

STATE OF WASHINGTON DEPARTMENT OF ECOLOGY 1250 W Alder St • Union Gap, WA 98903-0009 • (509) 575-2490

TECHNICAL MEMO

Assessment of Hydrogen Sulfide Release from Sodium Hydrosulfide Solutions

Holden Mine Water Treatment Plant (MWTP)

Chris Wend, PhD, PE 8-1-2017



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# Summary

The mine water treatment plant located at Holden Mine will utilize a 30% sodium hydrosulfide (NaHS) solution as a source of sulfide for a supplemental metals removal process in the event conditions do not allow the main process to remove metals below the required effluent levels. The possible release of hydrogen sulfide (H<sub>2</sub>S) gas from the bulk solution storage tank has been identified as an issue of concern and this document outlines an analysis of different release scenarios. Only three plausible release scenarios are outlined in this technical memo, largely because the requirements necessary to produce H<sub>2</sub>S gas from the 30% NaHS solution are extremely limiting. Ultimately, there is little support for a release of H<sub>2</sub>S in quantities that would impact offsite (outside MWTP site boundary) receptors (e.g., people at Holden Village).

NOTE: Although this technical memorandum, in outlining release scenarios, finds little risk for a H<sub>2</sub>S release from a 30% NaHS solution to Holden Village, it should not be interpreted as implying that 30% NaHS solution is not dangerous. In all cases, proper safety protocols, and standard operating procedures should be followed. Onsite personnel at the MWTP are most at risk, given their close proximity, and should be properly trained in handling the chemicals present as well as emergency response procedures.

The three plausible H<sub>2</sub>S release scenarios for a 30% NaHS solution that were considered are:

- 1. Rapid contact and mixing with sufficient quantities of a strong (>10 molar) acid, causing the generation of  $H_2S$  gas.
- 2. High solution temperatures. (This scenario could include a fire similar to the 2015 Wolverine Fire at Holden Village).
- 3. Dilution with water in a spill/fire situation. This scenario envisions a spill (perhaps during transport), release from secondary containment to storage pond, or localized fire in the immediate vicinity of the tank.

The results for these release scenarios are summarized below.

1. Rapid contact and mixing with sufficient quantities of a strong acid will cause the production and release of  $H_2S$  gas. However, given the lack of bulk acid at the site, this scenario is not likely.

- 2. High temperatures from a scenario like a long-burning, close proximity fire, could cause the NaHS solution to off-gas H<sub>2</sub>S. However, there are two very important limiting factors:
  - a. The first is the quantity of  $H_2S$  within the NaHS solution, which is a negligible (< 0.0001%) portion of the total sulfide mass in solution. The maximum amount of release would be limited to the quantity of  $H_2S$  in solution only.
  - b. The second limiting factor is heat. First, the temperature required to off-gas  $H_2S$  requires elevating tank temperatures above 80°C which would take a minimum of three days with a consistent, close proximity heat source > 800°C. Although fires can burn for a long time, they tend to move around. Another important point is that the autoignition temperature for  $H_2S$  is 260°C. In a forest fire situation, the  $H_2S$  would oxidize (essentially, burn up into the air).
- 3. Given that water is often the remedy for spills and small fires, this scenario contemplates diluting the solution with water. This would drop the pH, but also dilute the solution, keeping the  $H_2S$  dissolved (in liquid versus gas).

The results of chemical calculations below show that 30% NaHS solution chemistry at pH = 11.5 has very little H<sub>2</sub>S in the solution compared to the total sulfides in solution. There is still, however, sufficient mass of H<sub>2</sub>S to impact onsite receptors. The concentrations were found to be in the following amounts:

$$[H_2S] = 8.8e-6 \quad \frac{moles}{L}$$
$$[HS^-] = 8.6 \quad \frac{moles}{L}$$
$$[S^{2-}] = 1.59 \quad \frac{moles}{L}$$

The solution is strongly basic having been produced with a strong solution of sodium hydroxide greater than  $10 \frac{moles}{L}$ . This prohibits the production of H<sub>2</sub>S from the sulfide species and is why the concentration of H<sub>2</sub>S is so low. The concentration of the H<sub>2</sub>S is well below the solubility of H<sub>2</sub>S even at elevated temperatures which will further restrict releases under elevated temperature conditions.

In conclusion, release of sufficient amounts of  $H_2S$  from the MWTP that might impact offsite receptors does not appear to be possible under the scenarios investigated in this technical memorandum.

# Introduction

As part of the mine water treatment plant design at Holden Mine, there is a final process that will use sulfide addition to remove additional metals if the main process does not meet operating effluent metals concentrations. The main process is lime and flocculant addition followed by aeration to produce metal hydroxides around a neutral pH. The resulting flocs are removed in a high density sludge clarifier. With enough iron oxides and contact time the main process should remove most of the metals. However, with certain conditions created by mixing of groundwater, mine water and flow rates, the addition of sulfide is necessary.

# NaHS Chemistry

The source of sulfide for the mine water treatment plant is a 30% sodium hydrosulfide (NaHS) solution with an anticipated maximum daily usage of 8 gallons. The 30% NaHS solution is a good storage formulation for a sulfide source since the high pH effectively prohibits the formation of the  $H_2S$  species and leaves the sulfide available for reaction with metals in solutions.

#### **General NaHS Information**

NaHS may be produced by dissolving  $H_2S$  in a strong sodium hydroxide solution. The solution is typically available in concentrations ranging from 20-59 % by weight. These solutions have a freezing point between 0 and 80 °F with boiling points ranging from 220 to 260 °F.

The proposed 30% solution will have a freezing point of ~  $0^{\circ}$ F and a boiling point of ~  $235^{\circ}$ F.

Oxygen can react with the sulfide in solution turning the solution yellow to dark green. Weak (3-5%) hydrogen peroxide solution will oxidize the sulfides and can be used to mitigate H<sub>2</sub>S in a spill situation.

A confined head space can accumulate levels of  $H_2S$  gas which has a wide flammable range of 4% to 44% by volume in air.

NaHS is a strong base with a pH between 11.5 and 12.5.

Sources: Wireless Information System for Emergency Responders (WISER) created by the National Library of Medicine. <u>http://wiser.nlm.nih.gov</u>

Version: 5.0.9

Database Version: 5.0.2

and "Technical Guide for Solutions of Sodium Hydrosulfide" TDC, LLC, <u>www.tdc-home.com</u>, 800-422-6274.

## Hydrogen Sulfide Chemistry

 $H_2S$  is a diprotic acid in solution with the following reactions.

$$\begin{split} H_2S + H_2O &\leftrightarrow H^+ + HS^- \qquad pK_1 = 7.04 \\ HS^- + H_2O &\leftrightarrow H^+ + S^{2-} \qquad pK_2 = 11.96 \end{split}$$

Henry's law constant = 9.8 L atm/mole at  $25^{\circ}\text{C}$ 

Note that  $pK_2$  will vary with concentration of NaOH and production conditions pertaining to  $CO_2$  levels and temperature. See Mamrosh, D., Beitler C., Fisher, K., and Stem, S., 2008, "Consider Improved Scrubbing Designs for Acid Gases: Better application of process chemistry enables efficient sulfur abatement", Hydrocarbon Processing, January 2008. www.hydrocarbonprocessing.com

### H<sub>2</sub>S Solubility and Temperature

A temperature increase can reduce the solubility of the  $H_2S$  and release that species but the dissolved phase of  $H_2S$  in a 30% NaHS solution is well below the solubility even at higher temperatures. The following graph was produced using the solubility equation for  $H_2S$  from "Solubility of Selected Gases in Water" by L.H.Geventman. Here the solubility at 100°C (373.15 K) is above 0.0005 (5e-4) mole fraction. The liquid phase mole fraction of the 30% NaHS solution is 1.6e-7 which is well below the solubility (5e-4) at 100°C.

In addition to having concentrations below the maximum solubility, the process will be limited once the concentration has been exhausted since the high pH does not allow for more sulfide to form  $H_2S$  to be available for off-gassing. Also, without agitation of the liquid, the release of gas at the gas-liquid interface will rapidly become diffusion limited on the liquid side and will take many days to fully release the dissolved gas.



# 30% Sodium Hydrosulfide (NaHS) Chemistry

NaHS solutions represent a storage chemistry for sulfide via strong base solutions such as sodium hydroxide (NaOH). To determine the chemistry of a 30% by weight solution of NaHS produced with NaOH, it was useful to perform chemical equilibrium calculations for solutions with pH = 11.5 and pH = 12.5. This pH range is described in a typical safety data sheet (SDS) for NaHS solutions.

Preliminary chemical equilibrium modeling was performed using PHREEQC Version 3.0 by USGS. Documentation and computer programs may be downloaded at the link below. All output with input conditions are in Appendices A and B.

https://wwwbrr.cr.usgs.gov/projects/GWC\_coupled/phreeqc/

The purpose of the modeling was to

- 1. Understand sodium and sulfide solution chemistry of a 30% by weight NaHS solution at a pH of 11.5 to 12.5.
- 2. Develop a preliminary estimate of species distribution due to temperature increase.

3. Develop a preliminary estimate of species distribution as the solution is diluted and pH approaches 7.0.

The tables below summarize the results for the conditions in the tank. The 30% NaHS solution volume was assumed to be 14,939 L (3946.5 gal). This is based upon a 4385 gallon tank capacity at 90% fill. The 4385 gallon tank capacity is described in subsection 2.9A.1.1 Sulfide Reagent Storage System of section 2.9A System 900A – Sulfide Reagent Storage and Feed in Operating and Maintenance Manual Mine Water Treatment Plant, Holden Mine, March 2016.

рН	11.5		
Species	mole/L	Mole Fraction	Total Moles
H2S	8.88E-06	1.60E-07	1.33E-01
HS-	8.36E+00	1.51E-01	1.25E+05
S2-	1.59E+00	2.87E-02	2.38E+04
рН	12.5		
Species	mole/L	Mole Fraction	Total Moles
H2S	5.80E-08	1.05E-09	8.67E-04
HS-	3.72E+00	6.70E-02	5.56E+04
S2-	7.45E+00	1.34E-01	1.11E+05

The model calculations also estimated that the solution would be a strong base equivalent to a 12 molar NaOH solution for pH of 11.5 and a 19 molar NaOH solution for a pH of 12.5.

As can be seen from the mole fraction calculations, the mass of sulfide as  $H_2S$  in solution is negligible compared to the total mass of sulfide in the system. There is, however, sufficient mass in this state to produce a gas phase concentration in a head space that would present a risk to nearby workers (onsite receptors). There is not, however, sufficient mass to produce a plume to threaten offsite receptors.

See appendix B for complete model input and output for chemical speciation and other physical parameters of a pH = 11.5, 30% NaHS solution that is diluted with water through 3 orders of magnitude. It is important to note here that PHREEQC performs solution mixing on a mass basis. Hence the dilution reported in the table is on a mass basis and when converted to a volume basis it is not direct due to changes in fluid density. The table below summarizes the results of the dilutions.

					Total Volu	ume
Species	Dilution	mole/L	Total Moles	рН	Liters	Gallons
H2S	0	8.88E-06	1.33E-01	11.5	14939	3946.5
HS-	0	8.36E+00	1.25E+05	11.5	14939	3946.5
S2-	0	1.59E+00	2.38E+04	11.5	14939	3946.5
H2S	1.00E-01	6.67E-06	9.96E-01	11.616	1.49E+05	39465
HS-	1.00E-01	6.99E-01	1.04E+05	11.616	1.49E+05	39465
S2-	1.00E-01	1.21E-01	1.80E+04	11.616	1.49E+05	39465
H2S	1.00E-02	1.69E-06	2.52E+00	11.455	1.49E+06	394650
HS-	1.00E-02	7.42E-02	1.11E+05	11.455	1.49E+06	394650
S2-	1.00E-02	5.22E-03	7.79E+03	11.455	1.49E+06	394650
H2S	1.00E-03	1.82E-05	2.72E+02	9.515	1.49E+07	3946500
HS-	1.00E-03	7.73E-03	1.15E+05	9.515	1.49E+07	3946500
S2-	1.00E-03	4.29E-06	6.41E+01	9.515	1.49E+07	3946500

Here it can be seen that diluting the mass with 100 times the original mass in water does not change the pH much but does lower the corresponding concentrations as would be expected. The total moles of sulfide change slightly as sulfate species are in play with the dilution.

This also demonstrates the strength of the high pH solution and the need for a strong acid (> 10 molar) to affect pH with a comparable volume.

# Heat Transfer

Heat transfer calculations were performed to estimate energy and time requirements needed to increase the temperature of the tank. In the specifications found on page 63 section 2.9A.1.1 of the Operating and Maintenance Manual, Mine Water Treatment Plant, Holden Mine, Revision 0, March 2016, the tank has a factory-applied spray-on foam insulation polyurethane foam with a minimum "R" value of 6.3/inch.

The tank dimensions are also listed here as 10 feet 2.5 inches in diameter and a height of 10 feet. From this the radius can be calculated to be 155.6 cm and the height is 304.8 cm. Top surface area is 7.6e4 cm<sup>2</sup> and the lateral surface area is 2.98e5 cm<sup>2</sup>. For this analysis it was assumed that the top of the tank contributes to the heat transfer at the same rate as the lateral sides. This is conservative since the top will have some head space between the top of the tank and the liquid which would provide an additional heat transfer resistance to the calculation. The total surface area is estimated to be 3.74e5 cm<sup>2</sup>.

The standard heat transfer equation can be written below as

$$q = UA\Delta T$$

Where

$$q = heat \ transfer \ rate \ (watts, W)$$
$$U = overall \ coefficient \ of \ heat \ transfer \ \left(\frac{W}{m^2 K}\right)$$
$$A = area \ (m^2)$$
$$T = absolute \ temperature \ (K)$$

## **Insulated Tank**

 $R_{US}$  in US units is equal to 5.678 times  $R_{SI}$  in SI units which yields  $R_{SI} = 2.22$  using the R value reported above and assuming 2 inches of insulation. Assuming a wildfire with a temperature of  $800^{\circ}$  C = 1073K and assuming a beginning temperature of  $20^{\circ}$ C = 293K yields  $\Delta$ T = 780K. With a surface area of 3.74e5 cm<sup>2</sup> = 37.4 m<sup>2</sup> the resulting heat transfer rate is 13,141 W.

The specific heat capacity for a 30% solution of NaOH ranges from about 0.84 to 0.88  $\frac{cal}{g^{\circ}c}$ . Using a middle value of 0.86  $\frac{cal}{g^{\circ}c}$  and a density of 1.25 g/L for a 30% NaHS solution yields a specific heat capacity of 4.5  $\frac{J}{mL^{\circ}c}$ . To raise the temperature of 14,939L (tank capacity) of 30% NaHS from 20°C to 80°C will require 4.0033x10° J. With the calculated 13,141W heat transfer rate it will take approximately 3.5 days to raise the temperature 60°C from 20°C to 80°C.

# **Uninsulated Tank**

There is one more thing to consider with this scenario. Application of such an intense external heat source will consume the externally applied polyurethane foam insulation since the polyurethane foam will decompose above 180°C and has a flash ignition point of between 315°C and 370°C and an autoignition point between 370°C and 427°C.

Without the insulation the tank material will be the only heat transfer material to consider. Note that this was neglected in the insulated tank calculation above making the time estimate conservative. R values were difficult to obtain for cross-linked high density polyethylene and a fiberglass sheet value of  $R_{US} = 2.5/in$  was selected. Assuming a tank wall thickness of 0.5 in. an  $R_{SI} = 0.22$  was calculated. The resulting heat transfer rate was found to be 1.3e5 W which corresponds to an 8.6 hour heat up period to 80°C.

The difficulty with both of the above scenarios is that cross-linked high density polyethylene is not rated for use above  $60^{\circ}$ C to  $65^{\circ}$ C. At some point the tank will fail and the contents will flow into the secondary containment which is concrete on the ground. This will essentially stop the heating process since the secondary containment will provide adequate heat transfer to the ground to prevent additional temperature increases.

## **Mass Transfer**

Mass transfer describes the movement of the constituent of concern in liquid and gas phases and across the gas-liquid interface. In this discussion the transport of  $H_2S$  in the liquid phase will be examined. With no mixing only diffusion processes will be considered. This will be a limiting case since in many situations there may be advection as well such as convective currents during a heating process.

#### Fourier Number

The liquid side mass transfer resistance was investigated through a quick check with the Fourier number. When mass transfer has gone on for a sufficient amount of time the process approaches equilibrium and the Fourier number is approximately equal to one.

$$1 = \frac{z^{2}}{\sqrt{Dt}}$$

$$z = length (cm)$$

$$\mathcal{D} = diffusion \ coefficient \ \left(\frac{cm^{2}}{sec}\right)$$

$$t = time \ (sec)$$

From this equation a time to diffuse to a certain depth or the depth of diffusion for a given time may be estimated. The Fourier number indicates 6 months to go 17.6 cm or 16 years to go 100 cm for diffusion in water.

### **Diffusion Models**

Two models were also investigated to determine  $H_2S$  mass transport in the liquid phase. One was diffusion into a semi-infinite domain which represents unsteady diffusion and the other was decay of a pulse. Both of these models give some indication of the diffusion transport speed in solution. The comparison of these models to the tank situation is based upon the hypothesis that when the upper layer near the gas-liquid interface is depleted of  $H_2S$ , the diffusion from the lower volume will proceed at a rate similar to those estimated in these models for a semi-infinite domain.

See the following sections for a description of the partial differential equation, boundary conditions, and analytical solution. Computer script for the output was written in language that can be run in Matlab or Octave. See Appendix C for a copy of the scripts.

