6.74808e-4
CH3OH,4.18415e-4,4.18415e-4
H2S,5.30469e-5,5.30469e-5
SO2,1.00864e-3,1.00864e-3

NO2,8.50324e-5,8.50324e-5
BaCl2,1.69170e-6,1.69170e-6
CaCl2,0.0130454,0.0130454
CaO,3.95899e-3,3.95899e-3
FeCl2,7.16243e-5,7.16243e-5
MgCl2,7.03559e-3,7.03559e-3
NaCl,0.539233,0.539233
SO3,2.30558e-3,2.30558e-3
BaSO4,2.96859e-4,2.96859e-4
C6H14O4,8.84731e-6,8.84731e-6

Calculated Rates

Corrosion Rate,1.78945e-3,mm/yr
Corrosion Potential,-0.252505,V (SHE)
Repassivation Potential*,-0.161639,V (SHE)
Corrosion Current Density,1.64895e-3,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.2H2O (Gypsum),0.109377
,CaSO4 (Anhydrite),0.128696
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,28.0993,mol
Temperature,50.0000,°C
Pressure,3398.00,psia

Aqueous Properties
pH,3.46882,
Ionic Strength (x-based),0.0214001,mol/mol
Ionic Strength (m-based),1.26043,mol/kg
ORP,0.0549144,V (SHE)
Osmotic Pressure,1264.99,psia
Specific Electrical Conductivity,1.43072e5,µmho/cm
"Electrical Conductivity, molar",6.89603e-3,m2/ohm-mol
"Viscosity, absolute",0.632403,cP
"Viscosity, relative",1.15567,
Standard Liquid Volume,0.527087,L
"Volume, Std. Conditions",0.515270,L
"Total Dissolved Solids, Estimated",66347.1,mg/L
Hardness,4655.63,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,3.91824e-6,L

Thermodynamic Properties
,Unit,Total,Aqueous,Solid
Density,g/ml,1.05118,1.05107,4.52894
Enthalpy,J,-8.10977e6,-8.10933e6,-448.686

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
Mole (True),28.6755,28.6752,3.63352e-4
Mole (App),28.0988,28.0984,3.63352e-4
,g,g,g
Mass,543.236,543.158,0.0773202
,L,L,cm3
Volume,0.516786,0.516769,0.0170724

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
FeS2 (Pyrite),1.00000,42364.1
BaSO4 (Barite),1.00000,273.084
FeS2(marcasite) (Marcasite),0.288259,12211.8
CaSO4 (Anhydrite),0.128696,0.143236
CaSO4.2H2O (Gypsum),0.109377,0.121266
CaSO4.0.5H2O (Bassanite),0.0432886,0.0481329
NaCl (Halite),0.0144195,0.0143080
NaHCO3 (Nahcolite),3.13624e-3,0.0126851
CaCO3 (Calcite),1.06592e-3,0.0163186
Na2SO4 (Thenardite),9.91024e-4,1.10496e-3
CaCO3 (Aragonite),7.45268e-4,0.0114096
FeCO3 (Siderite),4.08242e-5,8.08533e-3
FeS (Pyrrhotite),1.11799e-6,6.65137e-3
FeS(mackinawite) (Mackinawite),2.61518e-8,1.55587e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
H2O,27.0247,27.0247,
Cl-1,0.579541,0.579541,
Na+1,0.53855,0.53855,
CO2,0.497592,0.497592,
Ca+2,0.0169077,0.0169077,
Mg+2,6.74536e-3,6.74536e-3,

N2,3.38271e-3,3.38271e-3,
SO4-2,2.70135e-3,2.70135e-3,
HCO3-1,2.02736e-3,2.02736e-3,
NH4+1,1.04283e-3,1.04283e-3,
CH3OH,4.18415e-4,4.18415e-4,
NaHCO3 (Nahcolite),3.96734e-4,3.96734e-4,0.0
BaSO4 (Barite),2.97365e-4,,2.97365e-4
NaSO4-1,2.86755e-4,2.86755e-4,
CO,2.12661e-4,2.12661e-4,
H+1,2.05208e-4,2.05208e-4,
MgHCO3+1,1.73078e-4,1.73078e-4,
MgSO4,1.17146e-4,1.17146e-4,0.0
CaSO4 (Anhydrite),9.62496e-5,9.62496e-5,0.0
FeS2 (Pyrite),6.59872e-5,,6.59872e-5
HSO4-1,2.47202e-5,2.47202e-5,
C6H14O4,8.84731e-6,8.84731e-6,
NH4SO4-1,7.9313e-6,7.9313e-6,
Fe+2,5.63038e-6,5.63038e-6,
Ba+2,8.77842e-7,8.77842e-7,
H2S,6.31889e-7,6.31889e-7,
BaCl(+1),2.94411e-7,2.94411e-7,
CaCl+1,2.79189e-7,2.79189e-7,
CaHCO3+1,1.40747e-7,1.40747e-7,
CaCO3 (Calcite),1.84423e-8,1.84423e-8,0.0
BaHCO3+1,1.37102e-8,1.37102e-8,
FeCl+1,5.86563e-9,5.86563e-9,
CO3-2,3.95398e-9,3.95398e-9,
NH3,3.73411e-9,3.73411e-9,
MgCO3 (Magnesite),1.14699e-9,1.14699e-9,0.0
NaCO3-1,7.53223e-10,7.53223e-10,
FeHCO3+1,7.16193e-10,7.16193e-10,
HS-1,7.11594e-10,7.11594e-10,
HCl,2.77114e-10,2.77114e-10,
OH-1,1.26523e-10,1.26523e-10,
MgOH+1,1.01919e-10,1.01919e-10,
FeCO3 (Siderite),6.26793e-11,6.26793e-11,0.0
S2O3-2,3.69681e-11,3.69681e-11,
FeHS+1,2.74005e-11,2.74005e-11,
NH2CO2-1,2.32039e-11,2.32039e-11,
NaS2O3-1,2.28154e-11,2.28154e-11,
CaOH+1,1.72078e-11,1.72078e-11,
FeOH+1,1.3906e-11,1.3906e-11,
FeCl2 (Lawrencite),9.76237e-12,9.76237e-12,0.0
HSO3-1,3.40745e-12,3.40745e-12,
H2,1.69404e-12,1.69404e-12,
Fe(NH3)+2,5.49672e-13,5.49672e-13,
SO2,8.7303e-14,8.7303e-14,
BaCO3 (Witherite),4.90873e-14,4.90873e-14,0.0
SO3-2,3.57894e-15,3.57894e-15,
FeOH+2,4.48681e-16,4.48681e-16,
Fe+3,2.06184e-16,2.06184e-16,
Fe(OH)2+1,3.59545e-17,3.59545e-17,
BaOH+1,3.14165e-17,3.14165e-17,
Fe(CO3)2-2,1.77723e-17,1.77723e-17,

CaCl2 (Hydrophilite),4.71648e-18,4.71648e-18,0.0
S-2,4.66366e-18,4.66366e-18,
FeCl2+1,3.27557e-18,3.27557e-18,
FeCl+2,2.10452e-18,2.10452e-18,
S2-2,1.05387e-18,1.05387e-18,
Fe(OH)3 (Bernalite),8.36749e-19,8.36749e-19,0.0
Fe(NH3)2+2,2.78579e-19,2.78579e-19,
FeSO4+1,2.6149e-19,2.6149e-19,
H2SO4,1.48646e-19,1.48646e-19,
S3-2,1.03895e-19,1.03895e-19,
FeCl3 (Molysite),4.99818e-20,4.99818e-20,0.0
S4-2,6.40017e-21,6.40017e-21,
FeS(HS)-1,2.61303e-21,2.61303e-21,
FeCl4-1,4.39813e-22,4.39813e-22,
S5-2,2.47076e-22,2.47076e-22,
SO3,2.49806e-23,2.49806e-23,
Fe(OH)4-1,1.44946e-23,1.44946e-23,
HFeO2-1,5.08819e-26,5.08819e-26,
Fe(NH3)3+2,3.84904e-26,3.84904e-26,
S2O5-2,1.79588e-27,1.79588e-27,
S2O4-2,2.84137e-28,2.84137e-28,
S2O6-2,7.31904e-29,7.31904e-29,
Na2S2O4,1.21167e-29,1.21167e-29,0.0
N2H5+1,1.05897e-33,1.05897e-33,
Fe2(OH)2+4,6.13623e-34,6.13623e-34,
Fe(NH3)4+2,1.01697e-35,1.01697e-35,
S5O6-2,2.21535e-36,2.21535e-36,
N2H4,5.21529e-38,5.21529e-38,
NH2OH,3.56114e-39,3.56114e-39,
Fe(NH3)5+2,2.68795e-45,2.68795e-45,
NO,9.41568e-47,9.41568e-47,
N2O,2.87652e-48,2.87652e-48,
HSO5-1,5.68546e-54,5.68546e-54,
Fe(NH3)6+2,7.10187e-55,7.10187e-55,
NO2-1,1.25393e-55,1.25393e-55,
HNO2,1.94382e-56,1.94382e-56,
O2,2.48549e-63,2.48549e-63,
S2O8-2,2.28823e-64,2.28823e-64,
FeO4-2,7.84191e-67,7.84191e-67,
NO2,1.28883e-68,1.28883e-68,
NO3-1,9.19125e-73,9.19125e-73,
NaNO3 (Nitratine),9.88391e-74,9.88391e-74,0.0
Ca(NO3)+1,2.16983e-74,2.16983e-74,
NH4NO3 (Gwihabaite),1.1614e-74,1.1614e-74,0.0
HNO3,9.71449e-81,9.71449e-81,
FeNO3+2,7.85092e-91,7.85092e-91,
Total (by phase),28.6755,28.6752,3.63352e-4

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid

,mol,mol,mol
H(+1),54.0565,54.0565,0.0
Na(+1),0.539233,0.539233,0.0
N(-3),1.05077e-3,1.05077e-3,0.0
Ba(+2),2.98551e-4,1.18596e-6,2.97365e-4
Ca(+2),0.0170043,0.0170043,0.0
Fe(+2),7.16243e-5,5.63708e-6,6.59872e-5
Mg(+2),7.03559e-3,7.03559e-3,0.0
Fe(+3),6.97349e-16,6.97349e-16,0.0
O(-2),28.042,28.0408,1.18946e-3
Cl(-1),0.579542,0.579542,0.0
C(+4),0.500189,0.500189,0.0
S(+4),3.49833e-12,3.49833e-12,0.0
S(+6),3.53152e-3,3.23416e-3,2.97365e-4
S(-2),6.66198e-5,6.32628e-7,6.59872e-5
S(+2),1.19567e-10,1.19567e-10,0.0
N(+3),1.44832e-55,1.44832e-55,0.0
N(+5),1.05128e-72,1.05128e-72,0.0
N(0),6.76543e-3,6.76543e-3,0.0
H(0),3.38807e-12,3.38807e-12,0.0
O(0),4.97099e-63,4.97099e-63,0.0
S(+8),5.68546e-54,5.68546e-54,0.0
S(+3),5.92508e-28,5.92508e-28,0.0
S(+5),1.46381e-28,1.46381e-28,0.0
S(+7),4.57646e-64,4.57646e-64,0.0
N(+2),9.41568e-47,9.41568e-47,0.0
N(+4),1.28883e-68,1.28883e-68,0.0
N(+1),5.75303e-48,5.75303e-48,0.0
N(-2),2.11805e-33,2.11805e-33,0.0
C(+2),2.12661e-4,2.12661e-4,0.0
Fe(+6),7.84191e-67,7.84191e-67,0.0
S(0),6.59872e-5,1.28185e-18,6.59872e-5
N(-1),3.56114e-39,3.56114e-39,0.0
METHANOL,4.18415e-4,4.18415e-4,0.0
TRIETLNGLY,8.84731e-6,8.84731e-6,0.0

Element Distribution

 ,Total,Total,Aqueous,Solid
,mol,mole %,% of Total,% of Total
H(+1),54.0565,64.542,100.0,0.0
Na(+1),0.539233,0.64383,100.0,0.0
N(-3),1.05077e-3,1.25459e-3,100.0,0.0
Ba(+2),2.98551e-4,3.56462e-4,0.39724,99.6028
Ca(+2),0.0170043,0.0203027,100.0,0.0
Fe(+2),7.16243e-5,8.55174e-5,7.87035,92.1297
Mg(+2),7.03559e-3,8.4003e-3,100.0,0.0
Fe(+3),6.97349e-16,8.32616e-16,100.0,0.0
O(-2),28.042,33.4814,99.9958,4.2417e-3
Cl(-1),0.579542,0.691957,100.0,0.0
C(+4),0.500189,0.597212,100.0,0.0
S(+4),3.49833e-12,4.17691e-12,100.0,0.0
S(+6),3.53152e-3,4.21654e-3,91.5797,8.42031