#### Semi-infinite

The partial differential equation along with the appropriate spatial and temporal boundary conditions is listed below. For the semi-infinite case, the following graph shows the concentration of  $H_2S$  versus depth for various times up to 190 years. Two of these profiles were selected and were used to predict a velocity of the front where there is zero concentration. See the second graph. This velocity was calculated to be 0.18 cm/day.

$$\frac{\partial c}{\partial t} = \mathcal{D} \frac{\partial^2 c}{\partial z^2}$$

$$c(z,0) = c_{\infty} = 0 \text{ where } z \in [0,\infty)$$

$$c(0,t) = c_{\circ} \text{ where } t \in (0,\infty)$$

$$c(\infty,t) = c_{\infty} = 0 \text{ where } t > 0$$

$$c(z,t) = c_{\circ} - c_{\circ} erf\left(\frac{z}{\sqrt{4\mathcal{D}t}}\right) = c_{\circ} erfc\left(\frac{z}{\sqrt{4\mathcal{D}t}}\right)$$

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_{0}^{x} e^{-s^2} ds$$

$$erfc(x) = 1 - erf(x)$$

c(z,t) = concentration as a function of position and time

$$z = length (cm)$$
$$\mathcal{D} = diffusion \ coefficient \left(\frac{cm^2}{sec}\right)$$
$$t = time \ (sec)$$





#### Pulse Decay Model

Using the pulse decay model, the profiles from selected times ranging from 134 to 6944 days are graphed. From this graph two profiles were selected to calculate a velocity for the diffusion front. See the second graph. The velocity was found to be about 0.25 cm/day.

$$\frac{\partial c}{\partial t} = \mathcal{D} \frac{\partial^2 c}{\partial z^2}$$

$$c(\infty, t) = c_{\infty} = 0 \text{ where } t > 0$$

$$c(0,0) = \frac{M}{A} \delta(z)$$

$$\frac{\partial c}{\partial z}\Big|_{z=0} \text{ where } t > 0$$

$$c(z,t) = \frac{\frac{M}{A}}{\sqrt{4\pi \mathcal{D}}} e^{\frac{-z^2}{4\pi \mathcal{D}}}$$

$$\delta(z) = \text{Dirac delta function}$$

$$M = \text{total mass}$$

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$$A = cross - sectional area for diffusion$$

$$c(z,t) = concentration as a function of position and time$$

$$z = length (cm)$$

$$\mathcal{D} = diffusion coefficient \left(\frac{cm^2}{sec}\right)$$

$$t = time (sec)$$





### **Plume Model**

To examine the threat from the  $H_2S$  in a 30% NaHS solution at pH = 11.5, the total amount of dissolved  $H_2S$  was assumed to be instantaneously released. It should be noted here that the previous section demonstrates that this is not likely.

The Pasquil-Gifford puff model in one dimension was used to determine downwind concentrations. A 12 m/s wind with stable (little mixing) condition was selected. The dispersion coefficients were derived from a linear regression of the figures 8.8 and 8.9 pages 416 and 417 found in *Air Pollution* Control by Cooper and Alley. See Appendix D for the script used to generate the graphs below.

$$C(x,t) = \frac{Q_m}{\sqrt{2}\pi^{2/3}\sigma_x\sigma_y\sigma_z} e^{\left\{-\frac{1}{2}\left[\left(\frac{x-ut}{\sigma_x}\right)^2\right]\right\}}$$

$$C(x,t) = concentration \left(\frac{mg}{m^3}\right)$$
  
$$\sigma_x = \sigma_y = 9.44x + 1.5 (x in km)$$
  
$$\sigma_z = 3.2z + 0.75 (z in km)$$

The graph below shows the concentration profile at 1500m with a maximum concentration of less than 0.5ppm. This concentration is less than the threshold value for an 8 hour time weighted average of 1ppm.



Plume after 125 seconds with 12 m/s wind (IDLH 100 ppm)

For the onsite exposure situation, the release will be below the IDLH within 200m of the release which will occur in less than 10 seconds. See the following graph.



#### Plume after 9 seconds with 12 m/s wind (IDLH 100 ppm)

### Discussion

Using the understanding of species distribution from the NaHS chemistry section, estimates of release mass and rate under changes in condition could be considered. The case with strong acid was not considered since there is no source for this at the site.

For a 30% by weight NaHS solution at a pH of 11.5, there will be approximately 8.88e-6  $\frac{\text{moles}}{L}$  of H<sub>2</sub>S in solution while there are 9.95  $\frac{\text{moles}}{L}$  of sulfide in solution. With the given Henry's Law constant a concentration of 87 ppm is estimated for a closed headspace such as the storage tank. The total mass of H<sub>2</sub>S available in the tank is 0.133 moles H<sub>2</sub>S or 5.42 g H<sub>2</sub>S. The volume of air needed to dilute this amount down to the IDLH of 100ppm is approximately 35m<sup>3</sup> (46 yd<sup>3</sup> or 10,000gal). This volume would not have sufficient radius to reach the boundaries of the plant site.

The ability to release this total amount in a reasonable time frame such as an hour is not feasible due to liquid side mass transfer resistance. Diffusion times for a meter below the surface can be on the order of years if no advection is present.

Heating the tank will not be successful in releasing this amount very fast either since the heating time to raise the tank temperature from 20°C to 80°C using an 800° C heat source is more than 3 days. In addition, the solubility of H<sub>2</sub>S is  $3.74 \frac{g}{L}$  at 21°C while the concentration of H<sub>2</sub>S in the 30% solution is  $3e-4 \frac{g}{L}$  at 21°C which means there is little chance that the solution will become supersaturated.

NaHS solutions may also be a byproduct of caustic scrubbers in the oil industry where  $H_2S$  removal occurs using the caustic solutions at temperatures as high as 100°C. This helps illustrate the robustness of the solution as an absorbent of  $H_2S$  and storage chemistry of sulfides.

Release scenarios 2 and 3 may both have localized releases that are close to the IDLH (100ppm) for near tank workers exposed to the head space of a closed tank but the majority of the sulfide will remain in solution as  $HS^-$  and  $S^{2-}$  and cannot be released as  $H_2S$ . An analysis of the chemistry of the NaHS solution reveals that under conditions that lower the pH either by strong acid addition or dilution it will retain greater than 90% of sulfide in solution until pH drops below 7. In the event of lower pH from dilution, the volume of water necessary to reduce the pH will allow for any  $H_2S$  produced to remain in solution. Also, any production of  $H_2S$  from sulfides will result in the consumption of  $H^+$  which will raise the pH slowing the production, and subsequent release, of  $H_2S$ . This significantly reduces the mass of  $H_2S$  that can be produced and there is little threat to offsite receptors.

Under release scenario 2, heat transfer calculations indicate that there is a period of days needed to raise the temperature of the tank contents to sufficient levels required for off-gassing of H<sub>2</sub>S. The total amount of H<sub>2</sub>S that could off-gas would be less than 6 grams which would impact at most 35 cubic meters (1236 cubic feet) of local air space before being diluted below the IDLH of 100ppm. In the absence of mixing or significant convective currents in the liquid phase, diffusional mass transfer on the liquid side of the gas-liquid interface will limit release due to liquid side mass transfer limitations. This will further reduce the release rate of any dissolved  $H_2S$ .

A 30% solution of sodium hydrosulfide (NaHS) can only release large amounts of  $H_2S$  gas if mixed with sufficient amounts of a strong acid. Other release scenarios such as heating will take much longer (on the order of days for the insulated tank) and in the case of open flame or high temperature any produced  $H_2S$  gas will autoignite at 260° C. With the absence of acid at the plant, the use of NaHS is considered safe from this scenario. In the event of an accidental release such as an accident during transport, the main threat to emergency responders is from the high pH since the 30% solution is also greater than a 10 molar sodium hydroxide solution and represents a strong base. Emergency response would follow accepted guidelines for NaHS spills as outlined by a standard SDS or more specific instructions from the manufacturer. Residual reactive sulfides can be oxidized with a weak (3-5%) hydrogen peroxide solution. This will prevent further generation of  $H_2S$  from the solution but the amount of hydrogen peroxide to sulfide needs to be at a 4:1 molar ratio. This would require 27L of 5% hydrogen peroxide for every liter of 30% NaHS.

If an emergency scenario includes excess water such as from firefighting, drainage of secondary contaiment to the storage pond, or release to the lake, the dilution of the 30% solution is sufficient to maintain the hydrogen sulfide in solution as the pH drops. While  $H_2S$  is of concern for emergency response personnel on the scene, the development of a significant plume that can affect offsite receptors is unlikely to occur.

# Conclusions

The three plausible H<sub>2</sub>S release scenarios for a 30% NaHS solution that were considered are:

- 1. Rapid contact and mixing with sufficient quantities of a strong (>10 molar) acid, causing the generation of  $H_2S$  gas.
- 2. High solution temperatures. (This scenario could include a fire similar to the 2015 Wolverine Fire at Holden Village).
- 3. Dilution with water in a spill/fire situation. This scenario envisions a spill (perhaps during transport), release from secondary containment to storage pond, or localized fire in the immediate vicinity of the tank.

The results for these release scenarios are summarized below.

- 1. Rapid contact and mixing with sufficient quantities of a strong acid will cause the production and release of  $H_2S$  gas. However, given the lack of bulk acid at the site, this scenario is not likely.
- 2. High temperatures from a scenario like a long-burning, close proximity fire, could cause the NaHS solution to off-gas H<sub>2</sub>S. However, there are two very important limiting factors:
  - a. The first is the quantity of  $H_2S$  within the NaHS solution, which is a negligible (< 0.0001%) portion of the total sulfide mass in solution. The maximum amount of release would be limited to the quantity of  $H_2S$  in solution only.

- b. The second limiting factor is heat. First, the temperature required to off-gas  $H_2S$  requires elevating tank temperatures above 80°C which would take a minimum of three days with a consistent, close proximity heat source > 800°C. Although fires can burn for a long time, they tend to move around. Another important point is that the autoignition temperature for  $H_2S$  is 260°C. In a forest fire situation, the  $H_2S$  would oxidize (essentially, burn up into the air).
- 3. Given that water is often the remedy for spills and small fires, this scenario contemplates diluting the solution with water. This would drop the pH, but also dilute the solution, keeping the H<sub>2</sub>S dissolved (in liquid versus gas).

The results of chemical calculations below show that 30% NaHS solution chemistry at pH = 11.5 has very little H<sub>2</sub>S in the solution compared to the total sulfides in solution. There is still, however, sufficient mass of H<sub>2</sub>S to impact onsite receptors. The concentrations were found to be in the following amounts:

$$[H_2S] = 8.8e-6 \frac{moles}{L}$$
  
 $[HS^-] = 8.6 \frac{moles}{L}$   
 $[S^{2-}] = 1.59 \frac{moles}{L}$ 

The solution is strongly basic having been produced with a strong solution of sodium hydroxide greater than  $10 \frac{moles}{L}$ . This prohibits the production of H<sub>2</sub>S from the sulfide species and is why the concentration of H<sub>2</sub>S is so low. The concentration of the H<sub>2</sub>S is well below the solubility of H<sub>2</sub>S even at elevated temperatures which will further restrict releases under elevated temperature conditions.

Heat transfer calculations were performed on the tank with the specified insulation. The results reveal that to raise the tank temperature to  $80^{\circ}$ C from  $20^{\circ}$ C with an  $800^{\circ}$ C external heat source it will take more than 3 days. During this time, any H<sub>2</sub>S that would escape will oxidize since the autoignition temperature for H<sub>2</sub>S is  $260^{\circ}$ C.

Calculations and models were examined to estimate liquid mass transport of H<sub>2</sub>S in solution. Results indicate that if conditions are quiescent the release of gas phase H<sub>2</sub>S will be reduced quickly due to diffusional resistance to H<sub>2</sub>S transport in the liquid phase. Estimates from the Fourier number indicate that only the top 20 cm of the tank would be depleted of H<sub>2</sub>S in 6 months. More detailed analyses indicate a transport velocity of 0.18 to  $0.25 \frac{cm}{day}$  in the liquid phase. All of this demonstrates the inability of the 30% NaHS solution to release the amount of H<sub>2</sub>S in solution instantaneously. A puff release model was evaluated to consider whether the mass of  $H_2S$  in solution could impact offsite receptors if all of it could be released at once (which is not plausible). The results show with a strong wind and stable conditions that the concentrations will be below the 100 ppm IDLH limit within 200m of the tank. With no wind or air movement, the amount of  $H_2S$  that could theoretically be released could not occupy a volume of air greater than 35 m<sup>3</sup> and still be above the IDLH of 100ppm.

The assumptions and calculations in this document attempt to provide a conservative estimate for the production and transport of hydrogren sulfide in a 30% sodium hydrosulfide solution. More rigorous calculations could be investigated, however the results indicating limited production of hydrogen sulfide from the sulfide solution and minimal release to the gas phase are unlikely to change.

In conclusion, release of sufficient amounts of  $H_2S$  from the MWTP that might impact offsite receptors does not appear to be possible under the scenarios investigated in this technical memorandum.

NOTE: Although this technical memorandum, in outlining release scenarios, finds little risk for a H<sub>2</sub>S release from a 30% NaHS solution to Holden Village, it should not be interpreted as implying that 30% NaHS solution is not dangerous. In all cases, proper safety protocols, and standard operating procedures should be followed. Onsite personnel at the MWTP are most at risk, given their close proximity, and should be properly trained in handling the chemicals present as well as emergency response procedures.

# References

Cooper, D. C., and Alley, F.C., 2002. Air Pollution Control (3rd Edition). Waveland Press.

Cussler, E. L., 1997. *Diffusion Mass Transfer in Fluid Systems*, 2<sup>nd</sup> Edition, Cambridge University Press.

Gevantman, L. H., *Solubility of Selected Gases in Water*. https://sites.chem.colostate.edu/diverdi/all\_courses/CRC%20reference%20data/solubility%20of %20gases%20in%20water.pdf

Lindeburg, Michael R. 1992. *Engineer-in-Training Reference Manual*. Professional Publications, Inc. Belmont, CA.

Mamrosh, D., Beitler, C., Fisher, K., and Stem, S., 2008. *Consider Improved Scrubbing Designs for Acid Gases: Better application of process chemistry enables efficient sulfur abatement.* Hydrocarbon Processing, January 2008, Pages 69-74. Gulf Publishing Company.

Operating and Maintenance Manual, Mine Water Treatment Plant, Holden Mine, Revision 0, March 2016

Perry, Robert H., 1997. *Perry's Chemical Engineers' Handbook* 7<sup>th</sup> Edition. The McGraw-Hill Companies, Inc.

TDC, LLC. *Technical Guide for Solutions of Sodium Hydrosulfide*. TDC a Genesis Energy Company, 1916 Farmerville Highway, Ruston, Louisiana, 71270. <u>www.tdc-home.com</u>.

Appendix A: 30% NaHS PHREEQC model results

#### pH 11.5

```
C:\get\usgs\phreeqc\work\holden\nahs\nahs_ph_11_5.out
                                                                                  1
       Input file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs ph 11 5
   3
       Output file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs ph 11 5.out
   4
       Database file: /home/cwend/get/usgs/phreeqc/phreeqc-3.3.5-10806/database/phreeqc.dat
   5
   6
   7
   8
      Initializing...
   9
  10
      End of Run after 0 Seconds.
  11
  12
          EXCHANGE MASTER SPECIES
  13
          EXCHANGE SPECIES
  14
          SURFACE MASTER SPECIES
  15
          SURFACE SPECIES
  16
          RATES
  17
          END
  18
         _____
                _____
  19
      Reading input data for simulation 1.
  20
        21
  22
          TITLE Sodium hydrosulfide equilibrium test.
  23
          SOLUTION 1 Tank Contents of 30% sodium hydrosulfide solution
  24
              pH 11.5 #charge
  25
                 density 1.3
  26
                        25.0
                 temp
  27
                 redox 0(0)/0(-2)
  28
                                 1.103e+04 charge
                 Na
  29
                                7.95e+3 #charge
                S(-2)
  30
              С
                      1e+02
  31
                 0(0)
                                 7
                                     02(g) -0.7
          SOLUTION MASTER_SPECIES
  32
          SOLUTION SPECIES
  33
  34
          EQUILIBRIUM PHASES 1
  35
         END
  36
       ____
  37
       TITLE
  38
       ----
  39
  40
       Sodium hydrosulfide equilibrium test.
  41
  42
       43
       Beginning of initial solution calculations.
  44
       _____
                   45
  46
       Initial solution 1. Tank Contents of 30% sodium hydrosulfide solution
  47
       -----Solution composition-----
  48
  49
  50
          Elements
                           Molality
                                        Moles
  51
  52
          С
                          1.000e-01
                                     1.000e-01
  53
          Na
                          9.423e+00
                                     9.423e+00
                                              Charge balance
                          4.419e-05
          0(0)
  54
                                     4.419e-05 Equilibrium with O2(g)
  55
          S(-2)
                          7.950e+00
                                     7.950e+00
  56
  57
       -----Description of solution-----
  58
  59
                                          pH = 11.500
                                          pe = 4.000
  60
  61
            Specific Conductance (µS/cm, 25°C)
                                             = 504414
  62
                                             = 1.25224
                             Density (g/cm<sup>3</sup>)
  63
                                  Volume (L) =
                                                1.18537
  64
                            Activity of water = 0.704
```

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Percent err	Mass o Total alkali: Total Temp Electrical 1 or, 100*(Cat- An	<pre>hic strength f water (kg) nity (eq/kg) CO2 (mol/kg) erature (°C) balance (eq) )/(Cat+ An ) Iterations Total F</pre>	$\begin{array}{rcl} & = & 1.06 \\ & = & 1.00 \\ & = & 9.42 \\ & = & 1.00 \\ & = & 25.00 \\ & = & 6.19 \\ & = & 0.00 \\ & = & 7 \\ H & = & 1.1769 \\ H & = & 1.0769 \end{array}$	3e+01 0e+00 3e+00 0e-01 8e-11 93e+02		
		Total C	) = 5.5811	31e+01		
Bedox co		Kedox co	ouples			
0(-2)/0(	0) 9.19	80 0 54	141			
	D	istribution	of openion			
	D	istribution	of species			
Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole cm³/mo
OH-	5.048e-03	2.254e-03	-2.297	-2.647	-0.350	10.5
H+ -	4.532e-12	3.162e-12	-11.344	-11.500	-0.156	0.0
H2O	5.551e+01	7.042e-01	1.744	-0.152	0.000	18.0
C(-4)	0.000e+00	0 000+00	-150 788	-1/9 725	1 063	35 /
C(4)	1.000e-01	0.00000000	100.700	-149.725	1.005	55.4
NaCO3-	7.899e-02	1.362e+00	-1.102	0.134	1.237	51.9
CO3-2	2.051e-02	2.145e-03	-1.688	-2.669	-0.981	11.9
HCO3-	2.544e-04	1.446e-04	-3.595	-3.840	-0.245	52.2
NaHCO3	2.397e-04	2.774e-03	-3.620	-2.557	1.063	1.8
C02	1.262e-10	1.460e-09	-9.899	-8.836	1.063	34.4
(CO2)2	3.384e-21	3.915e-20	-20.471	-19.407	1.063	68.8
H(U)	0.000e+00	0.0000+00	-45 600	-11 516	1 0.62	20
Na	9.423e+00	0.000000000	-45.609	-44.540	1.065	20.0
Na+	9.344e+00	3.410e+01	0.971	1.533	0.562	2.1
NaCO3-	7.899e-02	1.362e+00	-1.102	0.134	1.237	51.9
NaHCO3	2.397e-04	2.774e-03	-3.620	-2.557	1.063	1.8
NaOH	6.644e-13	7.686e-12	-12.178	-11.114	1.063	(0)
0(0)	4.419e-05					
02	2.209e-05	2.556e-04	-4.656	-3.592	1.063	30.4
5(-2)	7.950e+00	0 000-100	0.005	0 435	0.050	~~ ~
no- S-2	0.001e+00	2.9030+00	0.825	0.4/5	-0.350	23.6
H2S	7,129e-06	8.248e-05	-5.147	-4.084	1.063	(U) 37 1
1100	,.1256 00	0.2106-00	5.11/	4.004	1.005	57.1
		-Saturation	indices			
Phase	SI** lo	g IAP log	К(298 К,	1 atm)		
CH4(g)	-146.92 -1	49.72 -2.8	30 CH4			
CO2(g)	-7.37	-8.84 -1.4	17 CO2			
H2(g)	-41.44 -	44.55 -3.1	LO H2			
H20(g)	-1.66	-0.15 1.5	DU H2O			
$n_{23}(g)$	-0.70	-3.59 -2.9	39 02 Dv	0	2 atm nh	1 000
Sulfur	32.43	37.31 4.9	38 S	cosure U.	z acm, phi	1.000
			- M			
**For a das.	ST = log10(fugac)	ity), Fugaci	tv = press	ure * phi	/ 1 atm.	

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C:\get\usgs\	phreeqc\work\holden\na	hs\nahs_ph_11_5.out						3
129	Beginning of b	oatch-reaction ca	lculations.					
130								
131								
132	Reaction step	1.						
133								
134	Using solution	1 1. Tank Conte	nts of 30%	sodium hyd:	rosulfide s	olution		
135	Using pure pha	ase assemblage 1.						
136								
137		S	olution com	position				
138				-				
139	Elements	Molalit	y Mol	es				
140			-					
141	С	1.000e-0	1.000e-	01				
142	Na	9.424e+0	0 9.423e+	00				
143	S	7.950e+0	0 7.950e+	00				
144								
145		De	scription o	f solution				
146								
147			Ha	= 11.50	1 Char	ge balance		
148			pe	= -9.34	2 Adiu	sted to re	dox	
			ea	uilibrium		0000 00 10	aon	
149	Specific	Conductance (uS	(cm. 25°C)	= 504293				
150	opoolla	Dens	$itv (a/cm^3)$	= 1.25	232			
151		20110	Volume (L)	= 1.18	530			
152		Activi	ty of water	= 0.70	4			
153		Top	ic strength	= 1.06	10+01			
154		Mass of	Water (kg)	- 9.99	90-01			
155		Total alkalin	ity (og/kg)	- 9.99	70+00			
156		Total arkalin	1102 (mol/kg)	- 9.41	00-02			
157		Toran	voz (mor/kg)	- 25.00	00-02			
150		Floatwicel b	clarace ( C)	= 25.00	2			
150	Dowoont owner	Electrical c	((Catille))	= 0.20	Se-II			
159	Percent error	c, 100*(Cat-[An])	/(Cat+ An )	= 0.00				
160			Iterations	= 22				
161			Total H	=:1.1/69	93e+02			
162			Total O	= 5.5811	31e+01			
163				- ·				
164		D1	stribution	of species				
165						-		
166	a			Log	Log	Log	mole V	
167	Species	Molality	Activity	Molality	Activity	Gamma	cm³/mol	
168								
169	OH-	5.066e-03	2.262e-03	-2.295	-2.646	-0.350	10.53	
170	H+	4.517e-12	3.151e-12	-11.345	-11.501	-0.156	0.00	
171	H20	5.551e+01	7.042e-01	1.744	-0.152	0.000	18.07	
172	C(-4)	3.209e-03						
173	CH4	3.209e-03	3.716e-02	-2.494	-1.430	1.064	35.46	
174	C(4)	9.680e-02						
175	NaCO3-	7.646e-02	1.320e+00	-1.117	0.120	1.237	52.02	
176	CO3-2	1.986e-02	2.077e-03	-1.702	-2.683	-0.981	11.97	
177	HCO3-	2.455e-04	1.396e-04	-3.610	-3.855	-0.245	52.22	
178	NaHCO3	2.313e-04	2.678e-03	-3.636	-2.572	1.064	1.80	
179	CO2	1.213e-10	1.405e-09	-9.916	-8.852	1.064	34.43	
180	(CO2)2	3.127e-21	3.621e-20	-20.505	-19.441	1.064	68.87	
181	H(0)	5.879e-09						
182	H2	2.940e-09	3.403e-08	-8.532	-7.468	1.064	28.61	
183	Na	9.424e+00						
184	Na+	9.344e+00	3.412e+01	0.971	1.533	0.562	2.14	
185	NaCO3-	7.6460-02	1.320+00	-1 117	0 120	1.237	52 02	
186	NaSO4-	2 0310-02	1 6670-02	-2 533	-2 779	-0 245	16 53	
187	NaHCO3	2.3318-03	2 6780-03	-2.000	-2.170	1 064	1 00	
100	Nancus Nancus	2.313e-04	2.0/00-03	-3.030	-2.3/2	1.064	1.80	
100	NaOn	61-9000.0	/./1/e-12	-12.1/6	-11.113	1.064	(0)	
100	0(0)	0.00000+00	0.000000	70 010	77 740	1 0.04	20 10	
101	02	0.000e+00	0.000e+00	-/8.812	-//./48	1.064	30.40	
TAT	5(-2)	1.94/e+00						

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	6 6750+00	2 9800+00	0 824	0 171	-0 250	22 65
S=2	1 2720+00	1 1420-01	0.024	-0.942	-0.330	23.00
120	7 0930-06	9 2120-05	-5 140	-0.942	-1.047	27.14
S(6)	3 2200-03	0.2120-05	-5.149	-4.086	1.064	37.10
NaSO4-	2 9310-03	1 6670-03	-0 500	-2 770	0.245	16 E
SO1-2	2.9510-04	9.7480-06	-2.555	-2.770	-0.245	40.00
HSO/-	1 7300-16	2 0070-15	-3.339	-14 525	-1.4/2	20.70
H304-	1.7506-10	2.90/0-15	-12.702	-14.525	1.237	42.4.
		-Saturation i	ndices			
		Sacuración J	.nuices			
Phase	ST** lo	a TAP loa P	(298 K	1 atm)		
	01 10	g 1112 10g 1	(250 11)	1 acmy		
CH4 (g)	1.37	-1.43 -2.80	CH4			
CO2 (g)	-7.38	-8.85 -1.41	CO2			
H2 (g)	-4.37	-7.47 -3.10	H2			
$H_{20}(\alpha)$	-1.66	-0.15 1.50	H20			
H2S(g)	-3.03 -	11.03 -7.99	H2S			
02(q)	-74.86 -	77.75 -2.89	02			
Sulfur	-4.65	0.23 4.88	S			
		0.20 1.00	0			
**For a gas,	SI = log10(fugac	ity). Fugacit	v = press	ure * phi )	1 atm.	
For ideal	gases, phi = 1.					
End of simul	ation.					
Reading inpu	t data for simula	tion 2.				
End of Run a	fter 0 Seconds.					

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#### pH 12.5

```
C:\get\usgs\phreeqc\work\holden\nahs\nahs_ph_12_5.out
                                                                                     1
       Input file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs ph 12 5
   3
       Output file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs ph 12 5.out
   4
   5
       Database file: /home/cwend/get/usgs/phreeqc/phreeqc-3.3.5-10806/database/phreeqc.dat
   6
   8
       Initializing...
   9
  10
       End of Run after 0 Seconds.
  11
  12
           EXCHANGE MASTER SPECIES
   13
           EXCHANGE SPECIES
           SURFACE MASTER SPECIES
  14
           SURFACE_SPECIES
  15
  16
          RATES
  17
          END
  18
       _____
  19
       Reading input data for simulation 1.
  20
       _____
  21
  22
          TITLE Sodium hydrosulfide equilibrium test.
  23
           SOLUTION 1 Tank Contents of 30% sodium hydrosulfide solution
              pH 12.5 #charge
  24
  25
                  density 1.3
  26
                  temp
                         25.0
                  redox 0(0)/0(-2)
  27
  28
                                  1.103e+04 charge
                  Na
  29
                 S(-2)
                                7.95e+3 #charge
  30
              С
                      le+02
   31
                 0(0)
                                  7
                                      02(g) -0.7
   32
          SOLUTION MASTER SPECIES
          SOLUTION_SPECIES
EQUILIBRIUM_PHASES 1
  33
  34
  35
          END
  36
       ____
  37
       TITLE
   38
  39
  40
        Sodium hydrosulfide equilibrium test.
  41
  42
       _____
   43
       Beginning of initial solution calculations.
   44
                _____
   45
   46
       Initial solution 1. Tank Contents of 30% sodium hydrosulfide solution
   47
   48
       -----Solution composition-----
   49
          Elements
  50
                           Molality
                                          Moles
  51
           C
  52
                           1.000e-01
                                     1.000e-01
  53
           Na
                           1.350e+01
                                      1.350e+01
                                                Charge balance
  54
           0(0)
                           6.759e-06
                                     6.759e-06
                                                Equilibrium with O2(g)
  55
                                     7.950e+00
           S(-2)
                           7.950e+00
  56
  57
       -----Description of solution-----
  58
  59
                                           pH = 12.500
            pe = 4.000
Specific Conductance (µS/cm, 25°C) = 681117
  60
                                                  4.000
  61
   62
                              Density (g/cm^3) = 1.40581
   63
                                                  1.12017
                                   Volume (L) =
                             Activity of water = 0.634
   64
```

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Percent erre	Ion Mass o: Total alkalin Total ( Temp Electrical ) or, 100*(Cat- An )	hic strength f water (kg) hity (eq/kg) co22 (mol/kg) prature (°C) balance (eq) )/(Cat+ An ) Iterations Total F Total C	$\begin{array}{rcrr} n &=& 1.87\\ &=& 1.00\\ &=& 1.35\\ &=& 1.00\\ &=& 25.00\\ &=& -1.72\\ &=& -0.00\\ &=& 9\\ H &=& 1.1370\\ 0 &=& 5.5853\\ \text{ouples}{}\end{array}$	9e+01 0e+00 0e+01 2e-11 75e+02 72e+01		
Redox co	uple j	pe Eh (volt	s)			
0(-2)/0(	0) 8.22	09 0.48	363			
	D:	istribution	of species			
			Log	Log	Log	molo
Species	Molality	Activity	Molality	Activity	Gamma	cm <sup>3</sup> /mo
OH-	4.750e-02	2 0290-02	-1 323	-1 693	-0 369	20 4
H+	4.571e-13	3 162e-13	-12 340	-12 500	-0.160	20.4
H2O	5.551e+01	6.338e-01	1.744	-0.198	0.000	18 0
C(-4)	0.000e+00	0.0000 01		0.190	0.000	10.0
CH4	0.000e+00	0.000e+00	-153.374	-151.495	1.879	35.4
C(4)	1.000e-01					0011
NaCO3-	5.774e-02	1.666e+01	-1.239	1.222	2.460	91.2
CO3-2	4.217e-02	4.048e-03	-1.375	-2.393	-1.018	19.8
HCO3-	4.904e-05	2.730e-05	-4.309	-4.564	-0.254	71.9
NaHCO3	4.485e-05	3.392e-03	-4.348	-2.470	1.879	1.8
CO2	4.049e-13	3.062e-11	-12.393	-10.514	1.879	34.4
(CO2)2	2.275e-25	1.721e-23	-24.643	-22.764	1.879	68.8
H(O)	0.000e+00					
H2	0.000e+00	0.000e+00	-46.470	-44.592	1.879	28.6
Na	1.350e+01					
Na+	1.344e+01	2.210e+02	1.128	2.344	1.216	3.3
NaCO3-	5.774e-02	1.666e+01	-1.239	1.222	2.460	91.2
NaHCO3	4.485e-05	3.392e-03	-4.348	-2.470	1.879	1.8
NaOH	5.927e-12	4.483e-10	-11.227	-9.348	1.879	(0)
0(0)	6.759e-06					
02	3.380e-06	2.556e-04	-5.471	-3.592	1.879	30.4
5(-2)	7.950e+00	1 010 0-		0 0 0 0 0		
S-2	5.303e+00	4.319e-01	0.724	-0.365	-1.089	(0)
H5- H2C	2.64/e+00	1.131e+00	0.423	0.053	-0.369	24.6
п25	4.1346-08	3.1206-00	-/.384	-5.505	T.8/9	37.1
		-Saturation	indices			
Phase	SI** lo	g IAP log	K(298 K,	1 atm)		
CH4 (g)	-148.69 -1	51.49 -2.8	30 CH4			
CO2 (g)	-9.05 -	10.51 -1.4	17 CO2			
H2(g)	-41.49 -	44.59 -3.1	0 H2			
H2O(g)	-1.70	-0.20 1.5	50 H2O			
H2S(g)	-4.45 -	12.45 -7.9	99 H2S			
02 (g)	-0.70	-3.59 -2.8	39 O2 Pr	essure 0.	2 atm, ph:	i 1.000
Sulfur	31.05	35.94 4.8	38 S			
**For a gas.	SI = log10(fugac	ity). Fugaci	ity = press	ure * phi /	1 atm.	

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C:\get\usgs\phreeqc\work\holden\nahs\nahs\_ph\_12\_5.out 129 Beginning of batch-reaction calculations. 131 132 Reaction step 1. 133 134 Using solution 1. Tank Contents of 30% sodium hydrosulfide solution 135 Using pure phase assemblage 1. 136 137 -----Solution composition-----138 139 Elements Molality Moles 140 C 1.000e-01 1.000e-01 141 1.350e+01 7.950e+00 142 Na 1.350e+01 143 S 7.950e+00 144 -----Description of solution-----145 146 147 pH = 12.500Charge balance 148 pe = -10.565Adjusted to redox equilibrium Specific Conductance ( $\mu$ S/cm, 25°C) = 681091 149 150 Density (g/cm3) = 1.40580 Volume (L) = 1.12018 Activity of water = 0.634 Ionic strength = 1.879e+01 151 152 153 Mass of water (kg) = 1.000e+00 Total alkalinity (eq/kg) = 1.350e+01 Total CO2 (mol/kg) = 9.919e-02 154 155 156 157 Temperature (°C) = 25.00158 Electrical balance (eq) = -1.658e-11Percent error, 100\*(Cat-|An|)/(Cat+|An|) = -0.00159 160 Iterations = 24 Total H = 1.137075e+02 161 162 Total 0 = 5.585372e+01 163 -----Distribution of species-----164 165 Log Log mole V 166 Log 167 Species Molality Activity Molality Activity Gamma cm³/mol 168 4.753e-02 2.030e-02 169 OH--1.323-1.692-0.36920.43 H+ 4.568e-13 170 3.160e-13 -12.340-12.500-0.1600.00 171 H2O 5.551e+01 6.338e-01 1.744 -0.198 0.000 18.07 172 8.068e-04 C(-4) 173 CH4 8.068e-04 6.102e-02 -3.093 -1.215 1.879 35.46 9.919e-02 174 C(4) NaCO3-175 5.727e-02 1.652e+01 -1.242 1.218 2.460 91.36 176 CO3-2 4.183e-02 4.016e-03 -1.379 -2.396 -1.018 19.89 177 HCO3-4.861e-05 2.706e-05 -4.313 -4.568 -0.254 72.01 178 -2.473 NaHCO3 4.446e-05 3.362e-03 -4.352 1.879 1.80 179 CO2 4.010e-13 3.033e-11 -12.397 34.43 -10.5181.879 180 (CO2)2 2.232e-25 1.688e-23 -24.651 -22.773 1.879 68.87 2.521e-09 181 H(0) 182 H2 1.261e-09 9.535e-08 -8.899 -7.021 1.879 28.61 183 1.350e+01 Na Na+ 2.344 184 1.344e+012.210e+02 1.128 1.216 3.34 NaCO3-5.727e-02 185 1.652e+01 -1.242 1.218 2.460 91.36 186 NaSO4-7.813e-04 4.349e-04 -3.107 -3.362 -0.254 58.08 187 NaHCO3 4.446e-05 3.362e-03 -2.473 -4.352 1.879 1.80 188 NaOH 5.932e-12 4.486e-10 -11.227 -9.348 1.879 (0) 0.000e+00 189 0(0)190 02 0.000e+00 0.000e+00 -80.613 -78.735 1.879 30.40 7.949e+00 191 S(-2)

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	S-2	5.303e+00	4.3196	e-01	0.725	-0.365	-1.089	(0)
3	HS-	2.646e+00	1.1300	e+00	0.423	0.053	-0.369	24.60
	H2S	4.128e-08	3.1226	e-06	-7.384	-5.506	1.879	37.10
5	S(6)	8.085e-04						
5	NaSO4-	7.813e-04	4.3490	e-04	-3.107	-3.362	-0.254	58.08
	SO4-2	2.720e-05	3.9270	e-07	-4.565	-6.406	-1.841	30.7
	HSO4-	4.181e-20	1.2060	e-17	-19.379	-16.919	2.460	42.7
			Saturat	tion ir	dices			
	Phase	SI** 1	og IAP	log K	298 K,	1 atm)		
	CH4 (g)	1.59	-1.21	-2.80	CH4			
	CO2 (g)	-9.05	-10.52	-1.47	C02			
	H2(g)	-3.92	-7.02	-3.10	H2			
	H2O(g)	-1.70	-0.20	1.50	H2O			
	H2S(g)	-4.45	-12.45	-7.99	H2S			
	O2 (g)	-75.84	-78.73	-2.89	02			
	Sulfur	-6.52	-1.63	4.88	S			
	**For a gas	, SI = log10(fuga	city). Fu	ugacity	v = press	sure * phi /	1 atm.	
	**For a gas For ideal	, SI = log10(fuga gases, phi = 1.	city). Fu	ugacity	y = press	sure * phi /	1 atm.	
	**For a gas For ideal	, SI = log10(fuga gases, phi = 1.	city). Fu	ugacity	v = press	sure * phi /	1 atm.	
	**For a gas For ideal	, SI = log10(fuga gases, phi = 1.	city). Fu	ugacity	v = press	sure * phi /	1 atm.	
	**For a gas For ideal End of simu	, SI = log10(fuga gases, phi = 1.  lation.	city). Fu	ugacity	v = press	sure * phi /	1 atm.	
	**For a gas For ideal End of simu	, SI = log10(fuga gases, phi = 1.  lation.	city). Fu	ugacity	v = press	sure * phi /	1 atm.	
	**For a gas For ideal End of simu	, SI = log10(fuga gases, phi = 1.  lation.	city). Fi	ugacity	v = press	sure * phi /	1 atm.	
	**For a gas For ideal End of simu	<pre>, SI = log10(fuga gases, phi = 1.  lation. </pre>	city). Fu	ugacity	/ = press	sure * phi /	1 atm.	
	**For a gas For ideal End of simu Reading inpu	, SI = log10(fuga gases, phi = 1. lation.  ut data for simul	city). Fu	ugacity	/ = press	sure * phi /	l atm.	
	**For a gas For ideal End of simu Reading inpu	, SI = log10(fuga gases, phi = 1.  lation.  ut data for simul.	city). Fr	ugacity	n = press	sure * phi /	1 atm.	
	**For a gas For ideal End of simu Reading inp	, SI = log10(fuga gases, phi = 1. lation. ut data for simul	city). Fu	ugacity	7 = press	sure * phi /	1 atm.	
	**For a gas For ideal End of simu Reading inp	, SI = log10(fuga gases, phi = 1. lation. ut data for simul	city). Fn ation 2.	ugacity	7 = press	sure * phi /	1 atm.	
	**For a gas For ideal End of simu Reading inp End of Run	, SI = log10(fuga gases, phi = 1. lation. ut data for simul after 0 Seconds.	city). Fu	ugacity	7 = press	sure * phi /	1 atm.	