S(-2),6.66198e-5,7.95422e-5,0.949609,99.0504
S(+2),1.19567e-10,1.4276e-10,100.0,0.0
N(+3),1.44832e-55,1.72925e-55,100.0,0.0
N(+5),1.05128e-72,1.2552e-72,100.0,0.0
N(0),6.76543e-3,8.07774e-3,100.0,0.0
H(0),3.38807e-12,4.04527e-12,100.0,0.0
O(0),4.97099e-63,5.93523e-63,100.0,0.0
S(+8),5.68546e-54,6.78828e-54,100.0,0.0
S(+3),5.92508e-28,7.07439e-28,100.0,0.0
S(+5),1.46381e-28,1.74775e-28,100.0,0.0
S(+7),4.57646e-64,5.46417e-64,100.0,0.0
N(+2),9.41568e-47,1.12421e-46,100.0,0.0
N(+4),1.28883e-68,1.53883e-68,100.0,0.0
N(+1),5.75303e-48,6.86897e-48,100.0,0.0
N(-2),2.11805e-33,2.52889e-33,100.0,0.0
C(+2),2.12661e-4,2.53912e-4,100.0,0.0
Fe(+6),7.84191e-67,9.36303e-67,100.0,0.0
S(0),6.59872e-5,7.87869e-5,1.94258e-12,100.0
N(-1),3.56114e-39,4.25191e-39,100.0,0.0
METHANOL,4.18415e-4,4.99576e-4,100.0,0.0
TRIETLNGLY,8.84731e-6,1.05635e-5,100.0,0.0

Calculation Summary
06-2 Alloy-4 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2205

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,(NH4)2SO3
,C6H14O4

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,27.0272,27.0272
CO2,0.500189,0.500189
N2,3.52818e-3,3.52818e-3
CO,2.12661e-4,2.12661e-4
O2,1.11890e-5,1.11890e-5
NH3,6.74808e-4,6.74808e-4
CH3OH,4.18415e-4,4.18415e-4
H2S,5.30469e-5,5.30469e-5
SO2,1.00864e-3,1.00864e-3
NO2,8.50324e-5,8.50324e-5
BaCl2,1.69170e-6,1.69170e-6

CaCl2,0.0130454,0.0130454
CaO,3.95899e-3,3.95899e-3
FeCl2,7.16243e-5,7.16243e-5
MgCl2,7.03559e-3,7.03559e-3
NaCl,0.539233,0.539233
SO3,2.30558e-3,2.30558e-3
BaSO4,2.96859e-4,2.96859e-4
C6H14O4,8.84731e-6,8.84731e-6

Calculated Rates

Corrosion Rate,2.80983e-4,mm/yr
Corrosion Potential,-0.238963,V (SHE)
Repassivation Potential*,-0.0431660,V (SHE)
Corrosion Current Density,2.66112e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.2H2O (Gypsum),0.137014
,CaSO4 (Anhydrite),0.160771
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,28.0993,mol
Temperature,50.0000,°C
Pressure,3398.00,psia

Liquid 1 Properties
pH,3.51482,
Ionic Strength (x-based),0.0213857,mol/mol
Ionic Strength (m-based),1.25794,mol/kg
Dielectric Constant,53.6355,
ORP,0.0438736,V (SHE)
Osmotic Pressure,1326.66,psia
Specific Electrical Conductivity,1.41858e5,µmho/cm
"Viscosity, absolute",0.634788,cP
Thermal Conductivity,554.913,cal/hr m °C
Surface Tension,0.0711104,N/m
Interfacial Tension LLE,1.46705e-5,N/m
Standard Liquid Volume,0.525699,L
"Volume, Std. Conditions",0.515095,L
"Total Dissolved Solids, Estimated",66495.4,mg/L
Hardness,4662.46,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,4.47969e-6,L

Liquid 2 Properties
pH,2.48706,
Ionic Strength (x-based),6.22230e-3,mol/mol
Ionic Strength (m-based),52.3806,mol/kg
Dielectric Constant,4.89064,
Specific Electrical Conductivity,12798.1,µmho/cm
"Viscosity, absolute",0.562254,cP
Surface Tension,0.0644671,N/m
Thermal Conductivity,558.128,cal/hr m °C
Standard Liquid Volume,1.38272e-3,L
"Volume, Std. Conditions",2.70510e-3,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid,Liquid-2
Density,g/ml,1.04935,1.05031,4.47972,0.783855
Enthalpy,J,-8.11081e6,-8.09580e6,-436.940,-14579.9

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
Mole (True),28.6749,28.6372,2.97093e-4,0.0374239
Mole (App),28.0986,28.0608,2.97093e-4,0.0375170
,g,g,g,g
Mass,543.238,541.543,0.0693397,1.62489
,L,L,cm3,L
Volume,0.517692,0.515603,0.0154786,2.07295e-3

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,222.975
H2O,0.580334,0.580327
CaSO4 (Anhydrite),0.160771,0.174593
CaSO4.2H2O (Gypsum),0.137014,0.148790
CaSO4.0.5H2O (Bassanite),0.0455027,0.0494146
CaSO4.0.5H2O (Bassanite),0.0359083,0.0389953
FeS2 (Pyrite),0.0206929,0.0246339
NaCl (Halite),0.0151840,0.0151840
NaCl.2H2O (hydrohalite),9.38078e-3,9.38078e-3
FeS2(marcasite) (Marcasite),5.96444e-3,7.10038e-3
NaHCO3 (Nahcolite),3.03478e-3,3.03478e-3
CaCO3 (Calcite),1.92406e-3,1.92406e-3
CaCO3 (Aragonite),1.48574e-3,1.48574e-3
Na2SO4 (Thenardite),5.41321e-4,5.89339e-4
Na2SO4.CaSO4 (Glauberite),2.48126e-4,2.93361e-4
Na2SO4.10H2O (Mirabilite),1.80870e-4,1.96892e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H2O,27.0243,27.0241,0.0,2.46767e-4
Cl-1,0.579541,0.579525,,1.57566e-5
Na+1,0.538812,0.538812,,2.40524e-12
CO2,0.497678,0.462044,,0.0356345
Ca+2,0.0165336,0.0165336,,1.01824e-20
Mg+2,6.61458e-3,6.61458e-3,,1.70669e-21
N2,3.23387e-3,1.94362e-3,,1.29026e-3
SO4-2,2.45833e-3,2.45833e-3,,2.4925e-11
HCO3-1,2.36506e-3,2.365e-3,,5.54516e-8
NH4+1,1.20291e-3,1.20291e-3,,5.04374e-9
CaSO4 (Anhydrite),4.70055e-4,4.69358e-4,0.0,6.97088e-7
NaMgSO4+1,4.20948e-4,4.02635e-4,,1.83129e-5
CH3OH,4.18388e-4,4.18179e-4,,2.09429e-7
BaSO4 (Barite),2.97093e-4,,2.97093e-4,
CO,2.12661e-4,2.12427e-4,,2.34439e-7
NH2CO2-1,1.45536e-4,6.5155e-11,,1.45536e-4
H3O+1,1.02221e-4,1.02221e-4,,3.14647e-17
Fe+2,7.15247e-5,1.00451e-8,,7.15146e-5
HSO4-1,1.31658e-5,1.31658e-5,,1.25689e-11
C6H14O4,8.84729e-6,8.84718e-6,,1.08327e-10
H2S,4.4653e-6,4.33621e-6,,1.29095e-7
Ba+2,1.45762e-6,1.45762e-6,,1.43319e-27
CaCl2 (Hydrophilite),5.76252e-7,5.76252e-7,0.0,1.65108e-22
FeCO2+2,9.95885e-8,9.95885e-8,,2.97456e-108
MgSO4,5.8992e-8,5.88918e-8,0.0,1.00176e-10
CaCO3 (Calcite),3.61863e-8,3.61658e-8,0.0,2.04751e-11
CaClCH3OH+1,2.64143e-8,2.52965e-8,,1.11777e-9
CO3-2,5.11781e-9,5.11779e-9,,1.31204e-14
NH4OH,4.07646e-9,4.07569e-9,,7.70847e-13
HS-1,3.75538e-9,3.75491e-9,,4.62277e-13
Na2SO4.NaHSO4,3.72815e-9,3.72815e-9,0.0,3.89017e-18
MgCO3,1.93687e-9,1.93473e-9,0.0,2.13522e-12
NH3,1.45253e-9,1.45233e-9,,2.02158e-13
OH-1,1.8051e-10,1.80504e-10,,5.70714e-15
MgOH+1,1.34324e-10,1.32717e-10,,1.60666e-12
S2O3-2,1.2891e-10,1.28909e-10,,6.39736e-16
CaOH+1,7.86845e-11,7.81449e-11,,5.39682e-13
HCl,2.82044e-11,2.75494e-11,,6.54975e-13
HO(CH2CH2O)3CO2(-1),1.87663e-11,1.87648e-11,,1.54024e-15
FeCl+1,6.4626e-12,6.38152e-12,,8.10788e-14
MgClCH3OH+1,6.34662e-12,3.70469e-12,,2.64193e-12
H2,3.59666e-12,3.59158e-12,,5.08164e-15
HSO3-1,3.09284e-12,3.09251e-12,,3.3476e-16
CH5O+1,2.67587e-12,2.42957e-12,,2.46308e-13
CH3OH.HCl,1.74934e-12,1.74741e-12,,1.92819e-15
C6H15O4+1,1.02652e-12,1.00712e-12,,1.94011e-14

FeSO4,4.85506e-13,4.84971e-13,0.0,5.35227e-16
HS2O3-1,4.21059e-13,4.21014e-13,,4.48511e-17
BaCO3 (Witherite),3.0856e-13,3.08219e-13,0.0,3.40158e-16
SO2,7.06136e-14,6.97733e-14,,8.40353e-16
FeH(CO3)2-1,2.29871e-14,2.29847e-14,,2.44858e-18
H2SO4,1.84856e-14,1.84856e-14,,9.34033e-23
FeOH+1,1.7542e-14,1.73321e-14,,2.09821e-16
FeHS+1,6.09268e-15,6.01981e-15,,7.2875e-17
CH3O-1,5.9059e-15,5.90527e-15,,6.2953e-19
SO3-2,3.5839e-15,3.58388e-15,,1.92789e-20
BaOH+1,1.88528e-15,1.86586e-15,,1.94174e-17
Fe(NH3)+2,1.16569e-15,9.82317e-16,,1.83378e-16
CO2S,7.25746e-16,7.24946e-16,,8.00068e-19
NaOH,5.38839e-16,5.38827e-16,0.0,1.21441e-20
H2S2O3,5.25101e-16,5.24522e-16,,5.78875e-19
S1,4.92761e-16,4.92218e-16,,5.43223e-19
FeS (Pyrrhotite),1.91582e-16,1.91371e-16,0.0,2.11201e-19
NaOH.Na2SO4,1.78978e-16,1.78978e-16,,4.22116e-30
C6H13O4-1,1.72942e-16,1.72924e-16,,1.82602e-20
S2,1.46816e-17,1.46655e-17,,1.61852e-20
S2-2,9.54694e-18,9.54685e-18,,8.82387e-23
S3-2,2.72762e-18,2.7276e-18,,2.52104e-23
FeO+1,7.19069e-19,7.10468e-19,,8.60084e-21
FeOH+2,6.70454e-19,5.98964e-19,,7.14901e-20
S4-2,4.86969e-19,4.86965e-19,,4.50087e-24
S8 (Sulfur),4.58839e-19,1.62565e-19,0.0,2.96274e-19
S-2,4.52761e-19,4.5273e-19,,3.12341e-23
S3,4.37404e-19,4.36922e-19,,4.82198e-22
FeCl+2,4.33108e-19,3.90799e-19,,4.23096e-20
MgCl2,2.76873e-19,2.75683e-19,0.0,1.1898e-21
Fe+3,9.70316e-20,2.56875e-20,,7.13441e-20
S5-2,5.44828e-20,5.44823e-20,,5.03564e-25
NaOHCO3-2,4.1744e-20,4.17436e-20,,3.85824e-25
S4,1.30332e-20,1.30188e-20,,1.43679e-23
HFeO2,2.84941e-21,2.84627e-21,,3.14122e-24
FeO,2.3349e-21,2.33233e-21,,2.57401e-24
Fe(NH3)2+2,9.18443e-22,7.73961e-22,,1.44482e-22
S5,3.88365e-22,3.87937e-22,,4.28136e-25
FeCl2+1,1.16002e-22,1.15451e-22,,5.50909e-25
FeHSO4+2,6.35937e-23,5.67583e-23,,6.83547e-24
S6,1.15731e-23,1.15603e-23,,1.27582e-26
S2O5-2,6.73065e-24,6.73059e-24,,6.21767e-29
S7,3.4472e-25,3.4434e-25,,3.80022e-28
FeO2-1,1.08623e-26,1.08611e-26,,1.15705e-30
SO3,3.13364e-27,3.13364e-27,,1.32462e-33
S2O4-2,2.03437e-28,2.03435e-28,,1.88029e-33
Fe(NH3)3+2,1.97276e-28,1.66242e-28,,3.10338e-29
HFeO2-1,6.36207e-29,6.3614e-29,,6.77687e-33
S2O6-2,1.6047e-29,1.60469e-29,,1.48316e-34
N2H5+1,8.81337e-34,8.70797e-34,,1.05397e-35
S5O6-2,1.50645e-35,1.50644e-35,,1.39235e-40
NH2OH2+1,2.01133e-36,1.9873e-36,,2.40343e-38
N2H6+2,8.44683e-38,7.54632e-38,,9.00512e-39
Fe(NH3)4+2,8.10287e-38,6.82819e-38,,1.27468e-38

Fe2(OH)2+4,6.86356e-38,7.28289e-39,,6.13527e-38
N2H4,5.27025e-38,5.27013e-38,,1.14586e-42
NH2OH,1.31517e-38,1.3144e-38,0.0,7.68475e-42
HClO,6.97509e-43,6.9674e-43,,7.68939e-46
NH2Cl,4.19084e-43,4.18622e-43,,4.62001e-46
Cl2,2.48091e-43,2.47817e-43,,2.73497e-46
ClO-1,1.67206e-46,1.67188e-46,,1.78107e-50
NO,7.66107e-47,6.59795e-47,,1.06312e-47
Fe(NH3)5+2,3.32945e-47,2.80569e-47,,5.23762e-48
N2O,1.41223e-48,1.33813e-48,,7.41011e-50
NH3Cl+1,4.87657e-52,4.81824e-52,,5.8329e-54
HSO5-1,1.40861e-54,1.40846e-54,,1.50045e-58
NO2-1,3.3974e-56,3.39706e-56,,3.35711e-60
Fe(NH3)6+2,1.36753e-56,1.1524e-56,,2.15129e-57
HNO2,8.82919e-57,8.81946e-57,,9.73337e-60
O2,9.2069e-64,8.48745e-64,,7.19449e-65
S2O8-2,1.52799e-65,1.52798e-65,,1.41226e-70
NO2,1.61927e-69,1.49375e-69,,1.25516e-70
FeO4-2,1.62479e-70,1.62477e-70,,1.50173e-75
NO3-1,1.59978e-73,1.59977e-73,,3.90889e-79
HNO3,1.71399e-78,1.71399e-78,,1.90763e-84
NHCl2,9.95725e-80,9.94627e-80,,1.09769e-82
ClO2-1,3.18162e-85,3.18128e-85,,3.38906e-89
NH2Cl2+1,4.86821e-86,4.80998e-86,,5.8229e-88
HClO2,8.67896e-87,8.66939e-87,,9.56775e-90
NH4NO3.(NH4)2SO4,8.30508e-87,8.29593e-87,0.0,9.15559e-90
ClO2,6.34327e-102,6.33628e-102,,6.99287e-105
ClO3-1,3.76893e-111,3.76852e-111,,4.01465e-115
N2O3,1.08806e-114,2.90311e-118,,1.08777e-114
NCl3,8.99006e-117,2.14411e-117,,6.84595e-117
NHCl3+1,5.79658e-121,5.72725e-121,,6.93334e-123
Total (by phase),28.6749,28.6372,2.97093e-4,0.0374239

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H(+1),54.0569,54.0561,0.0,7.85151e-4
Na(+1),0.539233,0.539215,0.0,1.83129e-5
N(-3),1.34846e-3,1.20291e-3,0.0,1.45541e-4
Ba(+2),2.98551e-4,1.45762e-6,2.97093e-4,3.59576e-16
Ca(+2),0.0170043,0.0170036,0.0,6.98226e-7
Fe(+2),7.16243e-5,1.09641e-7,0.0,7.15146e-5
Mg(+2),7.03559e-3,7.01728e-3,0.0,1.8313e-5
Fe(+3),1.92269e-18,1.72894e-18,0.0,1.93755e-19
O(-2),28.042,27.969,1.18837e-3,0.0718832
Cl(-1),0.579542,0.579526,0.0,1.57577e-5
C(+4),0.500189,0.464409,0.0,0.0357801
S(+4),3.16704e-12,3.16586e-12,0.0,1.17513e-15
S(+6),3.65966e-3,3.34355e-3,2.97093e-4,1.90101e-5
S(-2),4.46906e-6,4.33996e-6,0.0,1.29095e-7

S(+2),2.58663e-10,2.58662e-10,0.0,1.37033e-15
N(+3),4.28032e-56,4.27901e-56,0.0,1.30905e-59
N(+5),1.59979e-73,1.59979e-73,0.0,3.90891e-79
N(0),6.46774e-3,3.88723e-3,0.0,2.58051e-3
H(0),7.19332e-12,7.18316e-12,0.0,1.01633e-14
O(0),1.84138e-63,1.69749e-63,0.0,1.4389e-64
S(+8),1.40861e-54,1.40846e-54,0.0,1.50045e-58
Cl(+1),1.36485e-42,1.36335e-42,0.0,1.50446e-45
Cl(+5),3.76893e-111,3.76852e-111,0.0,4.01465e-115
S(+3),4.06873e-28,4.06869e-28,0.0,3.76057e-33
S(+5),3.2094e-29,3.20937e-29,0.0,2.96633e-34
S(+7),3.05598e-65,3.05595e-65,0.0,2.82453e-70
N(+2),7.66107e-47,6.59795e-47,0.0,1.06312e-47
N(+4),1.61927e-69,1.49375e-69,0.0,1.25516e-70
Cl(+3),3.26841e-85,3.26798e-85,0.0,4.34583e-89
Cl(+4),6.34327e-102,6.33628e-102,0.0,6.99287e-105
N(+1),2.82446e-48,2.67626e-48,0.0,1.48202e-49
N(-2),1.76295e-33,1.74185e-33,0.0,2.10975e-35
C(+2),2.12661e-4,2.12427e-4,0.0,2.34439e-7
Fe(+6),1.62479e-70,1.62477e-70,0.0,1.50173e-75
S(0),1.26959e-15,1.26584e-15,0.0,3.74751e-18
MeO(-1),4.18415e-4,4.18204e-4,0.0,2.1055e-7
N(-1),2.02449e-36,2.00044e-36,0.0,2.4042e-38
TEGION,8.84731e-6,8.8472e-6,0.0,1.08348e-10

Element Distribution

 ,Total,Total,Liquid-1,Solid,Liquid-2
,mol,mole %,% of Total,% of Total,% of Total
H(+1),54.0569,64.5421,99.9985,0.0,1.45245e-3
Na(+1),0.539233,0.643827,99.9966,0.0,3.3961e-3
N(-3),1.34846e-3,1.61001e-3,89.2068,0.0,10.7932
Ba(+2),2.98551e-4,3.5646e-4,0.488232,99.5118,1.2044e-10
Ca(+2),0.0170043,0.0203026,99.9959,0.0,4.10617e-3
Fe(+2),7.16243e-5,8.5517e-5,0.153077,0.0,99.8469
Mg(+2),7.03559e-3,8.40026e-3,99.7397,0.0,0.260291
Fe(+3),1.92269e-18,2.29563e-18,89.9227,0.0,10.0773
O(-2),28.042,33.4813,99.7394,4.23783e-3,0.256341
Cl(-1),0.579542,0.691954,99.9973,0.0,2.719e-3
C(+4),0.500189,0.597209,92.8467,0.0,7.15331
S(+4),3.16704e-12,3.78134e-12,99.9629,0.0,0.0371051
S(+6),3.65966e-3,4.36951e-3,91.3625,8.11806,0.519451
S(-2),4.46906e-6,5.3359e-6,97.1114,0.0,2.88865
S(+2),2.58663e-10,3.08836e-10,99.9995,0.0,5.29774e-4
N(+3),4.28032e-56,5.11056e-56,99.9694,0.0,0.030583
N(+5),1.59979e-73,1.9101e-73,99.9998,0.0,2.44338e-4
N(0),6.46774e-3,7.72227e-3,60.1018,0.0,39.8982
H(0),7.19332e-12,8.58859e-12,99.8587,0.0,0.141288
O(0),1.84138e-63,2.19855e-63,92.1858,0.0,7.81424
S(+8),1.40861e-54,1.68183e-54,99.9893,0.0,0.010652
Cl(+1),1.36485e-42,1.62959e-42,99.8898,0.0,0.110229
Cl(+5),3.76893e-111,4.49997e-111,99.9893,0.0,0.010652
S(+3),4.06873e-28,4.85793e-28,99.9991,0.0,9.24261e-4

S(+5),3.2094e-29,3.83192e-29,99.9991,0.0,9.24261e-4
S(+7),3.05598e-65,3.64874e-65,99.9991,0.0,9.24261e-4
N(+2),7.66107e-47,9.14706e-47,86.1231,0.0,13.8769
N(+4),1.61927e-69,1.93335e-69,92.2486,0.0,7.75141
Cl(+3),3.26841e-85,3.90237e-85,99.9867,0.0,0.0132965
Cl(+4),6.34327e-102,7.57365e-102,99.8898,0.0,0.110241
N(+1),2.82446e-48,3.37232e-48,94.7529,0.0,5.24709
N(-2),1.76295e-33,2.1049e-33,98.8033,0.0,1.19672
C(+2),2.12661e-4,2.5391e-4,99.8898,0.0,0.110241
Fe(+6),1.62479e-70,1.93994e-70,99.9991,0.0,9.24261e-4
S(0),1.26959e-15,1.51585e-15,99.7048,0.0,0.295176
MeO(-1),4.18415e-4,4.99573e-4,99.9497,0.0,0.0503208
N(-1),2.02449e-36,2.41717e-36,98.8124,0.0,1.18756
TEGION,8.84731e-6,1.05634e-5,99.9988,0.0,1.22464e-3

Calculation Summary
06-2 Alloy-5 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2507

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,(NH4)2SO3
,C6H14O4

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,27.0272,27.0272
CO2,0.500189,0.500189
N2,3.52818e-3,3.52818e-3
CO,2.12661e-4,2.12661e-4
O2,1.11890e-5,1.11890e-5
NH3,6.74808e-4,6.74808e-4
CH3OH,4.18415e-4,4.18415e-4
H2S,5.30469e-5,5.30469e-5
SO2,1.00864e-3,1.00864e-3
NO2,8.50324e-5,8.50324e-5
BaCl2,1.69170e-6,1.69170e-6

CaCl2,0.0130454,0.0130454
CaO,3.95899e-3,3.95899e-3
FeCl2,7.16243e-5,7.16243e-5
MgCl2,7.03559e-3,7.03559e-3
NaCl,0.539233,0.539233
SO3,2.30558e-3,2.30558e-3
BaSO4,2.96859e-4,2.96859e-4
C6H14O4,8.84731e-6,8.84731e-6

Calculated Rates

Corrosion Rate,2.72371e-4,mm/yr
Corrosion Potential,-0.241040,V (SHE)
Repassivation Potential*,0.0212446,V (SHE)
Corrosion Current Density,2.65471e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.2H2O (Gypsum),0.137014
,CaSO4 (Anhydrite),0.160771
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,28.0993,mol
Temperature,50.0000,°C
Pressure,3398.00,psia

Liquid 1 Properties
pH,3.51482,
Ionic Strength (x-based),0.0213857,mol/mol
Ionic Strength (m-based),1.25794,mol/kg
Dielectric Constant,53.6355,
ORP,0.0438736,V (SHE)
Osmotic Pressure,1326.66,psia
Specific Electrical Conductivity,1.41858e5,µmho/cm
"Viscosity, absolute",0.634788,cP
Thermal Conductivity,554.913,cal/hr m °C
Surface Tension,0.0711104,N/m
Interfacial Tension LLE,1.46705e-5,N/m
Standard Liquid Volume,0.525699,L
"Volume, Std. Conditions",0.515095,L
"Total Dissolved Solids, Estimated",66495.4,mg/L
Hardness,4662.46,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,4.47969e-6,L

Liquid 2 Properties
pH,2.48706,
Ionic Strength (x-based),6.22230e-3,mol/mol
Ionic Strength (m-based),52.3806,mol/kg
Dielectric Constant,4.89064,
Specific Electrical Conductivity,12798.1,µmho/cm
"Viscosity, absolute",0.562254,cP
Surface Tension,0.0644671,N/m
Thermal Conductivity,558.128,cal/hr m °C
Standard Liquid Volume,1.38272e-3,L
"Volume, Std. Conditions",2.70510e-3,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid,Liquid-2
Density,g/ml,1.04935,1.05031,4.47972,0.783855
Enthalpy,J,-8.11081e6,-8.09580e6,-436.940,-14579.9

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
Mole (True),28.6749,28.6372,2.97093e-4,0.0374239
Mole (App),28.0986,28.0608,2.97093e-4,0.0375170
,g,g,g,g
Mass,543.238,541.543,0.0693397,1.62489
,L,L,cm3,L
Volume,0.517692,0.515603,0.0154786,2.07295e-3