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Appendix B. 11.5% NaHS solution dilution runs with PHREEQC

#### 1e-1 dilution

```
C:\get\usgs\phreeqc\work\holden\nahs\nahs7_1e1.out
                                                                                      1
       Input file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs7
   3
       Output file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs7.out
   4
   5
       Database file: /home/cwend/get/usgs/phreeqc/phreeqc-3.3.5-10806/database/phreeqc.dat
   6
   7
   8
       Initializing...
   9
  10
       End of Run after 0.01 Seconds.
  11
       XCHANGE MASTER SPECIES
  12
          EXCHANGE SPECIES
  13
          SURFACE MASTER SPECIES
  14
          SURFACE SPECIES
  15
          RATES
  16
          END
  17
       _____
                _____
  18
       Reading input data for simulation 1.
  19
       _____
  20
  21
          TITLE part 1 Sodium hydrosulfide solution pH 11.5
          SOLUTION 1 Tank Contents of 30% sodium hydrosulfide solution
  22
  23
              pH 11.5 #charge
  24
                  density 1.3
  25
                  temp
                         25.0
  26
                  redox 0(0)/0(-2)
  27
                                  1.103e+04 charge
                  Na
  28
                                 7.95e+3 #charge
                 S(-2)
  29
              С
                      1e+02
  30
                  0(0)
                                  7
                                      02(g) -0.7
          SOLUTION MASTER_SPECIES
  31
  32
          SOLUTION SPECIES
  33
          EQUILIBRIUM PHASES 1
  34
          SAVE solution 1
  35
         END
  36
       ____
  37
       TITLE
  38
       ____
  39
  40
       part 1 Sodium hydrosulfide solution pH 11.5
  41
  42
  43
       Beginning of initial solution calculations.
  44
                45
  46
       Initial solution 1. Tank Contents of 30% sodium hydrosulfide solution
  47
  48
       -----Solution composition-----
  49
  50
         Elements
                           Molality
                                         Moles
  51
          C
  52
                           1.000e-01
                                      1.000e-01
  53
                                      9.423e+00 Charge balance
          Na
                           9.423e+00
  54
          0(0)
                           4.419e-05
                                      4.419e-05
                                                Equilibrium with O2(g)
  55
          S(-2)
                           7.950e+00
                                      7.950e+00
  56
  57
          ------Description of solution------
  58
  59
                                           pH = 11.500
  60
                                           pe =
                                                  4.000
            Specific Conductance (\muS/cm, 25°C) = 504414
  61
  62
                              Density (g/cm<sup>3</sup>) = 1.25224
Volume (L) = 1.18537
  63
  64
                             Activity of water = 0.704
```

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Percent erro	Io Mass o Total alkali Total Temp Electrical or, 100*(Cat- An	nic strength f water (kg) nity (eq/kg) CO2 (mol/kg) erature (°C) balance (eq) )/(Cat+ An ) Iterations Total H Total (	$\begin{array}{rcrr} h &=& 1.06\\ =& 1.00\\ =& 9.42\\ =& 1.00\\ =& 25.00\\ =& 6.19\\ =& 0.00\\ =& 7\\ H &= 1.1769\\ D &= 5.5811 \end{array}$	30+01 100+00 130+00 1000-01 980-11 9930+02 1310+01		
		Redox co	ouples			
Redox cou	ple	pe Eh (volt	ts)			
0(-2)/0(0	9.19	80 0.54	141			
	D	istribution	of species			
			Log	Log	Log	mole
Species	Molality	Activity	Molality	Activity	Gamma	cm <sup>3</sup> /mc
OH-	5.048e-03	2.254e-03	-2.297	-2.647	-0.350	10.5
H+	4.532e-12	3.162e-12	-11.344	-11.500	-0.156	0.0
H20	5.551e+01	7.042e-01	1.744	-0.152	0.000	18.0
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-150.788	-149.725	1.063	35.4
NaCO3-	7.899e-02	1.362e+00	-1.102	0.134	1.237	51
C03-2	2.051e-02	2.145e-03	-1.688	-2.669	-0.981	11.9
HCO3-	2.544e-04	1.446e-04	-3.595	-3.840	-0.245	52.3
NaHCO3	2.397e-04	2.774e-03	-3.620	-2.557	1.063	1.
C02	1.262e-10	1.460e-09	-9.899	-8.836	1.063	34.4
(CO2)2	3.384e-21	3.915e-20	-20.471	-19.407	1.063	68.
H(0)	0.000e+00	0.000-100	15 600	11 510	1 0.00	~ ~
HZ	0.000e+00 9.423e+00	0.000e+00	-45.609	-44.546	1.063	28.
Na+	9.344e+00	3.410e+01	0.971	1.533	0.562	2
NaCO3-	7.899e-02	1.362e+00	-1.102	0.134	1.237	51.
NaHCO3	2.397e-04	2.774e-03	-3.620	-2.557	1.063	1.
NaOH	6.644e-13	7.686e-12	-12.178	-11.114	1.063	(0)
0(0)	4.419e-05					
02	2.209e-05	2.556e-04	-4.656	-3.592	1.063	30.
S(-2) .	7.950e+00	0.002-100	0.005	0 475	0.050	0.0
R5- S-2	1 269e+00	2.983e+00 1 139e-01	0.825	-0.9475	-0.350	23.
H2S	7.129e-06	8.248e-05	-5.147	-4.084	1.063	37.
		Coturation	indiana			
		-Saturation	Indices			
Phase	SI** lo	g IAP log	K(298 K,	l atm)		
CH4 (g)	-146.92 -1	49.72 -2.8	B0 CH4			
CO2 (g)	-7.37	-8.84 -1.4	47 CO2			
H2(g)	-41.44 -	44.55 -3.3	10 H2			
H2O(g)	-1.66	-0.15 1.5	50 H2O			
H2S(g)	-3.03 -	-3.59 -7.9	99 H2S		2 atm st	: 1 000
Sulfur	-0.70	37.31 4	88 S	lessure 0	.2 atm, ph	T T.000
Surrur	52.45	57.51 4.0	00 0			
**For a gas,	SI = log10(fugac	ity). Fugac:	ity = press	sure * phi	/ 1 atm.	
	2 . 2.					

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C:\get\usgs\phreeqc\work\holden\nahs\nahs7\_1e1.out 129 Beginning of batch-reaction calculations. 130 \_\_\_\_\_ 131 132 Reaction step 1. 133 134 Using solution 1. Tank Contents of 30% sodium hydrosulfide solution 135 Using pure phase assemblage 1. 136 137 -----Solution composition-----138 139 Elements Molality Moles 140 C 1.000e-01 1.000e-01 141 9.424e+00 9.423e+00 7.950e+00 7.950e+00 142 Na 143 S 144 -----Description of solution-----145 146 147 pH = 11.501 Charge balance 148 pe = -9.342Adjusted to redox equilibrium Specific Conductance ( $\mu$ S/cm, 25°C) = 504293 149 150 Density  $(g/cm^3) = 1.25232$ Volume (L) = 1.18530 Activity of water = 0.704 Ionic strength = 1.064e+01 151 152 153 Mass of water (kg) = 9.999e-01 Total alkalinity (eq/kg) = 9.417e+00 Total CO2 (mol/kg) = 9.680e-02 154 155 156 157 Temperature (°C) = 25.00Electrical balance (eq) = 6.203e-11Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.00 Iterations = 22 158 159 160 Total H = 1.176993e+02 161 Total O = 5.581131e+01 162 163 -----Distribution of species-----164 165 Log Log Log mole V 166 167 Species Molality Activity Molality Activity Gamma cm3/mol 168 ОН-Н+ Н2О 10.53 5.066e-03 2.262e-03 -2.295 169 -2.646 -0 350 -11.345 -11.501 4.517e-12 3.151e-12 5.551e+01 7.042e-01 170 -0.1560.00 171 1.744 -0.152 0.000 18.07 172 3.209e-03 C(-4) CH4 173 3.209e-03 3.716e-02 -2.494 -1.430 1.064 35.46 9.680e-02 174 C(4) NaCO3-175 7.646e-02 1.320e+00 -1.117 0.120 1.237 52.02 176 CO3-2 1.986e-02 2.077e-03 -1.702 -2.683 -0.981 11.97 177 HCO3-2.455e-04 1.396e-04 -3.610 -3.855 -0.245 52.22 2.313e-04 178 NaHCO3 2.678e-03 -3.636 -2.572 1.064 1.80 1.213e-10 179 CO2 1.405e-09 -9.916 -8.852 1.064 34.43 (CO2)2 180 3.127e-21 3.621e-20 -20.505 -19.441 1.064 68.87 181 H(0) 5.879e-09 182 H2 2.940e-09 3.403e-08 -8.532 -7.468 1.064 28.61 183 Na+ 9.424e+00 Na 1.533 0.120 9.344e+00 3.412e+01 0.971 184 0.562 2.14 NaCO3-7.646e-02 -1.117 185 1.320e+00 1.237 52.02 186 NaSO4-2.931e-03 1.667e-03 -2.533 -2.778 -0.245 46.53 187 NaHCO3 2.313e-04 2.678e-03 -3.636 -2.572 1.064 1.80 6.665e-13 188 7.717e-12 -12.176 1.064 (0) NaOH -11.1130(0) 0.000e+00 189 190 02 0.000e+00 0.000e+00 -78.812 -77.748 1.064 30.40 7.947e+00 191 S(-2)

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C:\get\usgs\phreeqc\work\holden\nahs\nahs7\_1e1.out 4 192 HS-6.675e+00 2.980e+00 0.824 0.104 0.474 -0.350 23.65 1.272e+00 1.142e-01 S-2 193 -0.942 -1.047 (0) H2S 194 7.093e-06 8.212e-05 -5.149 -4.086 1.064 37.16 195 S(6) 3.220e-03 196 NaSO4-2.931e-03 1.667e-03 -2.533 -2.778 -0.245 46.53 -5.011 197 9.748e-06 SO4-2 2.891e-04 -3.539 -1.472 26.70 198 HSO4-1.730e-16 2.987e-15 -15.762 -14.525 1.237 42.41 199 200 -----Saturation indices-----201 SI\*\* log IAP log K(298 K, 1 atm) 202 Phase 203 204 CH4 (g) 1.37 -1.43-2.80 CH4 205 CO2(g) -7.38 -8.85 -1.47 CO2 206 H2(g) -4.37 -7.47 -3.10 H2 207 H20(g) -1.66 -0.15 1.50 H2O 208 H2S(g) -3.03 -11.03 -7.99 H2S 209 02(g) -74.86 -2.89 02 -77.75 210 Sulfur -4.65 0.23 4.88 S 211 212 \*\*For a gas, SI = log10(fugacity). Fugacity = pressure \* phi / 1 atm. 213 For ideal gases, phi = 1. 214 215 ------216 End of simulation. 217 218 219 -------220 Reading input data for simulation 2. 221 222 223 TITLE --Part 2 water 224 SOLUTION 2 water pH 7.0 225 Temp 25.0 226 227 EQUILIBRIUM PHASES 228 CO2(g) -2.0 Calcite 0.0 229 SAVE solution 2 230 231 END 232 233 TITLE 234 \_\_\_\_ 235 236 --Part 2 water 237 238 239 Beginning of initial solution calculations. 240 241 242 Initial solution 2. water 243 244 -----Solution composition-----245 246 Elements Molality Moles 247 248 Pure water 249 250 -----Description of solution-----251 252 pH = 7.000 Specific Conductance  $(\mu S/cm, 25^{\circ}C) = 0$ 253 254 255 Density  $(g/cm^3) = 0.99704$ 

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		Volume (L)	= 1.00	297		
	Activ	ity of water	r = 1.00	0		
	Io	nic strength	h = 1.00	7e-07		
	Total alkali	i water (kg)	= 1.00	70-00		
	Total car	bon (mol/kg)	= 0.00	0e+00		
	Total	CO2 (mol/kg)	= 0.00	0e+00		
	Temp	erature (°C)	= 25.00	)		
D	Electrical	balance (eq)	= -1.21	7e-09		
Percent err	cor, 100*(Cat- An	)/(Cat+ An )	= -0.60	)		
		Total F	s = 0 t = 1 1101	240+02		
		Total C	= 5.5506	22e+01		
	D	istribution	of species			
	5	100110001001	or opeored			
Species	Molality	Activity	Log	Log	L	og mole
0000100	morarrey	ACCIVICY	HOTATICA	ACCIVICY	Gam	ma cmº/m
OH-	1.013e-07	1.012e-07	-6.995	-6.995	-0.0	00 -4.3
H+	1.001e-07	1.000e-07	-7.000	-7.000	-0.0	00 0.0
H2O	5.551e+01	1.000e+00	1.744	0.000	0.0	00 18.0
H(0)	1.416e-25	2 022 02	0.5			
HZ	7.079e-26	7.079e-26	-25.150	-25.150	0.0	28.
02	0.000e+00	0.000+00	-42 080	-42 080	0.0	0.0 20
	0.0000100	0.00000000	42.000	-42.000	0.0	50.4
		-Saturation	indices			
Phase	SI** lo	g IAP log	K(298 K,	1 atm)		
H2 (a)	-22.05 -	25.15 =3.1	0 112			
H2(g) H2O(g)	-22.05 -	25.15 -3.1	0 H2			
H2(g) H2O(g) O2(g)	-22.05 - -1.50 -39.19 -	25.15 -3.1 0.00 1.5 42.08 -2.8	0 H2 50 H20 89 O2			
H2(g) H2O(g) O2(g) **For a gas, For ideal	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1.	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci	0 H2 60 H2O 89 O2 ty = press	ure * phi	/ 1 atm	
H2(g) H2O(g) O2(g) **For a gas, For ideal 	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1.	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci  alculations.	0 H2 0 H2O 19 O2 ty = press	wure * phi	/ 1 atm	
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1.	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations.	0 H2 60 H20 9 O2 ty = press	ure * phi	/ 1 atm	
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1.	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations.	0 H2 60 H20 9 O2 ty = press	ure * phi	/ l atm	
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of  Reaction ste	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations.	0 H2 60 H20 9 O2 ty = press	ure * phi	/ 1 atm	
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c p 1. con 2. water bhase assemblage 1	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations.	0 H2 60 H20 9 O2 ty = press	ure * phi	/ 1 atm	
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c p 1. on 2. water water base assemblage 1	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations.	0 H2 0 H20 9 O2 ty = press	ure * phi	/ 1 atm	
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c p 1. con 2. water base assemblage 1	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations.	0 H2 0 H20 9 O2 ty = press	ure * phi	/ 1 atm	blage
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of  Reaction ste Using soluti Using pure p 	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. E batch-reaction c ep 1. con 2. water phase assemblage 1 SI log I	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations. Phase asse AP log K(T,	0 H2 0 H20 9 O2 ty = press	ure * phi Moles	/ 1 atm 	blage Delta
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of  Reaction ste Using soluti Using pure p  Phase CO2(g)	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c p 1. con 2. water bhase assemblage 1 SI log I -2.00 -3.	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations. Phase asse AP log K(T, 47 -1.47	0 H2 0 H20 9 O2 ty = press	Moles	/ 1 atm  in assem Final 98e+00	blage Delta -1.976e-03
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of  Reaction ste Using soluti Using pure p  Phase CO2(g) Calcite	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c p 1. con 2. water bhase assemblage 1 SI log I -2.00 -3. 0.00 -8.	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations. Phase asse AP log K(T, 47 -1.47 48 -8.48	0 H2 0 H20 9 O2 ty = press - - - P) Init 1.000e 1.000e	Moles ial +01 9.9 +01 9.9	/ 1 atm in assemu Final 98e+00 98e+00	blage Delta -1.976e-03 -1.646e-03
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c pp 1. con 2. water bhase assemblage 1 SI log I -2.00 -3. 0.00 -8.	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations. Phase asse AP log K(T, 47 -1.47 48 -8.48 Solution com	0 H2 0 H20 9 O2 ty = press  P) Init 1.000e 1.000e	Moles ial +01 9.9	/ 1 atm in assem Final 98e+00 98e+00	blage Delta -1.976e-03 -1.646e-03
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite Elements	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c pp 1. ton 2. water ohase assemblage 1 -2.00 -3. 0.00 -8. Molali	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations. Phase asse AP log K(T, 47 -1.47 48 -8.48 Solution com ty Mol	0 H2 0 H20 9 O2 ty = press mblage P) Init 1.000e 1.000e position	Moles ial +01 9.9	/ 1 atm in assemu Final 98e+00 98e+00	Delta -1.976e-03 -1.646e-03
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of  Reaction ste Using soluti Using pure p  Phase CO2(g) Calcite  Elements C	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c pp 1. on 2. water ohase assemblage 1 -2.00 -3. 0.00 -8. Molali	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci 	0 H2 0 H20 9 O2 ty = press mblage P) Init 1.000e 1.000e aposition es 03	Moles ial +01 9.9	/ 1 atm in assemu Final 98e+00 98e+00	Delta -1.976e-03 -1.646e-03
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of  Reaction ste Using soluti Using pure p  Phase CO2(g) Calcite  Elements C Ca	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c pp 1. con 2. water ohase assemblage 1 -2.00 -3. 0.00 -8. Molali 3.622e- 1.646e-	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci 	0 H2 0 H20 9 O2 ty = press mblage P) Init 1.000e 1.000e aposition es 03 03	Moles ial +01 9.9	/ 1 atm in assemu Final 98e+00 98e+00	Delta -1.976e-03 -1.646e-03
H2(g) H2O(g) O2(g) **For a gas, For ideal Beginning of  Reaction ste Using soluti Using pure p  Phase CO2(g) Calcite Elements C Ca	-22.05 - -1.50 -39.19 - SI = log10(fugac gases, phi = 1. batch-reaction c pp 1. con 2. water ohase assemblage 1 -2.00 -3. 0.00 -8. Molali 3.622e- 1.646e-	25.15 -3.1 0.00 1.5 42.08 -2.8 ity). Fugaci alculations. Phase asse AP log K(T, 47 -1.47 48 -8.48 Solution com ty Mol 03 3.622e- 03 1.646e-	0 H2 0 H20 9 O2 ty = press mblage P) Init 1.000e 1.000e aposition es 03 03	Moles ial +01 9.9	/ 1 atm in assemu Final 98e+00 98e+00	Delta -1.976e-03 -1.646e-03

0			DH	= 7.20	7 Char	re balance	0
1			pn	= -1.57	5 Adam	isted to m	edox
			eo	uilibrium	- AUJU		ouon
2	Specif	ic Conductance (u)	S/cm, 25°C)	= 306			
3	-1	Den	sity $(q/cm^3)$	= 0.99	726		
1			Volume (L)	= 1.00	300		
5		Activ	ity of water	= 1.00	0		
5		Io	nic strength	= 4.82	6e-03		
7		Mass	f water (kg)	= 1.00	00+00		
:		Total alkali	nity (ea/ka)	= 3.29	10-03		
3		Total	CO2 (mol/kg)	= 3.62	20-03		
)		Temp	erature (°C)	= 25.00	)		
		Electrical	palance (eq)	= -1.21	7e-09		
	Percent err	or, 100*(Cat- An	(Cat+ An )	= -0.00	)		
			Iterations	= 17			
			Total H	= 1,1101	24e+02		
			Total C	= 5.5515	11e+01		
		D	istribution	of species			
				Log	Loa	Log	mole
	Species	Molality	Activity	Molality	Activity	Gamma	cm <sup>3</sup> /mo
	-	- 1		1			,
	OH-	2.162e-07	2.005e-07	-6.665	-6.698	-0.033	-4.0
	H+	5.401e-08	5.048e-08	-7.268	-7.297	-0.029	0.0
	H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.0
	C(-4)	1.401e-25					20.0
	CH4	1.401e-25	1.403e-25	-24.854	-24.853	0.000	35.4
	C(4)	3.622e-03					
	HCO3-	3.224e-03	2.998e-03	-2.492	-2.523	-0.032	24.7
	CO2	3.399e-04	3.403e-04	-3.469	-3.468	0.000	34.4
	CaHCO3+	4.887e-05	4.549e-05	-4.311	-4.342	-0.031	9.7
	CaCO3	5.559e-06	5.565e-06	-5.255	-5.255	0.000	-14.6
	CO3-2	3.724e-06	2.785e-06	-5.429	-5.555	-0.126	-5.1
	(CO2)2	2.123e-09	2.125e-09	-8.673	-8.673	0.000	68.8
	Ca	1.646e-03					
	Ca+2	1.591e-03	1.189e-03	-2.798	-2.925	-0.126	-18.0
	CaHCO3+	4.887e-05	4.549e-05	-4.311	-4.342	-0.031	9.7
	CaCO3	5.559e-06	5.565e-06	-5.255	-5.255	0.000	-14.6
	CaOH+	4.213e-09	3.910e-09	-8.375	-8.408	-0.032	(0)
	H(0)	5.090e-15					
	H2	2.545e-15	2.548e-15	-14.594	-14.594	0.000	28.6
	0(0)	0.000e+00					
	02	0.000e+00	0.000e+00	-63.193	-63.192	0.000	30.4
			-Saturation	indices			
	Phase	SI** lo	g IAP log	K(298 K,	1 atm)		
	Aragonite	-0.14	-8.48 -8.3	4 CaCO3			
	Calcite	0.00	-8.48 -8.4	8 CaCO3			
	CH4 (g)	-22.05 -2	24.85 -2.8	0 CH4			
	CO2 (g)	-2.00	-3.47 -1.4	7 CO2 Pr	essure 0.	0 atm, ph	i 1.000
	H2(g)	-11.49 -	14.59 -3.1	0 H2			
	H2O(g)	-1.50	-0.00 1.5	0 H2O			
	02 (g)	-60.30 -	53.19 -2.8	9 02			
	**For a gas,	SI = log10(fugac	ity). Fugaci	ty = press	sure * phi /	1 atm.	
	For ideal	gases, phi = 1.					
	End of star						
	End of simul	ation.					

```
C:\get\usgs\phreeqc\work\holden\nahs\nahs7_1e1.out
 383 -----
  384
       Reading input data for simulation 3.
 385
       ------
 386
 387
           TITLE -- Part 3 mix the two
 388
          MIX 1
              1 0.1
2 0.9
  389
          1
 390
          SAVE solution 3
 391
 392
          END
 393
       ____
  394
       TITLE
 395
       ____
 396
 397
        -- Part 3 mix the two
 398
 399
  400
       Beginning of batch-reaction calculations.
 401
       402
 403
       Reaction step 1.
 404
 405
       Using mix 1.
 406
 407
       Mixture 1.
 408
 409
             1.000e-01 Solution 1 Solution after simulation 1.
             9.000e-01 Solution 2 Solution after simulation 2.
 410
 411
 412
       -----Solution composition-----
 413
 414
          Elements
                           Molality
                                          Moles
 415
                            1.326e-02 1.326e-02
1.481e-03 1.481e-03
          С
 416
 417
           Ca
 418
         Na
                           9.425e-01
                                      9.423e-01
 419
          S
                            7.951e-01
                                      7.950e-01
 420
       -----Description of solution-----
 421
 422
                                            pH = 11.616
pe = -9.368
 423
                                                            Charge balance
 424
                                                             Adjusted to redox
                                            equilibrium
            Specific Conductance (µS/cm, 25°C) = 65380
Density (g/cm<sup>3</sup>) = 1.03096
 425
 426
 427
                                    Volume (L) = 1.01717
                             Activity of water = 0.970
Ionic strength = 1.057e+00
 428
 429
                            Mass of water (kg) = 9.998e-01
alkalinity (eq/kg) = 9.447e-01
Total CO2 (mol/kg) = 1.290e-02
Temperature (°C) = 25.00
 430
 431
                       Total alkalinity (eq/kg)
 432
 433
 434
                        Electrical balance (eq) = -1.089e-09
 435
        Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
 436
                                    Iterations = 17
                                       Total H = 1.116811e+02
 437
 438
                                       Total O = 5.554473e+01
 439
             -----Distribution of species-----
 440
 441
 442
                                                         Log
                                                   Log
                                                                    Log mole V
                        Molality Activity Molality Activity Gamma cm³/mol
 443
         Species
 444
 445
         OH-
                         7.052e-03 4.055e-03 -2.152 -2.392
                                                                   -0.240
                                                                             -2.02
```

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6	H+	3.266e-12	2.4220-	-12	-11,486	-11.616	-0.130	0 0
7	H20	5.551e+01	9 7030-	-01	1 744	-0.013	0.100	18 0
8	C(-4)	3 6380-04	5.7056	0 I	1./44	-0.015	0.000	10.0
a	CHA	3 6380-04	1 6110-	-04	-3 130	-3 333	0 106	25 4
0	C(A)	1 2000-02	4.0416	04	-5.459	-3.355	0.100	55.4
1	NaCO3-	1.2906-02	7 4010	0.2	2 0 2 0	0 105	0 007	4 0
1	Nacus-	9.3626-03	7.491e-	-03	-2.029	-2.125	-0.097	4.8
2	003-2	3.2468-03	5.869e-	-04	-2.489	-3.231	-0.743	-1.0
3	CaCO3	2.339e-04	2.984e-	-04	-3.631	-3.525	0.106	-14.6
4	HCO3-	4.648e-05	3.031e-	-05	-4.333	-4.518	-0.186	28.0
5	NaHCO3	9.159e-06	1.168e-	-05	-5.038	-4.932	0.106	1.8
6	CaHCO3+	1.744e-07	1.170e-	-07	-6.758	-6.932	-0.173	9.9
7	CO2	1.333e-10	1.701e-	-10	-9.875	-9.769	0.106	34.4
B	(CO2)2	4.163e-22	5.310e-	-22	-21.381	-21.275	0.106	68.8
9	Ca	1.481e-03						
)	Ca+2	1.221e-03	3.026e-	-04	-2.913	-3.519	-0.606	-16.4
1	CaCO3	2.339e-04	2.984e-	-04	-3.631	-3.525	0.106	-14.6
2	CaOH+	2.515e-05	2.012e-	-05	-4.600	-4.696	-0.097	(0)
3	CaS04	1.2886-06	1 643e-	-06	-5 890	-5 784	0 106	7 5
1	CaHCO3+	1.7440=07	1 1700-	-07	-6 758	-6 932	-0 173	0.0
	CallCOST	3 2680-17	2 6150	-17	-16 100	-16 502	-0.1/3	9.9
<	U(A)	3.2000-17	Z.0106-	1/	-10.400	-10.303	-0.097	(0)
2	n(0)	3.3498-08	0.064	0.0	7 751	7 645	0 100	00.0
5	HZ	1.7/5e-08	2.264e-	-08	-/./51	-/.645	0.106	28.6
5	Na	9.425e-01						
9	Na+	9.329e-01	6.855e-	-01	-0.030	-0.164	-0.134	-0.2
)	NaCO3-	9.362e-03	7.491e-	-03	-2.029	-2.125	-0.097	4.8
-	NaSO4-	1.608e-04	1.049e-	-04	-3.794	-3.979	-0.186	23.2
2	NaHCO3	9.159e-06	1.168e-	-05	-5.038	-4.932	0.106	1.8
3	NaOH	2.179e-13	2.780e-	-13	-12.662	-12.556	0.106	(0)
	0(0)	0.000e+00						
5	02	0.000e+00	0.000e+	+00	-77.222	-77.116	0.106	30.4
5	S(-2)	7.948e-01						
7	HS-	6.776e-01	3.896e-	-01	-0.169	-0.409	-0.240	21 5
2	5-2	1 1710-01	1 9430-	-02	-0.931	_1 711	-0.790	(0)
à	428	6 4690-06	9 2510	06	-5.100	-1./11	-0.700	27 1
5	R/6)	2 6400-04	0.2016-	-00	-5.109	-5.064	0.100	37.1
	5(0)	3.6490-04	0.050	0.5	0 600		0.000	10.0
1	504-2	2.028e-04	3.052e-	-05	-3.693	-4.515	-0.822	18.2
2	NaSO4-	1.608e-04	1.049e-	-04	-3.794	-3.979	-0.186	23.2
3	CaSO4	1.288e-06	1.643e-	-06	-5.890	-5.784	0.106	7.5
4	HSO4-	8.982e-15	7.187e-	-15	-14.047	-14.143	-0.097	41.1
5	CaHSO4+	3.268e-17	2.615e-	-17	-16.486	-16.583	-0.097	(0)
5								
7			Saturati	ion in	dices			
3								
)	Phase	SI** lo	og IAP ]	log K(	298 К,	1 atm)		
L	Anhydrite	-3.76	-8.03 -	-4.28	CaSO4			
2	Aragonite	1.59	-6.75 -	-8.34	CaCO3			
3	Calcite	1.73	-6.75 -	-8.48	CaCO3			
1	CH4 (a)	-0.53	-3.33 -	-2.80	CH4			
5	CO2 (a)	-8.30	-9.77 -	-1.47	CO2			
2	Gunsum	-3.48	-8.06 -	_/ 50	CaS04 - 3	120		
7	up (a)	-3.40	-0.00 -	2 10	U2	HZU		
	n2(g)	-4.54	-7.05 -	-3.10	HZ			
5	H20(g)	-1.52	-0.01	1.50	HZO			
1	H2S(g)	-4.03 -	-12.03 -	-7.99	H2S			
)	O2(g)	-74.22 -	-77.12 -	-2.89	02			
1	Sulfur	-5.47	-0.59	4.88	S			
2								
5	For a gas,	SI = logl0(fugad gases, phi = 1.	city). Fug	gacity	= press	sure * phi	/latm.	
5								
5								

#### C:\get\usgs\phreeqc\work\holden\nahs\nahs7\_1e1.out

510 -----511 Reading input data for simulation 4. 512 -----513 514 -----515 End of Run after 0.01 Seconds. 516 517 518

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#### 1e-2 dilution

```
C:\get\usgs\phreeqc\work\holden\nahs\nahs7_1e2.out
                                                                                       1
       Input file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs7
   1
   2
   3
       Output file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs7.out
   4
   5
       Database file: /home/cwend/get/usgs/phreeqc/phreeqc-3.3.5-10806/database/phreeqc.dat
   6
   7
   8
      Initializing...
   9
  10
       End of Run after 0 Seconds.
  11
           EXCHANGE_MASTER_SPECIES
  13
           EXCHANGE SPECIES
  14
           SURFACE MASTER SPECIES
  15
           SURFACE_SPECIES
  16
          RATES
  17
          END
  18
       _____
  19
       Reading input data for simulation 1.
  20
  21
  22
           TITLE part 1 Sodium hydrosulfide solution pH 11.5
  23
           SOLUTION 1 Tank Contents of 30% sodium hydrosulfide solution
  24
              pH 11.5 #charge
  25
                  density 1.3
                  temp 25.0
redox O(0)/O(-2)
  26
  27
                                  1.103e+04 charge
  28
                  Na
                 S(-2)
le+02
O(0)
  29
                                 7.95e+3 #charge
  30
              С
  31
                                  7
                                       02(g) -0.7
          SOLUTION MASTER_SPECIES
SOLUTION_SPECIES
  32
  33
  34
           EQUILIBRIUM PHASES 1
  35
           SAVE solution 1
  36
          END
  37
       ____
  38
       TITLE
  39
       ____
  40
       part 1 Sodium hydrosulfide solution pH 11.5
  41
  42
  43
       _____
  44
       Beginning of initial solution calculations.
  45
  46
  47
       Initial solution 1. Tank Contents of 30% sodium hydrosulfide solution
  48
  49
       -----Solution composition-----
  50
  51
          Elements
                           Molality
                                          Moles
  52
          C
  53
                           1.000e-01
                                      1.000e-01
  54
          Na
                           9.423e+00
                                     9.423e+00 Charge balance
  55
                           4.419e-05
                                      4.419e-05 Equilibrium with O2(g)
           0(0)
                           7.950e+00
                                      7.950e+00
  56
           S(-2)
  57
       -----Description of solution-----
  58
  59
  60
                                           pH = 11.500
  61
                                            pe =
                                                   4.000
  62
            Specific Conductance (\muS/cm, 25°C) = 504414
  63
                               Density (g/cm^3) = 1.25224
  64
                                    Volume (L) = 1.18537
```

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Percent err	Activ Ior Mass c: Total alkalin Total ( Temp Electrical ) or, 100*(Cat- An )	ty of water hic strength f water (kg) hity (eq/kg) CO2 (mol/kg) erature (°C) balance (eq) )/(Cat+ An ) Iterations Total H Total C Redox co	$\begin{array}{rcl} &=& 0.76\\ &=& 1.06\\ &=& 1.00\\ &=& 9.42\\ &=& 1.00\\ &=& 25.00\\ &=& 6.19\\ &=& 0.00\\ &=& 7\\ &=& 1.1769\\ &=& 5.5811\\ \end{array}$	4 30e+01 30e+00 30e+00 90e-01 98e-11 993e+02 31e+01		
Redox co	uple	pe Eh (volt	s)			
0(-2)/0(	0) 9.19	80 0.54	41			
	D:	istribution	of species	;		
Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole cm³/mc
OH-	5.048e-03	2.254e-03	-2.297	-2.647	-0.350	10.5
H+	4.532e-12	3.162e-12	-11.344	-11.500	-0.156	0.0
H2O	5.551e+01	7.042e-01	1.744	-0.152	0.000	18.0
C(-4)	0.000e+00	0.000.000	150 300	1 4 0 5 0 5		
CH4	0.000e+00	0.000e+00	-150.788	-149.725	1.063	35.4
NaCO3-	7 8990-02	1 3620+00	-1 102	0 134	1 237	51 0
C03-2	2.051e-02	2.145e-03	-1.688	-2.669	-0.981	11.9
HCO3-	2.544e-04	1.446e-04	-3.595	-3.840	-0.245	52.2
NaHCO3	2.397e-04	2.774e-03	-3.620	-2.557	1.063	1.8
CO2	1.262e-10	1.460e-09	-9.899	-8.836	1.063	34.4
(CO2)2	3.384e-21	3.915e-20	-20.471	-19.407	1.063	68.8
H(0)	0.000e+00					
H2	0.000e+00	0.000e+00	-45.609	-44.546	1.063	28.6
Na	9.423e+00	0.410.401	0 071	1 500	0 5 6 0	
Na+	9.3440+00	3.410e+01	0.971	1.533	0.562	2.1
NaCO3-	2.3970-04	1.362e+00	-1.102	0.134	1.237	51.9
NaOH	6 6440-13	2.774e-03 7.686e-12	-12 178	-2.55/	1.063	1.8
0(0)	4.419e-05	1.0000 12	12.170	11.111	1.005	(0)
02	2.209e-05	2.556e-04	-4.656	-3.592	1.063	30.4
S(-2)	7.950e+00					
HS-	6.681e+00	2.983e+00	0.825	0.475	-0.350	23.6
S-2	1.269e+00	1.139e-01	0.103	-0.943	-1.047	(0)
H2S	7.129e-06	8.248e-05	-5.147	-4.084	1.063	37.1
		-Saturation	indices			
Phase	SI** log	g IAP log	K(298 K,	1 atm)		
CH4(g)	-146.92 -14	49.72 -2.8	0 CH4			
CO2 (g)	-7.37	-8.84 -1.4	7 CO2			
H2 (g)	-41.44 -4	44.55 -3.1	0 H2			
H20(g)	-1.66	-0.15 1.5	0 H2O			
n25(g)	-3.03 -	-3 50 -7.9	9 HZS		2 atra	1 000
02(9)	-0.70	-3.39 -2.8	9 02 Pr	essure 0.	z atm, ph	1 1.000
Sulfur	3/ / 3	3/3/ / 9	× ~			