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,222.975
H2O,0.580334,0.580327
CaSO4 (Anhydrite),0.160771,0.174593
CaSO4.2H2O (Gypsum),0.137014,0.148790
CaSO4.0.5H2O (Bassanite),0.0455027,0.0494146
CaSO4.0.5H2O (Bassanite),0.0359083,0.0389953
FeS2 (Pyrite),0.0206929,0.0246339
NaCl (Halite),0.0151840,0.0151791
NaCl.2H2O (hydrohalite),9.38078e-3,9.37755e-3
FeS2(marcasite) (Marcasite),5.96444e-3,7.10038e-3
NaHCO3 (Nahcolite),3.03478e-3,3.03200e-3
CaCO3 (Calcite),1.92406e-3,1.91575e-3
CaCO3 (Aragonite),1.48574e-3,1.47932e-3
Na2SO4 (Thenardite),5.41321e-4,5.89339e-4
Na2SO4.CaSO4 (Glauberite),2.48126e-4,2.93361e-4
Na2SO4.10H2O (Mirabilite),1.80870e-4,1.96892e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H2O,27.0243,27.0241,0.0,2.46767e-4
Cl-1,0.579541,0.579525,,1.57566e-5
Na+1,0.538812,0.538812,,2.40524e-12
CO2,0.497678,0.462044,,0.0356345
Ca+2,0.0165336,0.0165336,,1.01824e-20
Mg+2,6.61458e-3,6.61458e-3,,1.70669e-21
N2,3.23387e-3,1.94362e-3,,1.29026e-3
SO4-2,2.45833e-3,2.45833e-3,,2.4925e-11
HCO3-1,2.36506e-3,2.365e-3,,5.54516e-8
NH4+1,1.20291e-3,1.20291e-3,,5.04374e-9
CaSO4 (Anhydrite),4.70055e-4,4.69358e-4,0.0,6.97088e-7
NaMgSO4+1,4.20948e-4,4.02635e-4,,1.83129e-5
CH3OH,4.18388e-4,4.18179e-4,,2.09429e-7
BaSO4 (Barite),2.97093e-4,,2.97093e-4,
CO,2.12661e-4,2.12427e-4,,2.34439e-7
NH2CO2-1,1.45536e-4,6.5155e-11,,1.45536e-4
H3O+1,1.02221e-4,1.02221e-4,,3.14647e-17
Fe+2,7.15247e-5,1.00451e-8,,7.15146e-5
HSO4-1,1.31658e-5,1.31658e-5,,1.25689e-11
C6H14O4,8.84729e-6,8.84718e-6,,1.08327e-10
H2S,4.4653e-6,4.33621e-6,,1.29095e-7
Ba+2,1.45762e-6,1.45762e-6,,1.43319e-27
CaCl2 (Hydrophilite),5.76252e-7,5.76252e-7,0.0,1.65108e-22
FeCO2+2,9.95885e-8,9.95885e-8,,2.97456e-108
MgSO4,5.8992e-8,5.88918e-8,0.0,1.00176e-10
CaCO3 (Calcite),3.61863e-8,3.61658e-8,0.0,2.04751e-11
CaClCH3OH+1,2.64143e-8,2.52965e-8,,1.11777e-9
CO3-2,5.11781e-9,5.11779e-9,,1.31204e-14
NH4OH,4.07646e-9,4.07569e-9,,7.70847e-13
HS-1,3.75538e-9,3.75491e-9,,4.62277e-13
Na2SO4.NaHSO4,3.72815e-9,3.72815e-9,0.0,3.89017e-18
MgCO3,1.93687e-9,1.93473e-9,0.0,2.13522e-12
NH3,1.45253e-9,1.45233e-9,,2.02158e-13
OH-1,1.8051e-10,1.80504e-10,,5.70714e-15
MgOH+1,1.34324e-10,1.32717e-10,,1.60666e-12
S2O3-2,1.2891e-10,1.28909e-10,,6.39736e-16
CaOH+1,7.86845e-11,7.81449e-11,,5.39682e-13
HCl,2.82044e-11,2.75494e-11,,6.54975e-13
HO(CH2CH2O)3CO2(-1),1.87663e-11,1.87648e-11,,1.54024e-15
FeCl+1,6.4626e-12,6.38152e-12,,8.10788e-14
MgClCH3OH+1,6.34662e-12,3.70469e-12,,2.64193e-12
H2,3.59666e-12,3.59158e-12,,5.08164e-15
HSO3-1,3.09284e-12,3.09251e-12,,3.3476e-16
CH5O+1,2.67587e-12,2.42957e-12,,2.46308e-13
CH3OH.HCl,1.74934e-12,1.74741e-12,,1.92819e-15
C6H15O4+1,1.02652e-12,1.00712e-12,,1.94011e-14

FeSO4,4.85506e-13,4.84971e-13,0.0,5.35227e-16
HS2O3-1,4.21059e-13,4.21014e-13,,4.48511e-17
BaCO3 (Witherite),3.0856e-13,3.08219e-13,0.0,3.40158e-16
SO2,7.06136e-14,6.97733e-14,,8.40353e-16
FeH(CO3)2-1,2.29871e-14,2.29847e-14,,2.44858e-18
H2SO4,1.84856e-14,1.84856e-14,,9.34033e-23
FeOH+1,1.7542e-14,1.73321e-14,,2.09821e-16
FeHS+1,6.09268e-15,6.01981e-15,,7.2875e-17
CH3O-1,5.9059e-15,5.90527e-15,,6.2953e-19
SO3-2,3.5839e-15,3.58388e-15,,1.92789e-20
BaOH+1,1.88528e-15,1.86586e-15,,1.94174e-17
Fe(NH3)+2,1.16569e-15,9.82317e-16,,1.83378e-16
CO2S,7.25746e-16,7.24946e-16,,8.00068e-19
NaOH,5.38839e-16,5.38827e-16,0.0,1.21441e-20
H2S2O3,5.25101e-16,5.24522e-16,,5.78875e-19
S1,4.92761e-16,4.92218e-16,,5.43223e-19
FeS (Pyrrhotite),1.91582e-16,1.91371e-16,0.0,2.11201e-19
NaOH.Na2SO4,1.78978e-16,1.78978e-16,,4.22116e-30
C6H13O4-1,1.72942e-16,1.72924e-16,,1.82602e-20
S2,1.46816e-17,1.46655e-17,,1.61852e-20
S2-2,9.54694e-18,9.54685e-18,,8.82387e-23
S3-2,2.72762e-18,2.7276e-18,,2.52104e-23
FeO+1,7.19069e-19,7.10468e-19,,8.60084e-21
FeOH+2,6.70454e-19,5.98964e-19,,7.14901e-20
S4-2,4.86969e-19,4.86965e-19,,4.50087e-24
S8 (Sulfur),4.58839e-19,1.62565e-19,0.0,2.96274e-19
S-2,4.52761e-19,4.5273e-19,,3.12341e-23
S3,4.37404e-19,4.36922e-19,,4.82198e-22
FeCl+2,4.33108e-19,3.90799e-19,,4.23096e-20
MgCl2,2.76873e-19,2.75683e-19,0.0,1.1898e-21
Fe+3,9.70316e-20,2.56875e-20,,7.13441e-20
S5-2,5.44828e-20,5.44823e-20,,5.03564e-25
NaOHCO3-2,4.1744e-20,4.17436e-20,,3.85824e-25
S4,1.30332e-20,1.30188e-20,,1.43679e-23
HFeO2,2.84941e-21,2.84627e-21,,3.14122e-24
FeO,2.3349e-21,2.33233e-21,,2.57401e-24
Fe(NH3)2+2,9.18443e-22,7.73961e-22,,1.44482e-22
S5,3.88365e-22,3.87937e-22,,4.28136e-25
FeCl2+1,1.16002e-22,1.15451e-22,,5.50909e-25
FeHSO4+2,6.35937e-23,5.67583e-23,,6.83547e-24
S6,1.15731e-23,1.15603e-23,,1.27582e-26
S2O5-2,6.73065e-24,6.73059e-24,,6.21767e-29
S7,3.4472e-25,3.4434e-25,,3.80022e-28
FeO2-1,1.08623e-26,1.08611e-26,,1.15705e-30
SO3,3.13364e-27,3.13364e-27,,1.32462e-33
S2O4-2,2.03437e-28,2.03435e-28,,1.88029e-33
Fe(NH3)3+2,1.97276e-28,1.66242e-28,,3.10338e-29
HFeO2-1,6.36207e-29,6.3614e-29,,6.77687e-33
S2O6-2,1.6047e-29,1.60469e-29,,1.48316e-34
N2H5+1,8.81337e-34,8.70797e-34,,1.05397e-35
S5O6-2,1.50645e-35,1.50644e-35,,1.39235e-40
NH2OH2+1,2.01133e-36,1.9873e-36,,2.40343e-38
N2H6+2,8.44683e-38,7.54632e-38,,9.00512e-39
Fe(NH3)4+2,8.10287e-38,6.82819e-38,,1.27468e-38

Fe2(OH)2+4,6.86356e-38,7.28289e-39,,6.13527e-38
N2H4,5.27025e-38,5.27013e-38,,1.14586e-42
NH2OH,1.31517e-38,1.3144e-38,0.0,7.68475e-42
HClO,6.97509e-43,6.9674e-43,,7.68939e-46
NH2Cl,4.19084e-43,4.18622e-43,,4.62001e-46
Cl2,2.48091e-43,2.47817e-43,,2.73497e-46
ClO-1,1.67206e-46,1.67188e-46,,1.78107e-50
NO,7.66107e-47,6.59795e-47,,1.06312e-47
Fe(NH3)5+2,3.32945e-47,2.80569e-47,,5.23762e-48
N2O,1.41223e-48,1.33813e-48,,7.41011e-50
NH3Cl+1,4.87657e-52,4.81824e-52,,5.8329e-54
HSO5-1,1.40861e-54,1.40846e-54,,1.50045e-58
NO2-1,3.3974e-56,3.39706e-56,,3.35711e-60
Fe(NH3)6+2,1.36753e-56,1.1524e-56,,2.15129e-57
HNO2,8.82919e-57,8.81946e-57,,9.73337e-60
O2,9.2069e-64,8.48745e-64,,7.19449e-65
S2O8-2,1.52799e-65,1.52798e-65,,1.41226e-70
NO2,1.61927e-69,1.49375e-69,,1.25516e-70
FeO4-2,1.62479e-70,1.62477e-70,,1.50173e-75
NO3-1,1.59978e-73,1.59977e-73,,3.90889e-79
HNO3,1.71399e-78,1.71399e-78,,1.90763e-84
NHCl2,9.95725e-80,9.94627e-80,,1.09769e-82
ClO2-1,3.18162e-85,3.18128e-85,,3.38906e-89
NH2Cl2+1,4.86821e-86,4.80998e-86,,5.8229e-88
HClO2,8.67896e-87,8.66939e-87,,9.56775e-90
NH4NO3.(NH4)2SO4,8.30508e-87,8.29593e-87,0.0,9.15559e-90
ClO2,6.34327e-102,6.33628e-102,,6.99287e-105
ClO3-1,3.76893e-111,3.76852e-111,,4.01465e-115
N2O3,1.08806e-114,2.90311e-118,,1.08777e-114
NCl3,8.99006e-117,2.14411e-117,,6.84595e-117
NHCl3+1,5.79658e-121,5.72725e-121,,6.93334e-123
Total (by phase),28.6749,28.6372,2.97093e-4,0.0374239

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid,Liquid-2
,mol,mol,mol,mol
H(+1),54.0569,54.0561,0.0,7.85151e-4
Na(+1),0.539233,0.539215,0.0,1.83129e-5
N(-3),1.34846e-3,1.20291e-3,0.0,1.45541e-4
Ba(+2),2.98551e-4,1.45762e-6,2.97093e-4,3.59576e-16
Ca(+2),0.0170043,0.0170036,0.0,6.98226e-7
Fe(+2),7.16243e-5,1.09641e-7,0.0,7.15146e-5
Mg(+2),7.03559e-3,7.01728e-3,0.0,1.8313e-5
Fe(+3),1.92269e-18,1.72894e-18,0.0,1.93755e-19
O(-2),28.042,27.969,1.18837e-3,0.0718832
Cl(-1),0.579542,0.579526,0.0,1.57577e-5
C(+4),0.500189,0.464409,0.0,0.0357801
S(+4),3.16704e-12,3.16586e-12,0.0,1.17513e-15
S(+6),3.65966e-3,3.34355e-3,2.97093e-4,1.90101e-5
S(-2),4.46906e-6,4.33996e-6,0.0,1.29095e-7

S(+2),2.58663e-10,2.58662e-10,0.0,1.37033e-15
N(+3),4.28032e-56,4.27901e-56,0.0,1.30905e-59
N(+5),1.59979e-73,1.59979e-73,0.0,3.90891e-79
N(0),6.46774e-3,3.88723e-3,0.0,2.58051e-3
H(0),7.19332e-12,7.18316e-12,0.0,1.01633e-14
O(0),1.84138e-63,1.69749e-63,0.0,1.4389e-64
S(+8),1.40861e-54,1.40846e-54,0.0,1.50045e-58
Cl(+1),1.36485e-42,1.36335e-42,0.0,1.50446e-45
Cl(+5),3.76893e-111,3.76852e-111,0.0,4.01465e-115
S(+3),4.06873e-28,4.06869e-28,0.0,3.76057e-33
S(+5),3.2094e-29,3.20937e-29,0.0,2.96633e-34
S(+7),3.05598e-65,3.05595e-65,0.0,2.82453e-70
N(+2),7.66107e-47,6.59795e-47,0.0,1.06312e-47
N(+4),1.61927e-69,1.49375e-69,0.0,1.25516e-70
Cl(+3),3.26841e-85,3.26798e-85,0.0,4.34583e-89
Cl(+4),6.34327e-102,6.33628e-102,0.0,6.99287e-105
N(+1),2.82446e-48,2.67626e-48,0.0,1.48202e-49
N(-2),1.76295e-33,1.74185e-33,0.0,2.10975e-35
C(+2),2.12661e-4,2.12427e-4,0.0,2.34439e-7
Fe(+6),1.62479e-70,1.62477e-70,0.0,1.50173e-75
S(0),1.26959e-15,1.26584e-15,0.0,3.74751e-18
MeO(-1),4.18415e-4,4.18204e-4,0.0,2.1055e-7
N(-1),2.02449e-36,2.00044e-36,0.0,2.4042e-38
TEGION,8.84731e-6,8.8472e-6,0.0,1.08348e-10