Poginning o	f beteb weeetice .	- 1 1 - 4 /				
Beginning of	I Datch-reaction c	alculations.	-			
Reaction ste	ep 1.					
Using solut	ion 1. Tank Cont	ents of 30%	sodium buc	irosulfide a	alution	
Using pure	phase assemblage 1		Souran nyc	itosutitue s	SOLUCION	
		Solution com	aposition			
Element	s Molali	ty Mol	es			
С	1.000e-	01 1.000e-	-01			
Na	9.424e+	00 9.423e+	-00			
S	7.950e+	00 7.950e+	-00			
	D	escription of	of solution			
		coorrigeron c	JE SOLUCIOI			
		pH	I = 11.50	)1 Char	ge balance	e,
		pe	e = -9.34	IZ Adji	isted to re	edox
Speci	fic Conductance (u)	$S/cm$ , $25^{\circ}C$	= 504293	3		
1	Den	sity (g/cm <sup>3</sup> )	= 1.25	232		
		Volume (L)	= 1.18	3530		
	Activ	ity of water	= 0.70	)4		
	Io	nic strength	1.06	54e+01		
	Mass o:	f water (kg)	= 9.99	9e-01		
	Total alkali	nity (eg/kg)	= 9.41	./e+00		
	Temp	erature (°C)	= 9.68	0e-02		
	1 Onio	CTUCUTO ( C)				
	Electrical	palance (eq)	= 6.20	, )3e=11		
Percent er	Electrical ) ror, 100*(Cat- An	<pre>oalance (eq) )/(Cat+ An )</pre>	= 6.20	) 3e-11		
Percent er	Electrical ) ror, 100*(Cat- An )	oalance (eq) /(Cat+ An ) Iterations	= 6.20 = 0.00 = 22	) 3e-11 )		
Percent er	Electrical ) ror, 100*(Cat- An )	oalance (eq) /(Cat+ An ) Iterations Total H	$= 6.20 \\ = 0.00 \\ = 22 \\ = 1.1769$	) 3e-11 ) 993e+02		
Percent er	Electrical ) ror, 100*(Cat- An )	calance (eq) )/(Cat+ An ) Iterations Total H Total C	= 6.20 $= 0.00$ $= 22$ $= 1.1769$ $= 5.5811$	)3e-11 ) 993e+02 .31e+01		
Percent er:	Electrical ) ror, 100*(Cat- An )	oalance (eq) )/(Cat+ An ) Iterations Total H Total C istribution	$= 6.20 \\ = 0.00 \\ = 22 \\ = 1.1769 \\ = 5.5811 \\ of species$	)3e-11 ) 993e+02 .31e+01		
Percent er:	Electrical ) ror, 100*(Cat- An )	oalance (eq) )/(Cat+ An ) Iterations Total E Total C istribution	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species	)3e-11 ) 993e+02 .31e+01 ;	Log	mole
Percent er: Species	Electrical ) ror, 100*(Cat- An ) D: Molality	oalance (eq) )/(Cat+ An ) Iterations Total E Total C istribution Activity	= 6.20 = 0.00 = 22 H = 1.1769 = 5.5811 of species Log Molality	)3e-11 ) 93e+02 .31e+01 ; Log Activity	Log Gamma	mole cm³/mo
Percent er: Species	Electrical ) ror, 100*(Cat- An ) D: Molality	oalance (eq) /(Cat+ An ) Iterations Total E Total C istribution Activity	= 6.20 = 0.00 = 22 H = 1.1769 = 5.5811 of species Log Molality	)3e-11 ) 393e+02 .31e+01 ; Log Activity	Log Gamma	mole cm³/mc
Percent er: Species OH-	Electrical ) ror, 100*(Cat- An ) D: Molality 5.066e-03	<pre>balance (eq) /(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Molality -2.295	)3e-11 993e+02 .31e+01 ; Log Activity -2.646	Log Gamma -0.350	mole cm³/mc 10.5
Percent er: Species OH- H+ H2C	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12	<pre>balance (eq) /(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 2.000 000</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Log Molality -2.295 -11.345	)3e-11 )93e+02 .31e+01 ;	Log Gamma -0.350 -0.156	mole cm³/mo 10.5 0.0
Percent er: Species OH- H+ H2O C(-4)	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03	<pre>balance (eq) /(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01</pre>	= 6.20 = 0.00 = 22 i = 1.1769 0 = 5.5811 of species Log Molality -2.295 -11.345 1.744	)3e-11 )93e+02 .31e+01 ;	Log Gamma -0.350 -0.156 0.000	mole cm³/mo 10.5 0.0 18.0
Percent er: Species OH- H+ H2O C(-4) C(-4)	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 3.209e-03	<pre>balance (eq) )/(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Log Molality -2.295 -11.345 1.744	) ) ) ) ) ) ) ) ) ) ) ) ) )	Log Gamma -0.350 -0.156 0.000	mole cm³/mo 10.5 0.0 18.0
Percent er: Species OH- H+ H2O C(-4) CH4 C(4)	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 3.209e-03 9.680e-02	<pre>balance (eq) )/(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02</pre>	= 6.20 = 0.00 = 22 i = 1.1769 0 = 5.5811 of species Log Molality -2.295 -11.345 1.744 -2.494	093e-11 093e+02 .31e+01 	Log Gamma -0.350 -0.156 0.000 1.064	mole cm³/mo 10.5 0.0 18.0 35.4
Percent er: Species OH- H+ H2O C(-4) C(4) C(4) NaCO3-	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 3.209e-03 9.680e-02 7.646e-02	<pre>balance (eq) )/(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Log Molality -2.295 -11.345 1.744 -2.494 -1.117	038-11 093e+02 31e+01 s Activity -2.646 -11.501 -0.152 -1.430 0.120	Log Gamma -0.350 -0.156 0.000 1.064 1.237	mole cm³/mo 10.5 0.0 18.0 35.4
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3-2	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 3.209e-03 9.680e-02 7.646e-02 1.986e-02	<pre>balance (eq) )/(Cat+ An ) Iterations Total F Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03</pre>	= 6.20 = 0.00 = 22 i = 1.1769 0 = 5.5811 of species Log Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702	038-11 093e+02 31e+01 	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981	mole cm³/mo 10.5 0.0 18.0 35.4 52.0 11.0
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3-2 HCO3-	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04	<pre>balance (eq) )/(Cat+ An ) Iterations Total F Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04</pre>	= 6.20 = 0.00 = 22 i = 1.1769 0 = 5.5811 of species Log Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610	03e-11 093e+02 .31e+01 	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245	mole cm³/mo 10.5 0.0 18.0 35.4 52.0 11.5 52.2
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3-2 HCO3- NaHCO3	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04	<pre>balance (eq) /(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04 2.678e-03</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Log Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -3.636	03e-11 093e+02 .31e+01 	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064	mole cm³/md 10.5 0.0 18.0 35.4 52.0 11.5 2.2 1.5
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3- NaHCO3 CO2	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-10 3.209e-03 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04 1.213e-10	<pre>balance (eq) /(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04 2.678e-03 1.405e-09</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Log Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -3.636 -9.916	03e-11 093e+02 .31e+01 	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064	mole cm <sup>3</sup> /mo 10.9 0.0 18.0 35.4 52.0 11.9 52.2 1.8 34.4
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3-2 HCO3- NaHCO3 CO2 (CO2)2	Electrical ) ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21	<pre>balance (eq) &gt;/(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-03 1.405e-09 3.621e-20</pre>	= 6.20 = 0.00 = 22 i = 1.1769 0 = 5.5811 of species Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -9.916 -20.505	.33e-11 .31e+01 	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064 1.064	mole cm <sup>3</sup> /mo 10.9 0.0 18.0 35.4 52.0 11.9 52.2 1.8 34.4 68.8
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3-2 HCO3- NaHCO3 CO2 (CO2)2 H(0)	Electrical 3 ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21 5.879e-09	<pre>balance (eq) /(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04 2.678e-03 1.405e-09 3.621e-20</pre>	= 6.20 = 0.00 = 22 = 1.1769 0 = 5.5811 of species Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -9.916 -20.505	<pre>/3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //2e-2 //2e-</pre>	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064	mole cm <sup>3</sup> /mo 10.9 0.0 18.0 35.4 52.0 11.9 52.2 1.8 34.4 68.8
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3-2 HCO3- NaHCO3 CO2 (CO2)2 H(0) H2	Electrical 3 ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21 5.879e-09 2.940e-09	<pre>balance (eq) )/(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04 2.678e-03 1.405e-09 3.621e-20 3.403e-08</pre>	= 6.20 = 0.00 = 22 = 1.1769 0 = 5.5811 of species Log Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -9.916 -20.505 -8.532	038-11 093e+02 .31e+01 	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064 1.064	mole cm³/mo 10.9 0.0 18.0 35.4 52.0 11.9 52.2 1.8 34.4 68.8 28.6
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3-2 HCO3- NaHCO3 CO2 (CO2)2 H(0) H2 Na	Electrical 3 ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21 5.879e-09 2.940e-09 9.424e+00	<pre>balance (eq) )/(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04 2.678e-03 1.405e-09 3.621e-20 3.403e-08 2.412.02</pre>	= 6.20 = 0.00 = 22 i = 1.1769 0 = 5.5811 of species Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -3.636 -9.916 -20.505 -8.532	038-11 093e+02 31e+01 Comparison Compa	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064 1.064 1.064	mole cm³/mo 10.5 0.0 18.0 35.4 52.0 11.5 52.2 1.8 34.4 68.8 28.6
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- CO3-2 HCO3- NaHCO3 CO2 (CO2)2 H(0) H2 Na Na+ NaCO3-	Electrical 3 ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21 5.879e-09 2.940e-09 9.424e+00 9.344e+00	<pre>balance (eq) )/(Cat+ An ) Iterations Total F Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04 2.678e-03 1.405e-09 3.621e-20 3.403e-08 3.412e+01 1.202000</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -3.636 -9.916 -20.505 -8.532 0.971	038-11 093e+02 31e+01 	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064 1.064 1.064 1.064	mole cm³/mo 10.5 0.0 18.0 35.4 52.0 11.5 52.2 1.8 34.4 68.8 28.6 2.1
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- NaHCO3 CO2 (CO2)2 H(0) H2 Na Na+ NaCO3- NaSO4-	Electrical 3 ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21 5.879e-09 2.940e-09 9.424e+00 7.646e-02 2.934e+00 7.646e-02	<pre>balance (eq) )/(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04 2.678e-03 1.405e-09 3.621e-20 3.403e-08 3.412e+01 1.320e+00 1.672-02</pre>	= 6.20 = 0.00 = 22 i = 1.1769 0 = 5.5811 of species Log Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -3.636 -9.916 -20.505 -8.532 0.971 -1.117	<pre>//3e-11 /93e-11 /993e+02 /31e+01 ////30 ///2.646 -11.501 -0.152 -1.430 0.120 -2.683 -3.855 -2.572 -8.852 -19.441 -7.468 1.533 0.120</pre>	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064 1.064 1.064 1.064	mole cm³/mo 10.5 0.0 18.0 35.4 52.0 1.5 52.2 1.8 34.4 68.8 28.6 2.1 52.0
Percent er: Species OH- H+ H2O C(-4) CH4 C(4) NaCO3- NaHCO3 CO2 (CO2)2 H(0) H2 Na Na+ NaCO3- NaHCO3 NaHCO3 NaHCO3 NaHCO3 NaHCO3	Electrical 3 ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551+01 3.209e-03 9.680e-02 7.646e-02 1.986e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21 5.879e-09 2.940e-09 9.424e+00 7.646e-02 2.931e-03 2.213e-04	<pre>balance (eq) )/(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.396e-04 2.678e-03 1.405e-09 3.621e-20 3.403e-08 3.412e+01 1.320e+00 1.667e-03 2.672e-02</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -3.636 -9.916 -20.505 -8.532 0.971 -1.117 -1.117 -2.533	<pre>//3e-11 //3e-11 //3e-11 //2/31e+01 //2/2/2/2/2/2/2/2/2/2/2/2/2/2/2/2/2/2/</pre>	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064 1.064 1.064 1.064 1.064	mole cm³/mo 10.5 0.0 18.0 35.4 52.0 11.5 52.0 1.8 34.4 68.8 28.6 2.1 52.0 46.5
Percent er: Species OH- H+ H2O C(-4) C(4) NaCO3- NAHCO3 CO2 (CO2)2 H(0) H2 Na Na+ NaCO3- NASO4- NAHCO3 NaO4 NAHCO3 NAO4	Electrical 3 ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 9.680e-02 7.646e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21 5.879e-09 2.940e-09 9.424e+00 7.646e-02 2.931e-03 2.313e-04 6.655e-13	<pre>balance (eq) /(Cat+ An ) Iterations Total E Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.405e-09 3.621e-20 3.403e-08 3.412e+01 1.320e+00 1.667e-03 2.678e-03 2.678e-03 3.412e+01 3.20e+00 3.667e-03 3.20e+00 3.667e-03 3.412e+01 3.20e+00 3.412e+01 3.412e</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -20.505 -8.532 0.971 -1.117 -2.533 -3.636 -2.255 -3.2532 -3.253 -3.2532 -3.25522 -3.25	<pre>/3e-11 //3e-11 //ae-11 //</pre>	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064 1.064 1.064 1.064 1.064 1.064 1.237 -0.245 1.064	mole cm <sup>3</sup> /mo 10.9 0.0 18.0 35.4 52.0 11.9 52.2 1.8 34.4 68.8 28.6 2.1 52.0 46.5 1.8
Percent er: Species OH- H+ H2O C(-4) C(4) NaCO3- CO3-2 HCO3- NaHCO3 CO2 (CO2)2 H(0) H2 Na Na+ NaCO3- NaSO4- NaHCO3 NaO4- NaCO3- NaCO3- NaCO3- NaSO4- NaHCO3 NaO4- NaCO3- NACO3- N	Electrical 3 ror, 100*(Cat- An ) Molality 5.066e-03 4.517e-12 5.551e+01 3.209e-03 9.680e-02 7.646e-02 2.455e-04 2.313e-04 1.213e-10 3.127e-21 5.879e-09 2.940e-09 9.424e+00 7.646e-02 2.931e-03 2.313e-04 6.665e-13 0.000e+00	<pre>balance (eq) )/(Cat+ An ) Iterations Total F Total C istribution Activity 2.262e-03 3.151e-12 7.042e-01 3.716e-02 1.320e+00 2.077e-03 1.405e-09 3.621e-20 3.403e-08 3.412e+01 1.320e+00 1.667e-03 2.678e-03 7.717e-12</pre>	= 6.20 = 0.00 = 22 = 1.1769 = 5.5811 of species Molality -2.295 -11.345 1.744 -2.494 -1.117 -1.702 -3.610 -9.916 -20.505 -8.532 0.971 -1.117 -2.533 -3.636 -12.176	<pre>/3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //3e-11 //3e-2.646 //1.501 //2.683 //3.855 //2.572 //3e-2.572 //3e-2.572 //3e-2.572 //3e-2.572 //1.113</pre>	Log Gamma -0.350 -0.156 0.000 1.064 1.237 -0.981 -0.245 1.064 1.064 1.064 1.064 1.064 1.237 -0.245 1.237 -0.245 1.064 1.064	mole cm³/mo 10.5 0.0 18.0 35.4 52.0 11.9 52.2 1.8 34.4 68.8 28.6 2.1 52.0 46.5 1.8 (0)

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5(-2)	7 9170+00						
5(-2)	7.9476+00	0.000					
HS-	6.6/5e+00	2.980	0e+00	0.824	0.474	-0.350	23.6
S-2	1.272e+00	1.142	2e-01	0.104	-0.942	-1.047	(0)
H2S	7.093e-06	8.212	2e-05	-5.149	-4.086	1.064	37.1
S(6)	3.220e-03						
NaSO4-	2.931e-03	1.667	7e-03	-2.533	-2.778	-0.245	46.5
SO4-2	2.891e-04	9.748	8e-06	-3.539	-5.011	-1.472	26 7
HSO4-	1.730e-16	2 98	70-15	-15 762	-14 525	1 237	12
	1.7500 10	2.50	10 10	10.702	14.020	1.201	42.5
		Satura	ation i	ndices			
		oucure					
Phase	SI** 1	og IAP	log K	(298 K,	1 atm)		
CH4 (a)	1 37	_1 42	-2 00	CILLA			
CO2 (g)	1.37	-1.45	-2.00	CH4			
CO2 (g)	-7.38	-8.85	-1.4/	C02			
H2(g)	-4.37	-7.47	-3.10	H2			
H2O(g)	-1.66	-0.15	1.50	H2O			
H2S(g)	-3.03	-11.03	-7.99	H2S			
02 (a)	-74.86	-77.75	-2.89	02			
Sulfur	-4.65	0.23	4.88	S			
				~			
**For a gas,	, SI = log10(fuga	city). H	Fugacit	y = press	sure * phi /	1 atm.	
For ideal	gases, phi = 1.				Perm /		
End of simul	lation.						
			-				
Reading inpu	ut data for simul	ation 2.					
			-				
OT OT P	Dant 2 water						
TITLE	-Part 2 water						
TITLE SOLUTION	-Part 2 water N 2 water						
TITLE SOLUTION PH	-Part 2 water N 2 water 7.0						
TITLE SOLUTION PH Tem	-Part 2 water N 2 water 7.0 mp 25.0						
TITLE SOLUTION PH Tem EOUILIBE	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES						
TITLE SOLUTION PH Tem EQUILIBE	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (G) -2.0						
TITLE SOLUTION PH Tem EQUILIBH CO2	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0						
TITLE SOLUTION PH Tem EQUILIBE CO2 ( Calc	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0						
TITLE SOLUTION PH Tem EQUILIBN CO2 Calc SAVE sol	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 lution 2						
TITLE SOLUTION PH Ten EQUILIBF CO2 Calc SAVE SOJ END	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 Lution 2						
TITLE SOLUTION PH Tem EQUILIBE CO2 Calc SAVE sol END	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 site 0.0 Lution 2						
TITLE SOLUTION PH Tem EQUILIBF CO2 Calc SAVE sol END 	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 Lution 2						
TITLE SOLUTION PH Ten EQUILIBH CO2 Calc SAVE sol END TITLE	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 Lution 2						
TITLE	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 Lution 2						
TITLE	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 Lution 2						
TITLE SOLUTION PH Tem EQUILIBF CO2 Calc SAVE sol END 	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 lution 2						
TITLE SOLUTION PH Tem EQUILIBH CO2 Calc SAVE sol END  TITLE Part 2 wa	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 Lution 2						
TITLE SOLUTION pH Ten EQUILIBH CO2 Calc SAVE sol END  TITLE Part 2 wa	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2			-			
TITLE SOLUTION pH Ten EQUILIBH CO2 Calc SAVE sol END 	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2 ater	n calcul	lations	-			
TITLE SOLUTION PH Ten EQUILIBE CO2 Calc SAVE SOJ END TITLE Part 2 was Beginning of	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2 ater	n calcul	lations	- -			
TITLE SOLUTION PH Tem EQUILIBE CO2 Calc SAVE sol END Part 2 wa Beginning of	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio	n calcul	lations	-			
TITLE SOLUTION PH Tem EQUILING CO2 Calc SAVE sol END  TITLE Part 2 was Beginning of	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio	n calcul	lations	-			
TITLE SOLUTION pH Ten EQUILIBH CO2 Calc SAVE sol END  Part 2 wa Beginning of Initial solu	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 site 0.0 lution 2 ater f initial solutio	n calcul	lations	-			
TITLE SOLUTION pH Ten EQUILIBH CO2 Calc SAVE sol END  Part 2 wa Beginning of  Initial solu	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio	n calcul	lations	- - osition			
TITLE SOLUTION PH Tem EQUILIBF CO2 Calc SAVE sol END  FITLE Part 2 was Beginning of	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio	n calcul	lations on comp	- - osition			
TITLE SOLUTION pH Ten EQUILIBN CO2 Calc SAVE sol END  Part 2 wa Beginning of Initial solu Elements	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio ution 2. water	n calcul 	lations  on comp Mole.	- - osition			
TITLE SOLUTION pH Ten EQUILIBH CO2 Calc SAVE sol END  Part 2 wa Beginning of Initial solu Elements	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio ution 2. water	n calcul 	lations on comp Mole	- - osition			
TITLE SOLUTION pH Ten EQUILIBH CO2 Calc SAVE sol END  TITLE Part 2 was Beginning of  Initial solu Elements Pure wat	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio ution 2. water s Molal	-Solutio	lations on comp Mole	- - osition			
TITLE SOLUTION PH Tem EQUILIBE CO2 Calc SAVE sol END Part 2 wa Beginning of Initial solu Elements Pure wat	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio ution 2. water s Molal	-Solutic	lations on comp Mole	- - osition			
TITLE SOLUTION PH Ten EQUILIBN CO2 Calc SAVE sol END  Part 2 was Beginning of Initial solu Elements Pure wat	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio ution 2. water s Molal ter		lations on comp Mole tion of	- - s solution			
TITLE SOLUTION pH Ten EQUILIBH CO2 Calc SAVE sol END  Part 2 was Beginning of Initial solu Elements Pure wat	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio ation 2. water s Molal ter	n calcul Solutic ity Descript	lations on comp Mole tion of	- - s solution	J		
TITLE SOLUTION pH Ten EQUILIBH CO2 Calc SAVE sol END  Part 2 wa Beginning of Initial solu Elements Pure wat	-Part 2 water N 2 water 7.0 mp 25.0 RIUM PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio ation 2. water s Molal ter	-Solutio -Solutio ity Descript	lations on comp Mole tion of	- - s solution = 7 00			
TITLE SOLUTION PH Tem EQUILIBE CO2 Calc SAVE sol END Part 2 was Beginning of Initial solu Elements Pure wat	-Part 2 water N 2 water 7.0 mp 25.0 RIUM_PHASES (g) -2.0 cite 0.0 lution 2 ater f initial solutio ution 2. water s Molal ter	-Solutio	lations on comp Mole tion of pH		 200		

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	Dens	sity (g/cm <sup>3</sup> )	= 0.99	704		
		Volume (L)	= 1.00	297		
	Activ	itv of water	. = 1.00	0		
	Ior	nic strength	n = 1.00	7e-07		
	Mass of	f water (kg)	= 1.00	0e+00		
	Total alkalin	nity (eg/kg)	= 1.21	7e-09		
	Total car	oon (mol/kg)	= 0.00	0e+00		
	Total (	CO2 (mol/kg)	= 0.00	0e+00		
	Temp	erature (°C)	= 25.00	00100		
	Electrical	balance (eq)	= -1 21	70-09		
Percent err	cor, 100*(Cat- Anl)	/(Cat+lAnl)	= -0.60	10 05		
		Iterations	s = 0			
		Total H	I = 1.1101	24e+02		
		Total (	= 5.5506	22e+01		
	D:	istribution	of species			
			Ter	T		1
Species	Mololity	Activity	Log	Log	Log	mole
phecres	мотаттсу	ACCIVICY	MOLALITY	Activity	Gamma	cm³/mc
OH-	1 0130-07	1 0120-07	-6 005	-6 005	_0_000	4 1
U11 -	1 0010-07	1 0000-07	-0.995	-0.995	-0.000	-4.1
H20	5 5510+01	1.00000-07	-7.000	-7.000	-0.000	10.0
H(0)	1 4160-25	1.00000+00	1./44	0.000	0.000	18.0
H2	7 070-26	7 070- 26	-05 150	-0F 1F0	0.000	00.4
0(0)	0.0000+00	1.0/96-26	-23.150	-25.150	0.000	28.6
02	0.000000000	0.0000+00	-12 000	_10.000	0.000	20
02	0.000e+00	0.00000000	-42.080	-42.080	0.000	30.4
		-Saturation	indices			
Phase	SI** loc	g IAP log	K(298 K,	1 atm)		
H2(g)	-22.05 -2	25.15 -3.1	LO H2			
H2O(g)	-1.50	0.00 1.5	50 H2O			
O2 (g)	-39.19 -4	42.08 -2.8	39 02			
	CT - legit/function	ity). Fugaci	ty = press	ure * phi	/ 1 atm.	
**For a gas,	SI = IOGIU(IUGAC.					
**For a gas, For ideal	gases, phi = $1$ .					
**For a gas, For ideal	gases, phi = $1$ .					
**For a gas, For ideal	gases, phi = 1.					
**For a gas, For ideal Beginning of	<pre>gases, phi = 1. batch-reaction ca</pre>	alculations.	-			
**For a gas, For ideal Beginning of	<pre>gases, phi = 1. batch-reaction ca</pre>	alculations.	-			
**For a gas, For ideal Beginning of	gases, phi = 1.	alculations.	-			
**For a gas, For ideal Beginning of Reaction ste	<pre>gases, phi = 1. batch-reaction ca pp 1.</pre>	alculations.	-			
**For a gas, For ideal Beginning of Reaction ste	<pre>gases, phi = 1. batch-reaction ca p 1.</pre>	alculations				
**For a gas, For ideal Beginning of Reaction ste Using soluti	<pre>gases, phi = 1. batch-reaction call p 1. on 2. water</pre>	alculations.				
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p	<pre>gases, phi = 1. gases, phi = 1. batch-reaction call p 1. on 2. water hase assemblage 1.</pre>	alculations.	-			
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p	<pre>gases, phi = 1. gases, phi = 1. batch-reaction call p 1. con 2. water base assemblage 1.</pre>	alculations.				
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p	<pre>gases, phi = 1. gases, phi = 1. batch-reaction ca p 1. on 2. water base assemblage 1.</pre>	alculations.	emblage			
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p	<pre>gases, phi = 1. gases, phi = 1. gases, phi = 1. gases, phi = 1. gases, phi = 1. gase, phi =</pre>	alculations.	emblage			
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p	<pre>gases, phi = 1. f batch-reaction ca pp 1. on 2. water phase assemblage 1.</pre>	alculations.	emblage	Moles	in_assembla	age
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p  Phase	<pre>gases, phi = 1. gases, phi = 1. batch-reaction can p 1. on 2. water hase assemblage 1. SI log IA</pre>	alculations. Phase asse AP log K(T,	emblage P) Init	Moles	in assembla Final	age Delta
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase	<pre>gases, phi = 1. gases, phi = 1. batch-reaction can p 1. on 2. water hase assemblage 1. SI log IA</pre>	alculations. Phase asse AP log K(T,	emblage P) Init	Moles	in assembla Final	age Delta
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g)	<pre>gases, phi = 1. gases, phi = 1. batch-reaction can phase assemblage 1. SI log IA -2.00 -3.4</pre>	alculations. Phase asse AP log K(T, 47 -1.47	emblage P) Init 1.000e	Moles ial +01 9.9	in assembla Final 98e+00 -1.	age Delta 976e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite	<pre>gases, phi = 1. gases, phi = 1. batch-reaction ca gases assemblage 1. sin 2. water base assemblage 1. SI log IA -2.00 -3.4 0.00 -8.4</pre>	alculations. Phase asse AP log K(T, 47 -1.47 48 -8.48	P) Init 1.000e	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite	<pre>gases, phi = 1. gases, phi = 1. batch-reaction cate p 1. f batch-reaction cate phase assemblage 1. SI log IA -2.00 -3.4 0.00 -8.4</pre>	alculations. Phase asse AP log K(T, 47 -1.47 48 -8.48	emblage P) Init 1.000e 1.000e	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite	<pre>gases, phi = 1. gases, phi = 1. batch-reaction cate p 1. f batch-reaction cate sp 1. f base assemblage 1. f b</pre>	AP log K(T, 47 -1.47 48 -8.48 Solution com	P) Init 1.000e position	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite	<pre>gases, phi = 1. gases, phi = 1. batch-reaction can p 1. sp 1.</pre>	AP log K(T, 47 -1.47 48 -8.48 Solution com	P) Init P) Init 1.000e 1.000e	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite Elements	<pre>gases, phi = 1. gases, phi = 1. batch-reaction can phase assemblage 1. SI log IA -2.00 -3.4 0.00 -8.4 Molalit</pre>	AP log K(T, 47 -1.47 48 -8.48 Solution com	P) Init P) Init 1.000e 1.000e aposition	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite Elements	<pre>gases, phi = 1. gases, phi = 1. batch-reaction cate phase assemblage 1 SI log IA -2.00 -3.4 0.00 -8.4 Molalit</pre>	AP log K(T, 47 -1.47 48 -8.48 Solution com	P) Init P) Init 1.000e 1.000e	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite Elements C	gases, phi = 1. gases, phi = 1. batch-reaction can p 1. ion 2. water water bhase assemblage 1. SI log IA -2.00 -3.4 0.00 -8.4 Molalit 3.622e-0	AP log K(T, 47 -1.47 48 -8.48 Solution com ty Mol 03 3.622e-	P) Init 7 1.000e 3 1.000e aposition .es	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p Phase CO2(g) Calcite Elements C Ca	<pre>si = logit(Hugac. gases, phi = 1. batch-reaction ca p 1. lon 2. water whase assemblage 1 -2.00 -3.4 0.00 -8.4 </pre>	AP log K(T, 47 -1.47 48 -8.48 Solution com ty Mol 03 3.622e- 03 1.646e-	P) Init P) Init 1.000e 1.000e aposition les -03 -03	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03
**For a gas, For ideal Beginning of Reaction ste Using soluti Using pure p  Phase CO2(g) Calcite Elements C Ca	<pre>gases, phi = 1. gases, phi = 1. f batch-reaction can phase assemblage 1. SI log IM -2.00 -3.4 0.00 -8.4</pre>	alculations. Phase asse AP log K(T, 47 -1.47 48 -8.48 Solution com ty Mol 03 3.622e- 03 1.646e-	P) Init P) Init 1.000e 1.000e position les -03 -03	Moles ial +01 9.9 +01 9.9	in assembla Final 98e+00 -1. 98e+00 -1.	age Delta 976e-03 646e-03

		p	H = 7.2	297 Cl	harge balance	9
		p	e = -1.5	575 Ad	djusted to re	edox
		e	quilibrium	n		
Specifi	Lc Conductance (µ	S/cm, 25°C	) = 306			
	Den	sity (g/cm <sup>3</sup>	) = 0.9	99726		
		Volume (L	) = 1.0	0300		
	Activ:	ity of wate	r = 1.0	000		
	LOI	nic strengt	n = 4.8	326e-03		
	Mass of Total alkali	r water (kg	) = 1.0	000e+00		
	Total alkali	CO2 (mol/kg	) = 3.2	5220-03		
	Temp	erature (°C	) = 25.0	10		
	Electrical	balance (eq	) = -1.2	217e-09		
Percent erro	pr. 100*(Cat- An	)/(Cat+ An	) = -0.0	0		
	, ( ()	Iteration	s = 17			
		Total	H = 1.110	0124e+02		
		Total	0 = 5.551	L511e+01		
	D	istribution	of specie	es		
			Loc	J Lo	g Log	mole V
Species	Molality	Activity	Molality	/ Activit	y Gamma	cm³/mol
011	0 160- 07	0.005+.07	6 6 6 6		0 0 0 0 0 0 0	4 07
OH-	Z.162e-07	2.005e-07	-0.003	-6.69	8 -0.033	-4.07
H20	5.401e-08	5.048e-08	-/.200	-7.29	0.029	10.00
C(-4)	1 4016-25	9.9998-01	1./45	-0.00	0.000	10.07
CH4	1.401e-25	1.403e-25	-24.854	-24.85	3 0.000	35.46
C(4)	3.622e-03	1.1000 20	21.00	21.00	0.000	55.40
HCO3-	3.224e-03	2.998e-03	-2.492	-2.52	3 -0.032	24.73
CO2	3.399e-04	3.403e-04	-3.469	-3.46	8 0.000	34.43
CaHCO3+	4.887e-05	4.549e-05	-4.313	-4.34	2 -0.031	9.70
CaCO3	5.559e-06	5.565e-06	-5.255	5 -5.25	5 0.000	-14.60
CO3-2	3.724e-06	2.785e-06	-5.429	-5.55	5 -0.126	-5.13
(CO2)2	2.123e-09	2.125e-09	-8.673	-8.67	3 0.000	68.87
Ca	1.646e-03					
Ca+2	1.591e-03	1.189e-03	-2.798	3 -2.92	5 -0.126	-18.02
CaHCO3+	4.887e-05	4.549e-05	-4.31	-4.34	2 -0.031	9.70
CaCO3	5.559e-06	5.565e-06	-5.25	-5.25	5 0.000	-14.60
CaOH+	4.213e-09	3.9106-09	-8.375	-8.40	8 -0.032	(0)
u2	2 E450-15	2 5490-15	14 50	1 -14 50	4 0.000	20 61
2(0)	2.5450-15	2.0408-10	-14.59	-14.59	4 0.000	20.01
02	0.000000000	0 0000+00	-63 19	3 -63 19	2 0.000	30 40
02	0.00000.00	0.0000100	00.10	00.19	2 0.000	50.40
		-Saturation	indices-			
Phase	SI** lo	g IAP log	K(298 K,	1 atm)		
Aragonite	-0.14	-8.48 -8.	34 CaCO3			
Calcite	0.00	-8.48 -8.	48 CaCO3			
CH4 (g)	-22.05 -	24.85 -2.	80 CH4			
CO2 (g)	-2.00	-3.47 -1.	47 CO2 1	Pressure	0.0 atm, ph	i 1.000
H2(g)	-11.49 -	14.59 -3.	10 H2			
H2O(g)	-1.50	-0.00 1.	50 H2O			
02(g)	-60.30 -	03.19 -2.	89 02			
**For a gas, For ideal	SI = log10(fugac gases, phi = 1.	ity). Fugac	ity = pres	ssure * ph	i / 1 atm.	
End of simul	ation.					