Element Distribution

 ,Total,Total,Liquid-1,Solid,Liquid-2
,mol,mole %,% of Total,% of Total,% of Total
H(+1),54.0569,64.5421,99.9985,0.0,1.45245e-3
Na(+1),0.539233,0.643827,99.9966,0.0,3.3961e-3
N(-3),1.34846e-3,1.61001e-3,89.2068,0.0,10.7932
Ba(+2),2.98551e-4,3.5646e-4,0.488232,99.5118,1.2044e-10
Ca(+2),0.0170043,0.0203026,99.9959,0.0,4.10617e-3
Fe(+2),7.16243e-5,8.5517e-5,0.153077,0.0,99.8469
Mg(+2),7.03559e-3,8.40026e-3,99.7397,0.0,0.260291
Fe(+3),1.92269e-18,2.29563e-18,89.9227,0.0,10.0773
O(-2),28.042,33.4813,99.7394,4.23783e-3,0.256341
Cl(-1),0.579542,0.691954,99.9973,0.0,2.719e-3
C(+4),0.500189,0.597209,92.8467,0.0,7.15331
S(+4),3.16704e-12,3.78134e-12,99.9629,0.0,0.0371051
S(+6),3.65966e-3,4.36951e-3,91.3625,8.11806,0.519451
S(-2),4.46906e-6,5.3359e-6,97.1114,0.0,2.88865
S(+2),2.58663e-10,3.08836e-10,99.9995,0.0,5.29774e-4
N(+3),4.28032e-56,5.11056e-56,99.9694,0.0,0.030583
N(+5),1.59979e-73,1.9101e-73,99.9998,0.0,2.44338e-4
N(0),6.46774e-3,7.72227e-3,60.1018,0.0,39.8982
H(0),7.19332e-12,8.58859e-12,99.8587,0.0,0.141288
O(0),1.84138e-63,2.19855e-63,92.1858,0.0,7.81424
S(+8),1.40861e-54,1.68183e-54,99.9893,0.0,0.010652
Cl(+1),1.36485e-42,1.62959e-42,99.8898,0.0,0.110229
Cl(+5),3.76893e-111,4.49997e-111,99.9893,0.0,0.010652
S(+3),4.06873e-28,4.85793e-28,99.9991,0.0,9.24261e-4

S(+5),3.2094e-29,3.83192e-29,99.9991,0.0,9.24261e-4
S(+7),3.05598e-65,3.64874e-65,99.9991,0.0,9.24261e-4
N(+2),7.66107e-47,9.14706e-47,86.1231,0.0,13.8769
N(+4),1.61927e-69,1.93335e-69,92.2486,0.0,7.75141
Cl(+3),3.26841e-85,3.90237e-85,99.9867,0.0,0.0132965
Cl(+4),6.34327e-102,7.57365e-102,99.8898,0.0,0.110241
N(+1),2.82446e-48,3.37232e-48,94.7529,0.0,5.24709
N(-2),1.76295e-33,2.1049e-33,98.8033,0.0,1.19672
C(+2),2.12661e-4,2.5391e-4,99.8898,0.0,0.110241
Fe(+6),1.62479e-70,1.93994e-70,99.9991,0.0,9.24261e-4
S(0),1.26959e-15,1.51585e-15,99.7048,0.0,0.295176
MeO(-1),4.18415e-4,4.99573e-4,99.9497,0.0,0.0503208
N(-1),2.02449e-36,2.41717e-36,98.8124,0.0,1.18756
TEGION,8.84731e-6,1.05634e-5,99.9988,0.0,1.22464e-3

Calculation Summary
06-3 Alloy-1 Calculation

Unit Set: Custom

Automatic Chemistry Model
,Aqueous (H+ ion) Databanks:
,,Corrosion (AQ)
,,Aqueous (H+ ion)
,Second Liquid phase
,Redox selected
,Using K-fit Polynomials
,,T-span: 25.0 - 225.0
,,P-span: 1.0 - 1500.0

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Super13Cr stainless steel

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,48.7309,48.7309
CO2,0.874387,0.874387
BaCl2,3.11264e-6,3.11264e-6
CaCl2,0.0234816,0.0234816
CaO,7.12625e-3,7.12625e-3
FeCl2,1.28924e-4,1.28924e-4
MgCl2,0.0126641,0.0126641
NaCl,0.970620,0.970620
SO3,4.15012e-3,4.15012e-3

BaSO4,5.34279e-4,5.34279e-4
N2,9.84989e-3,9.84989e-3
CO,4.90814e-4,4.90814e-4
O2,2.99526e-5,2.99526e-5
NH3,1.34962e-4,1.34962e-4
CH3OH,8.82125e-5,8.82125e-5
H2S,5.32917e-5,5.32917e-5
SO2,2.08671e-4,2.08671e-4
NO2,1.16889e-4,1.16889e-4
C6H14O4,1.76951e-6,1.76951e-6

Calculated Rates

Corrosion Rate,1.77621e-3,mm/yr
Corrosion Potential,-0.259976,V (SHE)
Repassivation Potential*,-0.134830,V (SHE)
Corrosion Current Density,1.63674e-3,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,50.6349,mol
Temperature,50.0000,°C
Pressure,3398.00,psia

Aqueous Properties
pH,3.58688,
Ionic Strength (x-based),0.0213276,mol/mol
Ionic Strength (m-based),1.25541,mol/kg
ORP,0.0669979,V (SHE)
Osmotic Pressure,1252.66,psia
Specific Electrical Conductivity,1.42831e5,µmho/cm
"Electrical Conductivity, molar",6.98270e-3,m2/ohm-mol
"Viscosity, absolute",0.632254,cP
"Viscosity, relative",1.15540,
Standard Liquid Volume,0.949303,L
"Volume, Std. Conditions",0.928180,L
"Total Dissolved Solids, Estimated",66210.1,mg/L
Hardness,4652.27,mg/L as CaCO3

Solid Properties
Standard Liquid Volume,8.06059e-6,L

Thermodynamic Properties
,Unit,Total,Aqueous,Solid
Density,g/ml,1.05074,1.05063,4.47972

Enthalpy,J,-1.46094e7,-1.46086e7,-786.515

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
Mole (True),51.6730,51.6725,5.34579e-4
Mole (App),50.6348,50.6343,5.34579e-4
,g,g,g
Mass,978.112,977.988,0.124767
,L,L,cm3
Volume,0.930884,0.930856,0.0278516

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,199.137
CaSO4 (Anhydrite),0.0982777,0.107342
CaSO4.2H2O (Gypsum),0.0836203,0.0909770
CaSO4.0.5H2O (Bassanite),0.0330665,0.0360811
NaCl (Halite),0.0143876,0.0142409
NaHCO3 (Nahcolite),3.98701e-3,0.0206322
CaCO3 (Calcite),1.78582e-3,0.0458937
CaCO3 (Aragonite),1.24861e-3,0.0320878
FeCO3 (Siderite),8.66769e-4,0.0229482
Na2SO4 (Thenardite),7.52390e-4,8.22245e-4
FeS2 (Pyrite),2.17884e-4,43260.9
FeS2(marcasite) (Marcasite),6.28069e-5,12470.3
FeS (Pyrrhotite),3.81137e-8,0.0131186
FeS(mackinawite) (Mackinawite),8.91543e-10,3.06867e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Aqueous,Solid
,mol,mol,mol
H2O,48.7276,48.7276,
Cl-1,1.04317,1.04317,
Na+1,0.969316,0.969316,
CO2,0.86843,0.86843,
Ca+2,0.0304743,0.0304743,
Mg+2,0.0121071,0.0121071,
N2,9.86562e-3,9.86562e-3,
HCO3-1,4.64961e-3,4.64961e-3,
SO4-2,3.69739e-3,3.69739e-3,
NaHCO3 (Nahcolite),9.09873e-4,9.09873e-4,0.0
BaSO4 (Barite),5.34579e-4,,5.34579e-4
CO,4.90814e-4,4.90814e-4,

MgHCO3+1,3.96347e-4,3.96347e-4,
NaSO4-1,3.94035e-4,3.94035e-4,
H+1,2.81778e-4,2.81778e-4,
NH4+1,2.19122e-4,2.19122e-4,
MgSO4,1.60628e-4,1.60628e-4,0.0
CaSO4 (Anhydrite),1.32597e-4,1.32597e-4,0.0
Fe+2,1.28766e-4,1.28766e-4,
CH3OH,8.82125e-5,8.82125e-5,
HSO4-1,2.58578e-5,2.58578e-5,
Ba+2,2.07477e-6,2.07477e-6,
C6H14O4,1.76951e-6,1.76951e-6,
NH4SO4-1,1.27044e-6,1.27044e-6,
BaCl(+1),6.96779e-7,6.96779e-7,
CaCl+1,5.03948e-7,5.03948e-7,
CaHCO3+1,3.24032e-7,3.24032e-7,
FeCl+1,1.34231e-7,1.34231e-7,
CaCO3 (Calcite),5.57407e-8,5.57407e-8,0.0
BaHCO3+1,4.12919e-8,4.12919e-8,
FeHCO3+1,2.08819e-8,2.08819e-8,
CO3-2,1.18946e-8,1.18946e-8,
MgCO3 (Magnesite),3.45045e-9,3.45045e-9,0.0
FeCO3 (Siderite),2.40078e-9,2.40078e-9,0.0
NaCO3-1,2.26488e-9,2.26488e-9,
H2S,1.77515e-9,1.77515e-9,
NH3,1.03092e-9,1.03092e-9,
FeOH+1,4.182e-10,4.182e-10,
HCl,3.80714e-10,3.80714e-10,
OH-1,2.99511e-10,2.99511e-10,
MgOH+1,2.40728e-10,2.40728e-10,
FeCl2 (Lawrencite),2.23502e-10,2.23502e-10,0.0
CaOH+1,4.08272e-11,4.08272e-11,
NH2CO2-1,8.14559e-12,8.14559e-12,
HS-1,2.62285e-12,2.62285e-12,
Fe(NH3)+2,1.9278e-12,1.9278e-12,
FeHS+1,1.28045e-12,1.28045e-12,
HSO3-1,8.68671e-13,8.68671e-13,
H2,7.44961e-13,7.44961e-13,
BaCO3 (Witherite),1.94283e-13,1.94283e-13,0.0
S2O3-2,7.88478e-14,7.88478e-14,
NaS2O3-1,4.86899e-14,4.86899e-14,
FeOH+2,2.07848e-14,2.07848e-14,
SO2,1.69598e-14,1.69598e-14,
Fe+3,7.24335e-15,7.24335e-15,
Fe(OH)2+1,2.19083e-15,2.19083e-15,
SO3-2,1.19386e-15,1.19386e-15,
Fe(CO3)2-2,1.13359e-15,1.13359e-15,
FeCl2+1,1.15595e-16,1.15595e-16,
BaOH+1,9.76094e-17,9.76094e-17,
FeCl+2,7.4201e-17,7.4201e-17,
Fe(OH)3 (Bernalite),6.70175e-17,6.70175e-17,0.0
CaCl2 (Hydrophilite),8.52063e-18,8.52063e-18,0.0
FeSO4+1,7.0375e-18,7.0375e-18,
FeCl3 (Molysite),1.76502e-18,1.76502e-18,0.0
Fe(NH3)2+2,1.49521e-19,1.49521e-19,

H2SO4,1.18596e-19,1.18596e-19,
S-2,2.25218e-20,2.25218e-20,
FeCl4-1,1.55052e-20,1.55052e-20,
Fe(OH)4-1,1.52273e-21,1.52273e-21,
S2-2,3.25063e-23,3.25063e-23,
SO3,1.99192e-23,1.99192e-23,
HFeO2-1,2.63609e-24,2.63609e-24,
FeS(HS)-1,3.28207e-25,3.28207e-25,
S3-2,2.04813e-26,2.04813e-26,
Fe(NH3)3+2,3.16155e-27,3.16155e-27,
S2O5-2,6.45447e-29,6.45447e-29,
S2O6-2,1.07984e-29,1.07984e-29,
S4-2,8.06378e-30,8.06378e-30,
S2O4-2,2.48812e-30,2.48812e-30,
Fe2(OH)2+4,7.26671e-31,7.26671e-31,
Na2S2O4,1.06065e-31,1.06065e-31,0.0
S5-2,1.98958e-33,1.98958e-33,
N2H5+1,1.39698e-34,1.39698e-34,
Fe(NH3)4+2,1.27835e-37,1.27835e-37,
N2H4,9.03949e-39,9.03949e-39,
NH2OH,4.0356e-39,4.0356e-39,
S5O6-2,8.52962e-44,8.52962e-44,
NO,8.86584e-46,8.86584e-46,
N2O,3.44413e-47,3.44413e-47,
Fe(NH3)5+2,5.17079e-48,5.17079e-48,
HSO5-1,2.44079e-53,2.44079e-53,
NO2-1,3.13653e-54,3.13653e-54,
HNO2,3.70927e-55,3.70927e-55,
Fe(NH3)6+2,2.09075e-58,2.09075e-58,
O2,7.55471e-62,7.55471e-62,
FeO4-2,8.967e-64,8.967e-64,
S2O8-2,5.68807e-64,5.68807e-64,
NO2,4.98133e-67,4.98133e-67,
NO3-1,9.50598e-71,9.50598e-71,
NaNO3 (Nitratine),1.01578e-71,1.01578e-71,0.0
Ca(NO3)+1,2.23401e-72,2.23401e-72,
NH4NO3 (Gwihabaite),1.39216e-73,1.39216e-73,0.0
HNO3,7.6091e-79,7.6091e-79,
FeNO3+2,1.57767e-87,1.57767e-87,
Total (by phase),51.673,51.6725,5.34579e-4

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Aqueous,Solid
,mol,mol,mol
H(+1),97.4623,97.4623,0.0
Na(+1),0.97062,0.97062,0.0
N(-3),2.20393e-4,2.20393e-4,0.0
Ba(+2),5.37392e-4,2.81284e-6,5.34579e-4
Ca(+2),0.0306078,0.0306078,0.0
Fe(+2),1.28924e-4,1.28924e-4,0.0

Mg(+2),0.0126641,0.0126641,0.0
Fe(+3),3.04846e-14,3.04846e-14,0.0
O(-2),50.5026,50.5004,2.13832e-3
Cl(-1),1.04318,1.04318,0.0
C(+4),0.874387,0.874387,0.0
S(+4),8.86825e-13,8.86825e-13,0.0
S(+6),4.94636e-3,4.41178e-3,5.34579e-4
S(-2),1.77905e-9,1.77905e-9,0.0
S(+2),2.55076e-13,2.55076e-13,0.0
N(+3),3.50746e-54,3.50746e-54,0.0
N(+5),1.07591e-70,1.07591e-70,0.0
N(0),0.0197312,0.0197312,0.0
H(0),1.48992e-12,1.48992e-12,0.0
O(0),1.51094e-61,1.51094e-61,0.0
S(+8),2.44079e-53,2.44079e-53,0.0
S(+3),5.18837e-30,5.18837e-30,0.0
S(+5),2.15967e-29,2.15967e-29,0.0
S(+7),1.13761e-63,1.13761e-63,0.0
N(+2),8.86584e-46,8.86584e-46,0.0
N(+4),4.98133e-67,4.98133e-67,0.0
N(+1),6.88825e-47,6.88825e-47,0.0
N(-2),2.79413e-34,2.79413e-34,0.0
C(+2),4.90814e-4,4.90814e-4,0.0
Fe(+6),8.967e-64,8.967e-64,0.0
S(0),3.25473e-23,3.25473e-23,0.0
N(-1),4.0356e-39,4.0356e-39,0.0
METHANOL,8.82125e-5,8.82125e-5,0.0
TRIETLNGLY,1.76951e-6,1.76951e-6,0.0

Element Distribution

 ,Total,Total,Aqueous,Solid
,mol,mole %,% of Total,% of Total
H(+1),97.4623,64.5777,100.0,0.0
Na(+1),0.97062,0.643125,100.0,0.0
N(-3),2.20393e-4,1.46031e-4,100.0,0.0
Ba(+2),5.37392e-4,3.56071e-4,0.523424,99.4766
Ca(+2),0.0306078,0.0202805,100.0,0.0
Fe(+2),1.28924e-4,8.54238e-5,100.0,0.0
Mg(+2),0.0126641,8.39111e-3,100.0,0.0
Fe(+3),3.04846e-14,2.01989e-14,100.0,0.0
O(-2),50.5026,33.4626,99.9958,4.23407e-3
Cl(-1),1.04318,0.6912,100.0,0.0
C(+4),0.874387,0.579362,100.0,0.0
S(+4),8.86825e-13,5.87603e-13,100.0,0.0
S(+6),4.94636e-3,3.27742e-3,89.1925,10.8075
S(-2),1.77905e-9,1.17878e-9,100.0,0.0
S(+2),2.55076e-13,1.69011e-13,100.0,0.0
N(+3),3.50746e-54,2.32401e-54,100.0,0.0
N(+5),1.07591e-70,7.12889e-71,100.0,0.0
N(0),0.0197312,0.0130738,100.0,0.0
H(0),1.48992e-12,9.87211e-13,100.0,0.0
O(0),1.51094e-61,1.00114e-61,100.0,0.0

S(+8),2.44079e-53,1.61725e-53,100.0,0.0
S(+3),5.18837e-30,3.43777e-30,100.0,0.0
S(+5),2.15967e-29,1.43098e-29,100.0,0.0
S(+7),1.13761e-63,7.53774e-64,100.0,0.0
N(+2),8.86584e-46,5.87443e-46,100.0,0.0
N(+4),4.98133e-67,3.30059e-67,100.0,0.0
N(+1),6.88825e-47,4.5641e-47,100.0,0.0
N(-2),2.79413e-34,1.85137e-34,100.0,0.0
C(+2),4.90814e-4,3.25209e-4,100.0,0.0
Fe(+6),8.967e-64,5.94146e-64,100.0,0.0
S(0),3.25473e-23,2.15656e-23,100.0,0.0
N(-1),4.0356e-39,2.67396e-39,100.0,0.0
METHANOL,8.82125e-5,5.84489e-5,100.0,0.0
TRIETLNGLY,1.76951e-6,1.17247e-6,100.0,0.0

Calculation Summary
06-3 Alloy-4 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2205

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,48.7309,48.7309
CO2,0.874387,0.874387
BaCl2,3.11264e-6,3.11264e-6
CaCl2,0.0234816,0.0234816
CaO,7.12625e-3,7.12625e-3
FeCl2,1.28924e-4,1.28924e-4
MgCl2,0.0126641,0.0126641
NaCl,0.970620,0.970620
SO3,4.15012e-3,4.15012e-3
BaSO4,5.34279e-4,5.34279e-4
N2,9.84989e-3,9.84989e-3

CO,4.90814e-4,4.90814e-4
O2,2.99526e-5,2.99526e-5
NH3,1.34962e-4,1.34962e-4
CH3OH,8.82125e-5,8.82125e-5
H2S,5.32917e-5,5.32917e-5
SO2,2.08671e-4,2.08671e-4
NO2,1.16889e-4,1.16889e-4
C6H14O4,1.76951e-6,1.76951e-6

Calculated Rates

Corrosion Rate,2.51415e-4,mm/yr
Corrosion Potential,-0.242290,V (SHE)
Repassivation Potential*,-0.0148511,V (SHE)
Corrosion Current Density,2.38109e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.2H2O (Gypsum),0.102063
,CaSO4 (Anhydrite),0.119974
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,50.6349,mol
Temperature,50.0000,°C
Pressure,3398.00,psia

Liquid 1 Properties
pH,3.63231,
Ionic Strength (x-based),0.0213036,mol/mol
Ionic Strength (m-based),1.25399,mol/kg
Dielectric Constant,53.5521,
ORP,0.0597411,V (SHE)
Osmotic Pressure,1346.00,psia
Specific Electrical Conductivity,1.41234e5,µmho/cm
"Viscosity, absolute",0.634431,cP
Thermal Conductivity,554.949,cal/hr m °C
Surface Tension,0.0713282,N/m
Standard Liquid Volume,0.949303,L
"Volume, Std. Conditions",0.934470,L
"Total Dissolved Solids, Estimated",66150.8,mg/L
Hardness,4648.24,mg/L as CaCO3

Solid Properties

Standard Liquid Volume,8.04968e-6,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid
Density,g/ml,1.04983,1.04973,4.47972
Enthalpy,J,-1.46113e7,-1.46105e7,-785.149

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
Mole (True),51.6730,51.6725,5.33855e-4
Mole (App),50.6348,50.6343,5.33855e-4
,g,g,g
Mass,978.116,977.991,0.124598
,L,L,cm3
Volume,0.931691,0.931663,0.0278138

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,170.430
H2O,0.579818,0.579814
CaSO4 (Anhydrite),0.119974,0.134225
CaSO4.2H2O (Gypsum),0.102063,0.114186
CaSO4.0.5H2O (Bassanite),0.0339409,0.0379727
CaSO4.0.5H2O (Bassanite),0.0267844,0.0299660
NaCl (Halite),0.0152891,0.0152842
NaCl.2H2O (hydrohalite),9.42891e-3,9.42582e-3
NaHCO3 (Nahcolite),4.17384e-3,4.17145e-3
CaCO3 (Calcite),3.53645e-3,3.52497e-3
CaCO3 (Aragonite),2.73081e-3,2.72194e-3
FeCO3 (Siderite),4.56609e-4,7.19325e-30
Na2SO4 (Thenardite),4.00758e-4,4.49411e-4
Na2SO4.CaSO4 (Glauberite),1.37082e-4,1.71985e-4
Na2SO4.10H2O (Mirabilite),1.32717e-4,1.48821e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
H2O,48.7276,48.7276,0.0
Cl-1,1.04317,1.04317,
Na+1,0.97006,0.97006,
CO2,0.868471,0.868471,
Ca+2,0.0299717,0.0299717,
Mg+2,0.0121041,0.0121041,

N2,9.86564e-3,9.86564e-3,
HCO3-1,5.8002e-3,5.8002e-3,
SO4-2,3.20444e-3,3.20444e-3,
CaSO4 (Anhydrite),6.3494e-4,6.3494e-4,0.0
NaMgSO4+1,5.59872e-4,5.59872e-4,
BaSO4 (Barite),5.33855e-4,,5.33855e-4
CO,4.90814e-4,4.90814e-4,
NH4+1,2.20345e-4,2.20345e-4,
H3O+1,1.38637e-4,1.38637e-4,
FeCO2+2,1.15442e-4,1.15442e-4,
CH3OH,8.8207e-5,8.8207e-5,
Fe+2,1.34725e-5,1.34725e-5,
HSO4-1,1.31595e-5,1.31595e-5,
Ba+2,3.53667e-6,3.53667e-6,
C6H14O4,1.76951e-6,1.76951e-6,
CaCl2 (Hydrophilite),1.04457e-6,1.04457e-6,0.0
CaCO3 (Calcite),1.20352e-7,1.20352e-7,0.0
MgSO4,8.0541e-8,8.0541e-8,0.0
CO3-2,1.65164e-8,1.65164e-8,
FeCl+1,8.44054e-9,8.44054e-9,
MgCO3,6.51207e-9,6.51207e-9,0.0
CaClCH3OH+1,5.49804e-9,5.49804e-9,
H2S,4.01942e-9,4.01942e-9,
Na2SO4.NaHSO4,2.7675e-9,2.7675e-9,0.0
NH4OH,9.83937e-10,9.83937e-10,
FeSO4,4.65821e-10,4.65821e-10,0.0
OH-1,4.26993e-10,4.26993e-10,
NH3,3.49728e-10,3.49728e-10,
MgOH+1,3.2851e-10,3.2851e-10,
CaOH+1,1.91359e-10,1.91359e-10,
FeH(CO3)2-1,7.39869e-11,7.39869e-11,
HCl,3.79781e-11,3.79781e-11,
FeOH+1,3.01543e-11,3.01543e-11,
NH2CO2-1,2.18089e-11,2.18089e-11,
HO(CH2CH2O)3CO2(-1),4.88728e-12,4.88728e-12,
HS-1,4.54125e-12,4.54125e-12,
BaCO3 (Witherite),1.37662e-12,1.37662e-12,0.0
H2,1.21365e-12,1.21365e-12,
MgClCH3OH+1,8.18223e-13,8.18223e-13,
HSO3-1,5.77254e-13,5.77254e-13,
CH5O+1,3.93171e-13,3.93171e-13,
CH3OH.HCl,2.79846e-13,2.79846e-13,
Fe(NH3)+2,1.74362e-13,1.74362e-13,
C6H15O4+1,1.47269e-13,1.47269e-13,
S2O3-2,8.61526e-14,8.61526e-14,
H2SO4,1.4014e-14,1.4014e-14,
SO2,9.93815e-15,9.93815e-15,
BaOH+1,6.12476e-15,6.12476e-15,
FeHS+1,5.33056e-15,5.33056e-15,
FeO+1,2.8642e-15,2.8642e-15,
FeOH+2,1.8451e-15,1.8451e-15,
CH3O-1,1.63356e-15,1.63356e-15,
NaOH,1.29021e-15,1.29021e-15,0.0
FeCl+2,9.15739e-16,9.15739e-16,

SO3-2,8.76036e-16,8.76036e-16,
NaOH.Na2SO4,3.12804e-16,3.12804e-16,
FeS (Pyrrhotite),2.21938e-16,2.21938e-16,0.0
HS2O3-1,2.14658e-16,2.14658e-16,
Fe+3,6.04895e-17,6.04895e-17,
C6H13O4-1,4.33881e-17,4.33881e-17,
HFeO2,1.50146e-17,1.50146e-17,
FeO,5.31438e-18,5.31438e-18,
CO2S,3.72673e-18,3.72673e-18,
S1,2.43708e-18,2.43708e-18,
MgCl2,5.17514e-19,5.17514e-19,0.0
FeCl2+1,2.68483e-19,2.68483e-19,
H2S2O3,2.03889e-19,2.03889e-19,
NaOHCO3-2,1.79086e-19,1.79086e-19,
FeHSO4+2,7.38866e-20,7.38866e-20,
Fe(NH3)2+2,1.8316e-20,1.8316e-20,
S-2,7.21536e-22,7.21536e-22,
S2,1.98261e-22,1.98261e-22,
FeO2-1,7.51506e-23,7.51506e-23,
S2-2,4.13851e-23,4.13851e-23,
HFeO2-1,1.89955e-25,1.89955e-25,
S2O5-2,1.29574e-25,1.29574e-25,
S3-2,3.22845e-26,3.22845e-26,
S3,1.61278e-26,1.61278e-26,
SO3,2.38078e-27,2.38078e-27,
Fe(NH3)3+2,5.2452e-28,5.2452e-28,
S4-2,1.57377e-29,1.57377e-29,
S2O6-2,1.65804e-30,1.65804e-30,
S4,1.31212e-30,1.31212e-30,
S2O4-2,7.30391e-31,7.30391e-31,
Fe2(OH)2+4,3.82247e-32,3.82247e-32,
S5-2,4.80759e-33,4.80759e-33,
N2H5+1,1.15072e-34,1.15072e-34,
S5,1.06756e-34,1.06756e-34,
NH2OH2+1,1.96747e-36,1.96747e-36,
Fe(NH3)4+2,2.87235e-38,2.87235e-38,
NH2OH,1.70374e-38,1.70374e-38,0.0
N2H4,9.04848e-39,9.04848e-39,
S6,8.68619e-39,8.68619e-39,
N2H6+2,7.61981e-39,7.61981e-39,
S8 (Sulfur),9.1532e-40,9.1532e-40,0.0
HClO,5.14752e-42,5.14752e-42,
Cl2,1.39173e-42,1.39173e-42,
S7,7.06443e-43,7.06443e-43,
NH2Cl,4.12712e-43,4.12712e-43,
S5O6-2,3.16842e-44,3.16842e-44,
ClO-1,1.62014e-45,1.62014e-45,
NO,1.07319e-45,1.07319e-45,
N2O,3.58971e-47,3.58971e-47,
Fe(NH3)5+2,1.57355e-48,1.57355e-48,
NH3Cl+1,3.62699e-52,3.62699e-52,
HSO5-1,7.56895e-54,7.56895e-54,
NO2-1,1.66365e-54,1.66365e-54,
HNO2,3.29481e-55,3.29481e-55,

Fe(NH3)6+2,8.617e-59,8.617e-59,
O2,4.47536e-62,4.47536e-62,
S2O8-2,4.54351e-65,4.54351e-65,
FeO4-2,1.83275e-65,1.83275e-65,
NO2,1.31706e-67,1.31706e-67,
NO3-1,4.18975e-71,4.18975e-71,
HNO3,3.43005e-76,3.43005e-76,
NHCl2,3.99867e-79,3.99867e-79,
ClO2-1,1.6538e-83,1.6538e-83,
HClO2,3.43597e-85,3.43597e-85,
NH2Cl2+1,1.47649e-85,1.47649e-85,
NH4NO3.(NH4)2SO4,1.65949e-87,1.65949e-87,0.0
ClO2,5.81909e-100,5.81909e-100,
ClO3-1,1.05096e-108,1.05096e-108,
N2O3,2.25648e-115,2.25648e-115,
NCl3,3.53491e-116,3.53491e-116,
NHCl3+1,7.16909e-120,7.16909e-120,
HNO3(SO3)2,6.85723e-128,6.85723e-128,
Total (by phase),51.673,51.6725,5.33855e-4

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid
,mol,mol,mol
H(+1),97.4623,97.4623,0.0
Na(+1),0.97062,0.97062,0.0
N(-3),2.20346e-4,2.20346e-4,0.0
Ba(+2),5.37392e-4,3.53667e-6,5.33855e-4
Ca(+2),0.0306078,0.0306078,0.0
Fe(+2),1.28924e-4,1.28924e-4,0.0
Mg(+2),0.0126641,0.0126641,0.0
Fe(+3),5.70088e-15,5.70088e-15,0.0
O(-2),50.5026,50.5004,2.13542e-3
Cl(-1),1.04318,1.04318,0.0
C(+4),0.874387,0.874387,0.0
S(+4),5.88068e-13,5.88068e-13,0.0
S(+6),4.94636e-3,4.4125e-3,5.33855e-4
S(-2),4.02397e-9,4.02397e-9,0.0
S(+2),1.72735e-13,1.72735e-13,0.0
N(+3),1.99313e-54,1.99313e-54,0.0
N(+5),4.18978e-71,4.18978e-71,0.0
N(0),0.0197313,0.0197313,0.0
H(0),2.4273e-12,2.4273e-12,0.0
O(0),8.95072e-62,8.95072e-62,0.0
S(+8),7.56895e-54,7.56895e-54,0.0
Cl(+1),6.95358e-42,6.95358e-42,0.0
Cl(+5),1.05096e-108,1.05096e-108,0.0
S(+3),1.46078e-30,1.46078e-30,0.0
S(+5),3.31607e-30,3.31607e-30,0.0
S(+7),9.08702e-65,9.08702e-65,0.0
N(+2),1.07319e-45,1.07319e-45,0.0

N(+4),1.31706e-67,1.31706e-67,0.0
Cl(+3),1.68816e-83,1.68816e-83,0.0
Cl(+4),5.81909e-100,5.81909e-100,0.0
N(+1),7.17942e-47,7.17942e-47,0.0
N(-2),2.30178e-34,2.30178e-34,0.0
C(+2),4.90814e-4,4.90814e-4,0.0
Fe(+6),1.83275e-65,1.83275e-65,0.0
S(0),6.16425e-18,6.16425e-18,0.0
MeO(-1),8.82125e-5,8.82125e-5,0.0
N(-1),1.98451e-36,1.98451e-36,0.0
TEGION,1.76951e-6,1.76951e-6,0.0

Element Distribution

,Total,Total,Liquid-1,Solid
,mol,mole %,% of Total,% of Total
H(+1),97.4623,64.5777,100.0,0.0
Na(+1),0.97062,0.643125,100.0,0.0
N(-3),2.20346e-4,1.46e-4,100.0,0.0
Ba(+2),5.37392e-4,3.56071e-4,0.658119,99.3419
Ca(+2),0.0306078,0.0202805,100.0,0.0
Fe(+2),1.28924e-4,8.54238e-5,100.0,0.0
Mg(+2),0.0126641,8.3911e-3,100.0,0.0
Fe(+3),5.70088e-15,3.77736e-15,100.0,0.0
O(-2),50.5026,33.4626,99.9958,4.22834e-3
Cl(-1),1.04318,0.691199,100.0,0.0
C(+4),0.874387,0.579361,100.0,0.0
S(+4),5.88068e-13,3.89649e-13,100.0,0.0
S(+6),4.94636e-3,3.27741e-3,89.2071,10.7929
S(-2),4.02397e-9,2.66625e-9,100.0,0.0
S(+2),1.72735e-13,1.14453e-13,100.0,0.0
N(+3),1.99313e-54,1.32063e-54,100.0,0.0
N(+5),4.18978e-71,2.77611e-71,100.0,0.0
N(0),0.0197313,0.0130738,100.0,0.0
H(0),2.4273e-12,1.60831e-12,100.0,0.0
O(0),8.95072e-62,5.93067e-62,100.0,0.0
S(+8),7.56895e-54,5.01512e-54,100.0,0.0
Cl(+1),6.95358e-42,4.60739e-42,100.0,0.0
Cl(+5),1.05096e-108,6.96361e-109,100.0,0.0
S(+3),1.46078e-30,9.67902e-31,100.0,0.0
S(+5),3.31607e-30,2.1972e-30,100.0,0.0
S(+7),9.08702e-65,6.02098e-65,100.0,0.0
N(+2),1.07319e-45,7.11086e-46,100.0,0.0
N(+4),1.31706e-67,8.72675e-68,100.0,0.0
Cl(+3),1.68816e-83,1.11856e-83,100.0,0.0
Cl(+4),5.81909e-100,3.85568e-100,100.0,0.0
N(+1),7.17942e-47,4.75702e-47,100.0,0.0
N(-2),2.30178e-34,1.52514e-34,100.0,0.0
C(+2),4.90814e-4,3.25209e-4,100.0,0.0
Fe(+6),1.83275e-65,1.21436e-65,100.0,0.0
S(0),6.16425e-18,4.08438e-18,100.0,0.0
MeO(-1),8.82125e-5,5.84489e-5,100.0,0.0
N(-1),1.98451e-36,1.31492e-36,100.0,0.0

TEGION,1.76951e-6,1.17247e-6,100.0,0.0

Calculation Summary
06-3 Alloy-5 Calculation

Unit Set: Custom

Automatic Chemistry Model
,MSE (H3O+ ion) Databanks:
,,Corrosion (MSE)
,,MSE (H3O+ ion)
,Second Liquid phase
,Redox selected
,Using Helgeson Direct

Single Point
No secondary survey selected

Polarization Curve Range
,Range,,-2.0 to 2.0 V (SHE)
,Step size,0.01 V (SHE)
,No. steps,400

Metal: Stainless steel
,Duplex stainless 2507

Flow Type: Complete Agitation
Scales included - passivating films included.

There are species for which the kinetic data has not been calibrated:

,CH3OH
,SO2
,C6H14O4
,(NH4)2SO3

It is not known if this will affect the calculation accuracy.
,

Stream Inflows
Row Filter Applied: Only Non Zero Values

,Input,Output
Species,mol,mol
H2O,48.7309,48.7309
CO2,0.874387,0.874387
BaCl2,3.11264e-6,3.11264e-6
CaCl2,0.0234816,0.0234816
CaO,7.12625e-3,7.12625e-3
FeCl2,1.28924e-4,1.28924e-4
MgCl2,0.0126641,0.0126641
NaCl,0.970620,0.970620
SO3,4.15012e-3,4.15012e-3
BaSO4,5.34279e-4,5.34279e-4
N2,9.84989e-3,9.84989e-3

CO,4.90814e-4,4.90814e-4
O2,2.99526e-5,2.99526e-5
NH3,1.34962e-4,1.34962e-4
CH3OH,8.82125e-5,8.82125e-5
H2S,5.32917e-5,5.32917e-5
SO2,2.08671e-4,2.08671e-4
NO2,1.16889e-4,1.16889e-4
C6H14O4,1.76951e-6,1.76951e-6

Calculated Rates

Corrosion Rate,2.43919e-4,mm/yr
Corrosion Potential,-0.243899,V (SHE)
Repassivation Potential*,0.125300,V (SHE)
Corrosion Current Density,2.37740e-4,A/sq-m
*Calculated at repassivation current density = 1.0e-2 A/sq-m

,Rate may be reduced because of saturation with the following solids:,

,Species,Scaling Tendency,
,BaSO4 (Barite),1.0

,Rate may ,also be reduced because of substantial saturation indices of:

,Species,Scaling Tendency,
,CaSO4.2H2O (Gypsum),0.102063
,CaSO4 (Anhydrite),0.119974
Stream Parameters
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

Mixture Properties
Stream Amount,50.6349,mol
Temperature,50.0000,°C
Pressure,3398.00,psia

Liquid 1 Properties
pH,3.63231,
Ionic Strength (x-based),0.0213036,mol/mol
Ionic Strength (m-based),1.25399,mol/kg
Dielectric Constant,53.5521,
ORP,0.0597411,V (SHE)
Osmotic Pressure,1346.00,psia
Specific Electrical Conductivity,1.41234e5,µmho/cm
"Viscosity, absolute",0.634431,cP
Thermal Conductivity,554.949,cal/hr m °C
Surface Tension,0.0713282,N/m
Standard Liquid Volume,0.949303,L
"Volume, Std. Conditions",0.934470,L
"Total Dissolved Solids, Estimated",66150.8,mg/L
Hardness,4648.24,mg/L as CaCO3

Solid Properties

Standard Liquid Volume,8.04968e-6,L

Thermodynamic Properties
,Unit,Total,Liquid-1,Solid
Density,g/ml,1.04983,1.04973,4.47972
Enthalpy,J,-1.46113e7,-1.46105e7,-785.149

Total and Phase Flows (Amounts)
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
Mole (True),51.6730,51.6725,5.33855e-4
Mole (App),50.6348,50.6343,5.33855e-4
,g,g,g
Mass,978.116,977.991,0.124598
,L,L,cm3
Volume,0.931691,0.931663,0.0278138

Scaling Tendencies
Row Filter Applied: Values > 1.0e-4

Solids,Post-Scale,Pre-Scale
BaSO4 (Barite),1.00000,170.430
H2O,0.579818,0.579814
CaSO4 (Anhydrite),0.119974,0.134225
CaSO4.2H2O (Gypsum),0.102063,0.114186
CaSO4.0.5H2O (Bassanite),0.0339409,0.0379727
CaSO4.0.5H2O (Bassanite),0.0267844,0.0299660
NaCl (Halite),0.0152891,0.0152842
NaCl.2H2O (hydrohalite),9.42891e-3,9.42582e-3
NaHCO3 (Nahcolite),4.17384e-3,4.17145e-3
CaCO3 (Calcite),3.53645e-3,3.52497e-3
CaCO3 (Aragonite),2.73081e-3,2.72194e-3
FeCO3 (Siderite),4.56609e-4,7.19325e-30
Na2SO4 (Thenardite),4.00758e-4,4.49411e-4
Na2SO4.CaSO4 (Glauberite),1.37082e-4,1.71985e-4
Na2SO4.10H2O (Mirabilite),1.32717e-4,1.48821e-4

Species Output (True Species)
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

,Total,Liquid-1,Solid
,mol,mol,mol
H2O,48.7276,48.7276,0.0
Cl-1,1.04317,1.04317,
Na+1,0.97006,0.97006,
CO2,0.868471,0.868471,
Ca+2,0.0299717,0.0299717,
Mg+2,0.0121041,0.0121041,

N2,9.86564e-3,9.86564e-3,
HCO3-1,5.8002e-3,5.8002e-3,
SO4-2,3.20444e-3,3.20444e-3,
CaSO4 (Anhydrite),6.3494e-4,6.3494e-4,0.0
NaMgSO4+1,5.59872e-4,5.59872e-4,
BaSO4 (Barite),5.33855e-4,,5.33855e-4
CO,4.90814e-4,4.90814e-4,
NH4+1,2.20345e-4,2.20345e-4,
H3O+1,1.38637e-4,1.38637e-4,
FeCO2+2,1.15442e-4,1.15442e-4,
CH3OH,8.8207e-5,8.8207e-5,
Fe+2,1.34725e-5,1.34725e-5,
HSO4-1,1.31595e-5,1.31595e-5,
Ba+2,3.53667e-6,3.53667e-6,
C6H14O4,1.76951e-6,1.76951e-6,
CaCl2 (Hydrophilite),1.04457e-6,1.04457e-6,0.0
CaCO3 (Calcite),1.20352e-7,1.20352e-7,0.0
MgSO4,8.0541e-8,8.0541e-8,0.0
CO3-2,1.65164e-8,1.65164e-8,
FeCl+1,8.44054e-9,8.44054e-9,
MgCO3,6.51207e-9,6.51207e-9,0.0
CaClCH3OH+1,5.49804e-9,5.49804e-9,
H2S,4.01942e-9,4.01942e-9,
Na2SO4.NaHSO4,2.7675e-9,2.7675e-9,0.0
NH4OH,9.83937e-10,9.83937e-10,
FeSO4,4.65821e-10,4.65821e-10,0.0
OH-1,4.26993e-10,4.26993e-10,
NH3,3.49728e-10,3.49728e-10,
MgOH+1,3.2851e-10,3.2851e-10,
CaOH+1,1.91359e-10,1.91359e-10,
FeH(CO3)2-1,7.39869e-11,7.39869e-11,
HCl,3.79781e-11,3.79781e-11,
FeOH+1,3.01543e-11,3.01543e-11,
NH2CO2-1,2.18089e-11,2.18089e-11,
HO(CH2CH2O)3CO2(-1),4.88728e-12,4.88728e-12,
HS-1,4.54125e-12,4.54125e-12,
BaCO3 (Witherite),1.37662e-12,1.37662e-12,0.0
H2,1.21365e-12,1.21365e-12,
MgClCH3OH+1,8.18223e-13,8.18223e-13,
HSO3-1,5.77254e-13,5.77254e-13,
CH5O+1,3.93171e-13,3.93171e-13,
CH3OH.HCl,2.79846e-13,2.79846e-13,
Fe(NH3)+2,1.74362e-13,1.74362e-13,
C6H15O4+1,1.47269e-13,1.47269e-13,
S2O3-2,8.61526e-14,8.61526e-14,
H2SO4,1.4014e-14,1.4014e-14,
SO2,9.93815e-15,9.93815e-15,
BaOH+1,6.12476e-15,6.12476e-15,
FeHS+1,5.33056e-15,5.33056e-15,
FeO+1,2.8642e-15,2.8642e-15,
FeOH+2,1.8451e-15,1.8451e-15,
CH3O-1,1.63356e-15,1.63356e-15,
NaOH,1.29021e-15,1.29021e-15,0.0
FeCl+2,9.15739e-16,9.15739e-16,

SO3-2,8.76036e-16,8.76036e-16,
NaOH.Na2SO4,3.12804e-16,3.12804e-16,
FeS (Pyrrhotite),2.21938e-16,2.21938e-16,0.0
HS2O3-1,2.14658e-16,2.14658e-16,
Fe+3,6.04895e-17,6.04895e-17,
C6H13O4-1,4.33881e-17,4.33881e-17,
HFeO2,1.50146e-17,1.50146e-17,
FeO,5.31438e-18,5.31438e-18,
CO2S,3.72673e-18,3.72673e-18,
S1,2.43708e-18,2.43708e-18,
MgCl2,5.17514e-19,5.17514e-19,0.0
FeCl2+1,2.68483e-19,2.68483e-19,
H2S2O3,2.03889e-19,2.03889e-19,
NaOHCO3-2,1.79086e-19,1.79086e-19,
FeHSO4+2,7.38866e-20,7.38866e-20,
Fe(NH3)2+2,1.8316e-20,1.8316e-20,
S-2,7.21536e-22,7.21536e-22,
S2,1.98261e-22,1.98261e-22,
FeO2-1,7.51506e-23,7.51506e-23,
S2-2,4.13851e-23,4.13851e-23,
HFeO2-1,1.89955e-25,1.89955e-25,
S2O5-2,1.29574e-25,1.29574e-25,
S3-2,3.22845e-26,3.22845e-26,
S3,1.61278e-26,1.61278e-26,
SO3,2.38078e-27,2.38078e-27,
Fe(NH3)3+2,5.2452e-28,5.2452e-28,
S4-2,1.57377e-29,1.57377e-29,
S2O6-2,1.65804e-30,1.65804e-30,
S4,1.31212e-30,1.31212e-30,
S2O4-2,7.30391e-31,7.30391e-31,
Fe2(OH)2+4,3.82247e-32,3.82247e-32,
S5-2,4.80759e-33,4.80759e-33,
N2H5+1,1.15072e-34,1.15072e-34,
S5,1.06756e-34,1.06756e-34,
NH2OH2+1,1.96747e-36,1.96747e-36,
Fe(NH3)4+2,2.87235e-38,2.87235e-38,
NH2OH,1.70374e-38,1.70374e-38,0.0
N2H4,9.04848e-39,9.04848e-39,
S6,8.68619e-39,8.68619e-39,
N2H6+2,7.61981e-39,7.61981e-39,
S8 (Sulfur),9.1532e-40,9.1532e-40,0.0
HClO,5.14752e-42,5.14752e-42,
Cl2,1.39173e-42,1.39173e-42,
S7,7.06443e-43,7.06443e-43,
NH2Cl,4.12712e-43,4.12712e-43,
S5O6-2,3.16842e-44,3.16842e-44,
ClO-1,1.62014e-45,1.62014e-45,
NO,1.07319e-45,1.07319e-45,
N2O,3.58971e-47,3.58971e-47,
Fe(NH3)5+2,1.57355e-48,1.57355e-48,
NH3Cl+1,3.62699e-52,3.62699e-52,
HSO5-1,7.56895e-54,7.56895e-54,
NO2-1,1.66365e-54,1.66365e-54,
HNO2,3.29481e-55,3.29481e-55,

Fe(NH3)6+2,8.617e-59,8.617e-59,
O2,4.47536e-62,4.47536e-62,
S2O8-2,4.54351e-65,4.54351e-65,
FeO4-2,1.83275e-65,1.83275e-65,
NO2,1.31706e-67,1.31706e-67,
NO3-1,4.18975e-71,4.18975e-71,
HNO3,3.43005e-76,3.43005e-76,
NHCl2,3.99867e-79,3.99867e-79,
ClO2-1,1.6538e-83,1.6538e-83,
HClO2,3.43597e-85,3.43597e-85,
NH2Cl2+1,1.47649e-85,1.47649e-85,
NH4NO3.(NH4)2SO4,1.65949e-87,1.65949e-87,0.0
ClO2,5.81909e-100,5.81909e-100,
ClO3-1,1.05096e-108,1.05096e-108,
N2O3,2.25648e-115,2.25648e-115,
NCl3,3.53491e-116,3.53491e-116,
NHCl3+1,7.16909e-120,7.16909e-120,
HNO3(SO3)2,6.85723e-128,6.85723e-128,
Total (by phase),51.673,51.6725,5.33855e-4

Element Balance
Row Filter Applied: Only Non Zero Values
column Filter Applied: Only Non Zero Values

 ,Total,Liquid-1,Solid
,mol,mol,mol
H(+1),97.4623,97.4623,0.0
Na(+1),0.97062,0.97062,0.0
N(-3),2.20346e-4,2.20346e-4,0.0
Ba(+2),5.37392e-4,3.53667e-6,5.33855e-4
Ca(+2),0.0306078,0.0306078,0.0
Fe(+2),1.28924e-4,1.28924e-4,0.0
Mg(+2),0.0126641,0.0126641,0.0
Fe(+3),5.70088e-15,5.70088e-15,0.0
O(-2),50.5026,50.5004,2.13542e-3
Cl(-1),1.04318,1.04318,0.0
C(+4),0.874387,0.874387,0.0
S(+4),5.88068e-13,5.88068e-13,0.0
S(+6),4.94636e-3,4.4125e-3,5.33855e-4
S(-2),4.02397e-9,4.02397e-9,0.0
S(+2),1.72735e-13,1.72735e-13,0.0
N(+3),1.99313e-54,1.99313e-54,0.0
N(+5),4.18978e-71,4.18978e-71,0.0
N(0),0.0197313,0.0197313,0.0
H(0),2.4273e-12,2.4273e-12,0.0
O(0),8.95072e-62,8.95072e-62,0.0
S(+8),7.56895e-54,7.56895e-54,0.0
Cl(+1),6.95358e-42,6.95358e-42,0.0
Cl(+5),1.05096e-108,1.05096e-108,0.0
S(+3),1.46078e-30,1.46078e-30,0.0
S(+5),3.31607e-30,3.31607e-30,0.0
S(+7),9.08702e-65,9.08702e-65,0.0
N(+2),1.07319e-45,1.07319e-45,0.0

N(+4),1.31706e-67,1.31706e-67,0.0
Cl(+3),1.68816e-83,1.68816e-83,0.0
Cl(+4),5.81909e-100,5.81909e-100,0.0
N(+1),7.17942e-47,7.17942e-47,0.0
N(-2),2.30178e-34,2.30178e-34,0.0
C(+2),4.90814e-4,4.90814e-4,0.0
Fe(+6),1.83275e-65,1.83275e-65,0.0
S(0),6.16425e-18,6.16425e-18,0.0
MeO(-1),8.82125e-5,8.82125e-5,0.0
N(-1),1.98451e-36,1.98451e-36,0.0
TEGION,1.76951e-6,1.76951e-6,0.0

Element Distribution

,Total,Total,Liquid-1,Solid
,mol,mole %,% of Total,% of Total
H(+1),97.4623,64.5777,100.0,0.0
Na(+1),0.97062,0.643125,100.0,0.0
N(-3),2.20346e-4,1.46e-4,100.0,0.0
Ba(+2),5.37392e-4,3.56071e-4,0.658119,99.3419
Ca(+2),0.0306078,0.0202805,100.0,0.0
Fe(+2),1.28924e-4,8.54238e-5,100.0,0.0
Mg(+2),0.0126641,8.3911e-3,100.0,0.0
Fe(+3),5.70088e-15,3.77736e-15,100.0,0.0
O(-2),50.5026,33.4626,99.9958,4.22834e-3
Cl(-1),1.04318,0.691199,100.0,0.0
C(+4),0.874387,0.579361,100.0,0.0
S(+4),5.88068e-13,3.89649e-13,100.0,0.0
S(+6),4.94636e-3,3.27741e-3,89.2071,10.7929
S(-2),4.02397e-9,2.66625e-9,100.0,0.0
S(+2),1.72735e-13,1.14453e-13,100.0,0.0
N(+3),1.99313e-54,1.32063e-54,100.0,0.0
N(+5),4.18978e-71,2.77611e-71,100.0,0.0
N(0),0.0197313,0.0130738,100.0,0.0
H(0),2.4273e-12,1.60831e-12,100.0,0.0
O(0),8.95072e-62,5.93067e-62,100.0,0.0
S(+8),7.56895e-54,5.01512e-54,100.0,0.0
Cl(+1),6.95358e-42,4.60739e-42,100.0,0.0
Cl(+5),1.05096e-108,6.96361e-109,100.0,0.0
S(+3),1.46078e-30,9.67902e-31,100.0,0.0
S(+5),3.31607e-30,2.1972e-30,100.0,0.0
S(+7),9.08702e-65,6.02098e-65,100.0,0.0
N(+2),1.07319e-45,7.11086e-46,100.0,0.0
N(+4),1.31706e-67,8.72675e-68,100.0,0.0
Cl(+3),1.68816e-83,1.11856e-83,100.0,0.0
Cl(+4),5.81909e-100,3.85568e-100,100.0,0.0
N(+1),7.17942e-47,4.75702e-47,100.0,0.0
N(-2),2.30178e-34,1.52514e-34,100.0,0.0
C(+2),4.90814e-4,3.25209e-4,100.0,0.0
Fe(+6),1.83275e-65,1.21436e-65,100.0,0.0
S(0),6.16425e-18,4.08438e-18,100.0,0.0
MeO(-1),8.82125e-5,5.84489e-5,100.0,0.0
N(-1),1.98451e-36,1.31492e-36,100.0,0.0

TEGION,1.76951e-6,1.17247e-6,100.0,0.0