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```
C:\get\usgs\phreeqc\work\holden\nahs\nahs7_1e2.out
 383
  384
 385
      Reading input data for simulation 3.
 386
       387
 388
          TITLE -- Part 3 mix the two
  389
          MIX 1
           1 0.01
 390
              2 0.99
 391
 392
           SAVE solution 3
 393
         END
  394
       -----
 395
       TITLE
 396
       ____
 397
        -- Part 3 mix the two
 398
  399
       ------
 400
 401
       Beginning of batch-reaction calculations.
 402
       ------
 403
  404
       Reaction step 1.
 405
 406
       Using mix 1.
 407
 408
       Mixture 1.
  409
 410
             1.000e-02 Solution 1 Solution after simulation 1.
 411
             9.900e-01 Solution 2 Solution after simulation 2.
 412
 413
       -----Solution composition-----
  414
 415
          Elements
                            Molality
                                          Moles
 416
          C
 417
                            4.586e-03 4.585e-03
 418
          Ca
                            1.629e-03 1.629e-03
  419
           Na
                            9.424e-02
                                        9.423e-02
                                       7.950e-02
 420
                            7.951e-02
          S
 421
       -----Description of solution-----
 422
 423
                                            pH = 11.455
pe = -9.078
                                                           Charge balance
Adjusted to redox
  424
 425
                                             equilibrium
 426
             Specific Conductance (\muS/cm, 25°C) = 9468
 427
                               Density (g/cm^3) = 1.00082
                              Volume (L) = 1.00427
Activity of water = 0.997
 428
 429
                                 Ionic strength = 1.034e-01
s of water (kg) = 9.999e-01
alinity (eq/kg) = 9.726e-02
al CO2 (mol/kg) = 4.466e-03
 430
 431
                             Mass of water (kg)
 432
                        Total alkalinity (eq/kg)
 433
                             Total CO2 (mol/kg)
                               Temperature (°C) = 25.00
  434
 435
                        Electrical balance (eq) = -1.286e-09
00*(Cat-|An|)/(Cat+|An|) = -0.00
 436
        Percent error, 100*(Cat-|An|)/(Cat+|An|)
                                     Iterations = 19
  437
                                        Total H = 1.110793e+02
Total O = 5.551807e+01
 438
  439
 440
       -----Distribution of species-----
 441
 442
 443
                                                             Log Log mole V
vity Gamma cm³/mol
                                                    Log
                         Molality Activity Molality Activity
 444
          Species
 445
```

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6	OH-	3.792e-03	2.878e-03	-2.421	-2.541	-0.120	-3.71
7	H+	4 2550-12	3 5060-12	-11 371	-11 /55	-0.094	0.00
8	H20	5 5510+01	9 9690-01	1 744	-0.001	0.000	19.01
q	C(-4)	1 1990-04	J.JUJE 01	1./44	-0.001	0.000	10.0
0	CU/	1 1000-04	1 229 - 04	2 0.01	2 011	0 010	25 4
1	C/4	1.1990-04	1.2208-04	-3.921	-3.911	0.010	33.40
1 2	C(4)	4.4000-03	0 750- 04	0 640	2 050	0 410	
2	003-2	2.290e-03	8./50e-04	-2.640	-3.058	-0.418	-4.1.
3	NaCO3-	1.518e-03	1.183e-03	-2.819	-2.927	-0.108	-0.2
4	CaCO3	5.722e-04	5.860e-04	-3.242	-3.232	0.010	-14.60
5	HCO3-	8.320e-05	6.541e-05	-4.080	-4.184	-0.104	25.1
6	NaHCO3	2.608e-06	2.671e-06	-5.584	-5.573	0.010	1.8
7	CaHCO3+	4.192e-07	3.327e-07	-6.378	-6.478	-0.100	9.8
8	CO2	5.051e-10	5.172e-10	-9.297	-9.286	0.010	34.4
9	(CO2)2	4.795e-21	4.911e-21	-20.319	-20.309	0.010	68.8
0	Ca	1.629e-03					
1	Ca+2	1.030e-03	3.986e-04	-2.987	-3.399	-0.412	-17.4
2	CaCO3	5.722e-04	5.860e-04	-3.242	-3.232	0.010	-14.6
3	CaOH+	2.414e-05	1.881e-05	-4.617	-4.726	-0.108	(0)
4	CaSO4	2.560e-06	2.621e-06	-5.592	-5.581	0.010	7.5
5	CaHCO3+	4.192e-07	3.327e-07	-6.378	-6.478	-0,100	9.8
6	CaHSO4+	7.751e-17	6.041e-17	-16.111	-16,219	-0.108	(0)
7	H(0)	2.4340-08	0.011C T/		10.213	0.100	(0)
8	H2	1.2176-08	1.2460-08	-7 915	-7 904	0 010	28 6
a	Na	9 1210-02	1.2406-00	-7.915	-7.504	0.010	20.0
0	Na±	9.2700-02	7 2600-02	_1 022	_1 120	-0 106	1 0
1	Na+	1 5100 02	1.1030.03	-1.033	-1.139	-0.100	-1.0
- -	Nacos-	1.5186-05	1.1830-03	-2.819	-2.92/	-0.108	-0.2
2	NaSO4-	1./11e-05	1.345e-05	-4.767	-4.8/1	-0.104	16.3
3	NaHCO3	2.6086-06	2.6/1e-06	-5.584	-5.5/3	0.010	1.8
4	NaOH	2.040e-14	2.090e-14	-13.690	-13.680	0.010	(0)
5	0(0)	0.000e+00					
6	02	0.000e+00	0.000e+00	-76.584	-76.574	0.010	30.4
7	S(-2)	7.939e-02					
8	HS-	7.417e-02	5.630e-02	-1.130	-1.249	-0.120	20.8
9	S-2	5.212e-03	1.940e-03	-2.283	-2.712	-0.429	(0)
0	H2S	1.685e-06	1.726e-06	-5.773	-5.763	0.010	37.1
1	S(6)	1.200e-04					
2	SO4-2	1.003e-04	3.698e-05	-3.999	-4.432	-0.433	15.6
3	NaSO4-	1.711e-05	1.345e-05	-4.767	-4.871	-0.104	16.3
4	CaSO4	2.560e-06	2.621e-06	-5.592	-5.581	0.010	7.5
5	HSO4-	1.617e-14	1.260e-14	-13.791	-13.899	-0.108	40.5
6	CaHSO4+	7.751e-17	6.041e-17	-16.111	-16.219	-0.108	(0)
7							(-)
8			-Saturation	indices			
9				21102000			
0	Phase	ST** 10	a IAP log	K(298 K	1 atm)		
1			209				
2	Anhydrite	-3.55	-7.83 -4 3	CaSO4			
3	Aragonite	1.88	-6.46 -8 3	4 Cacos			
4	Calcito	2.00	-6.46 -0.3	9 Cacoo			
74 5	CUALCILLE	2.02	-0.40 -8.4	o CaCO3			
6	CO2 (~)	-1.11	-3.31 -2.8	7 000			
0	CO2 (g)	-7.82	-9.29 -1.4	7 CO2			
1	Gypsum	-3.25	-7.83 -4.5	8 CaSO4:2	H20		
8	H2(g)	-4.80	-7.90 -3.1	.0 H2			
9	H2O(g)	-1.50	-0.00 1.5	0 H2O			
0	H2S(g)	-4.71 -	12.70 -7.9	9 H2S			
1	O2(g)	-73.68 -	76.57 -2.8	9 02			
2	Sulfur	-5.89	-1.01 4.8	8 S			
3							
4	**For a gas,	SI = log10(fugac	ity). Fugaci	ty = press	ure * phi	/ 1 atm.	
5	. For ideal (	gases, phi = 1.	_				
6							
7							

#### C:\get\usgs\phreeqc\work\holden\nahs\nahs7\_1e2.out

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#### 1e-3 dilution

```
C:\get\usgs\phreeqc\work\holden\nahs\nahs7_1e3.out
```

```
1
    Input file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs7
2
    Output file: /home/cwend/get/usgs/phreeqc/work/holden/nahs/nahs7.out
3
4
5
    Database file: /home/cwend/get/usgs/phreeqc/phreeqc-3.3.5-10806/database/phreeqc.dat
6
8
    Initializing...
9
10
    End of Run after 0.01 Seconds.
    XCHANGE_MASTER_SPECIES
11
12
        EXCHANGE SPECIES
13
        SURFACE MASTER SPECIES
14
        SURFACE SPECIES
15
        RATES
16
        END
17
    ____
18
    Reading input data for simulation 1.
19
                  _____
20
21
        TITLE part 1 Sodium hydrosulfide solution pH 11.5
22
        SOLUTION 1 Tank Contents of 30% sodium hydrosulfide solution
23
            pH 11.5 #charge
24
               density 1.3
               temp 25.0
redox 0(0)/0(-2)
25
26
27
               Na
                               1.103e+04 charge
28
                               7.95e+3 #charge
              S(-2)
29
            С
                   1e+02
30
               0(0)
                                    02(g) -0.7
                                7
        SOLUTION_MASTER_SPECIES
31
32
        SOLUTION SPECIES
33
        EQUILIBRIUM PHASES 1
34
        SAVE solution 1
35
       END
36
    ___
37
    TITLE
38
39
40
     part 1 Sodium hydrosulfide solution pH 11.5
41
42
    _____
43
    Beginning of initial solution calculations.
44
                 _____
        ____
45
46
    Initial solution 1. Tank Contents of 30% sodium hydrosulfide solution
47
48
    -----Solution composition-----
49
50
                         Molality
       Elements
                                        Moles
51
                                   1.000e-01
        C
52
                         1.000e-01
53
        Na
                         9.423e+00
                                    9.423e+00
                                               Charge balance
54
        0(0)
                         4.419e-05
                                    4.419e-05 Equilibrium with O2(g)
55
        S(-2)
                                    7.950e+00
                         7.950e+00
56
57
    -----Description of solution-----
58
59
                                         pH = 11.500
          Specific Conductance (\muS/cm, 25°C) = 504414
60
                                                4.000
61
                           Density (g/cm<sup>3</sup>) = 1.25224
Volume (L) = 1.18537
Activity of water = 0.704
62
63
64
```

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	Io	nic strength	n = 1.06	3e+01		
	Mass o	f water (kg)	= 1.00	0e+00		
	Total alkali:	nity (eq/kg)	= 9.42	3e+00		
	Total	CO2 (mol/kg)	= 1.00	0e-01		
	Temp	erature (°C)	= 25.00	0		
Porgont orro	Electrical .	balance (eq)	= 6.19	8e-11		
rercent erro	r, 100^(Cat- An	)/(Cat+ An )	= 0.00			
		Total F	s = 7 s = 1,1760	930+02		
		Total C	= 5.5811	310+01		
		iotai t	/ _ 0.0011	516+01		
		Redox co	ouples			
Redox cou	ple	pe Eh (volt	s)			
0(-2)/0(0	) 9.19	80 0.54	41			
	D	istribution	of species			
			Log		Tog	molo
Species	Molality	Activity	Molality	Activity	Gamma	cm <sup>3</sup> /mo
OH-	5.048e-03	2.254e-03	-2.297	-2 647	-0.350	10
H+	4.532e-12	3.162e-12	-11.344	-11.500	-0.156	10.1
H2O	5.551e+01	7.042e-01	1.744	-0.152	0.000	18.0
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-150.788	-149.725	1.063	35.4
C(4)	1.000e-01					
NaCO3-	7.899e-02	1.362e+00	-1.102	0.134	1.237	51.
CO3-2	2.051e-02	2.145e-03	-1.688	-2.669	-0.981	11.
HCO3-	2.544e-04	1.446e-04	-3.595	-3.840	-0.245	52.
NaHCO3	2.397e-04	2.774e-03	-3.620	-2.557	1.063	1.
C02	1.262e-10	1.460e-09	-9.899	-8.836	1.063	34.
(CO2)2	3.384e-21	3.915e-20	-20.471	-19.407	1.063	68.1
H(U)	0.000e+00	0.000.000	15 600			
nz No	0.000e+00	0.000e+00	-45.609	-44.546	1.063	28.
Na	9.4230+00	2 410-101	0 071	1 500	0 5 6 0	0
NaCO3-	7 8990-02	1 3620+00	_1 102	1.533	1 227	Z.,
NaHCO3	2 3970-04	2 7740-03	-3.620	-2 557	1.237	JI.3
NaOH	6.644e-13	7.6860-12	-12 178	-11 114	1 063	(0)
0(0)	4.419e-05	1.0006-12	12.1/0	11.113	1.003	(0)
02	2.209e-05	2.556e-04	-4.656	-3.592	1,063	30
S(-2)	7.950e+00			0.052	1.000	50.
HS-	6.681e+00	2.983e+00	0.825	0.475	-0.350	23.0
S-2	1.269e+00	1.139e-01	0.103	-0.943	-1.047	(0)
H2S	7.129e-06	8.248e-05	-5.147	-4.084	1.063	37.1
		-Saturation	indices			
Phase	SI** lo	g IAP loa	К(298 К,	1 atm)		
0114.4.5						
CH4 (g)	-146.92 -1	49.72 -2.8	CH4			
COZ(g)	-7.37	-8.84 -1.4	7 CO2			
H20/~)	-41.44 -	44.55 -3.1	0 HZ			
H20(g)	-3.03	-U.ID I.5	H20			
$\Omega^{2}(q)$	-0.70	-3 59 -2 9	9 02 02	00001170	2 otm who	1 000
Sulfur	32.43	-3.35 -2.8 37.31 / 9	18 S	essure U.	z atm, ph	T T.000
- ur r ur	52.45	J.J. 4.0				
**For a gas,	SI = log10(fugac	ity). Fugaci	ty = press	ure * phi /	/ 1 atm.	

C:\get\usgs\phreeqc\work\holden\nahs\nahs7\_1e3.out 129 Beginning of batch-reaction calculations. \_\_\_\_\_ 131 132 Reaction step 1. 133 Using solution 1. Tank Contents of 30% sodium hydrosulfide solution 134 135 Using pure phase assemblage 1. 136 137 -----Solution composition-----138 139 Molality Elements Moles 140 C 1.000e-01 1.000e-01 141 9.424e+00 9.423e+00 7.950e+00 7.950e+00 142 Na 143 S 144 -----Description of solution-----145 146 Charge balance 147 pH = 11.501 148 pe = -9.342Adjusted to redox equilibrium Specific Conductance ( $\mu$ S/cm, 25°C) = 504293 149 150 Density  $(g/cm^3) = 1.25232$ Volume (L) = 1.18530 Activity of water = 0.704 Ionic strength = 1.064e+01 151 152 153 Mass of water (kg) = 9.999e-01 Total alkalinity (eq/kg) = 9.417e+00 Total CO2 (mol/kg) = 9.680e-02 154 155 156 157 Temperature (°C) = 25.00Electrical balance (eq) = 6.203e-11Percent error, 100\*(Cat-|An|)/(Cat+|An|) = 0.00 Iterations = 22 158 159 160 Total H = 1.176993e+02 161 162 Total O = 5.581131e+01 163 -----Distribution of species-----164 165 Log Log mole V 166 Log 167 Species Molality Activity Molality Activity Gamma cm³/mol 168 169 OH-5.066e-03 2.262e-03 -2.295 10.53 -2.646 -0 350 H+ 4.517e-12 3.151e-12 5.551e+01 7.042e-01 170 -11.345-11.501 -0.1560.00 171 H2O 1.744 -0.152 0.000 18.07 C(-4) 172 3.209e-03 173 CH4 3.209e-03 3.716e-02 -2.494 -1.430 1.064 35.46 C(4) 9.680e-02 174 NaCO3-175 7.646e-02 -1.117 1.320e+00 0.120 1.237 52.02 176 CO3-2 1.986e-02 2.077e-03 -1.702-2.683 -0.981 11.97 177 HCO3-2.455e-04 1.396e-04 -3.610 -3.855 -0.245 52.22 178 2.313e-04 NaHCO3 2.678e-03 -3.636 -2.572 1.064 1.80 1.213e-10 -9.916 179 C02 1.405e-09 -8.852 1.064 34.43 180 (CO2)2 3.127e-21 3.621e-20 -20.505 -19.441 1.064 68.87 5.879e-09 181 H(0) 182 H2 2.940e-09 3.403e-08 -8.532 -7.468 1.064 28.61 183 Na+ 9.424e+00 Na 1.533 0.120 184 9.344e+00 3.412e+01 0.971 0.562 2.14 NaCO3--1.117 185 7.646e-02 1.320e+00 1.237 52.02 186 NaSO4-2.931e-03 1.667e-03 -2.533 -2.778 -0.245 46.53 187 NaHCO3 2.313e-04 2.678e-03 -3.636 -2.572 1.064 1.80 188 NaOH 6.665e-13 7.717e-12 -12.176 1.064 -11.113(0) 189 0.000e+00 0(0) 190 02 0.000e+00 0.000e+00 -78.812 -77.748 1.064 30.40 7.947e+00 191 S(-2)

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HS-	6 6750+00	2 000	00+00	0 00/	0 474	0 250	
n5-	0.0750+00	2.900	00+00	0.824	0.4/4	-0.350	23.8
5-2	1.2/2e+00	1.142	2e-01	0.104	-0.942	-1.047	(0)
HZS	7.093e-06	8.212	2e-05	-5.149	-4.086	1.064	37.1
S(6)	3.220e-03						
NaSO4-	2.931e-03	1.667	/e-03	-2.533	-2.778	-0.245	46.
SO4-2	2.891e-04	9.748	8e-06	-3.539	-5.011	-1.472	26.
HSO4-	1.730e-16	2.987	e-15	-15.762	-14.525	1.237	42
		Cotumo					
		Satura	ition in	alces			
Phase	SI** lo	og IAP	log K(	298 K,	1 atm)		
CH4 (a)	1.37	-1.43	-2.80	CH4			
CO2 (g)	-7.38	-8.85	-1 47	CO2			
$H_2(\alpha)$	-4.37	-7 47	-3 10	U2			
H20(a)	1.57	0.15	-3.10	п <u>2</u>			
H20(g)	-1.00	-0.15	1.50	HZO			
HZS(g)	-3.03 -	-11.03	-7.99	H2S			
02 (g)	-74.86 -	-77.75	-2.89	02			
Sulfur	-4.65	0.23	4.88	S			
**For a gas, S For ideal ga	I = log10(fugac ses, phi = 1.	city). F	fugacity	y = press	ure * phi /	′l atm.	
End of simulat	ion						
End of simulat	100.						
Reading input	data for simula	ation 2.					
TITLEPa SOLUTION 2 pH 7.	rt 2 water water 0						
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END  TITLE  Part 2 wate Beginning of i	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solutior	calcul	ations.				
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END  TITLE Part 2 wate Beginning of i	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution	n calcul	ations.				
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END 	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution on 2. water	calcul	ations.				
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END  TITLE  Part 2 wate Beginning of i	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution on 2. water	calcul Solutio	ations.	sition			
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END Part 2 wate Beginning of i Initial soluti	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution on 2. water Molali	calcul Solutio	ations. on compo Moles	sition			
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END Part 2 wate Beginning of i Initial soluti Elements Pure water	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution on 2. water Molali	calcul Solutio	ations. on compo Moles	sition			
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END  TITLE Part 2 wate Beginning of i Initial soluti Elements Pure water	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution on 2. water  Molali	Solutio ty	ations. on compo Moles	solution			
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END TITLE Part 2 wate Beginning of i Initial soluti Elements Pure water	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution on 2. water Molali	Solutio ty	ations. on compo Moles tion of pH	sition solution = 7.00	0		
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END  TITLE Part 2 wate Beginning of i Initial soluti Elements Pure water	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution on 2. water Molali	Solutio ty	ations. on compo Moles tion of pH pe	solution = 7.00 = 4.00	0		
TITLEPa SOLUTION 2 pH 7. Temp EQUILIBRIU CO2(g) Calcit SAVE solut END  TITLE Part 2 wate Beginning of i Initial soluti Elements Pure water	rt 2 water water 0 25.0 M_PHASES -2.0 e 0.0 ion 2 r nitial solution on 2. water Molali E Conductance (p	Solutio ty escript	ations. on compo Moles tion of pH pe 25°C)	solution = 7.00 = 4.00	0		

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Activity of water = 1.0009' Ionic strength = 1.0009'0 Mass of water (kg) = 1.007e-07 Total alkalinity (eq/kg) = 1.217e-09 Total alkalinity (eq/kg) = 0.000e+00 Total carbon (mol/kg) = 0.000e+00 Total carbon (mol/kg) = 0.000e+00 Tetal carbon (mol/kg) = 0.000e+00 Tetal carbon (eq) = -1.217e-09 Percent error, 100*(Cat+lAnl) / (Cat+lAnl) = -0.60 Iterations = 0 Total 1 = 1.110124e+02 Total 0 = 5.550622e+01 Distribution of species Distribution of species			Volume (	$I_{1}$ = 1 0	0297				
<pre>Indic strangth = 1.007=07 Mass of vater (kg) = 1.017=09 Total alkalinity (eg/kg) = 0.000e+00 Total (cdmol/kg) = 0.000e+00 Temperature (*C) = 25.00 Electrical balance (eg) = -1.217e-09 Percent error, 100*(Cat-[An])/(Cat+[An]) = -0.60 Total 0 = 5.5506220+01 Total 0 = 5.5506220+01 Total 0 = 5.5506220+01 Distribution of species Distribution of species Distribution of species</pre>	Activity of water = 1.000								
Mass of water (kg)         1.0000+00           Total alkalinity (eg/kg)         1.217e-09           Total common (m0/kg)         0.0000+00           Temperature (*C)         25.00           Electrical balance (eg)         -1.217e-09           Percent error, 100*(Cat+[An])/(Cat+[An])         -0.60           Iterations         0           Total # = 1.110124e+02         Total # = 1.110124e+02           Total # = 1.100*(Cat+[An])/(Cat		net	Tonic streng	th = 1.0	070-07				
Total alkalinity (eq/kg)         1.217e-09           Total carbon (mc)/kg)         0.000e+00           Temperature (*C)         2.5.00           Electrical balance (eq)         -1.217e-09           Percent error, 100*(Cat-[An])/(Cat+[An]))         -0.60           Total C2         Total C2           Percent error, 100*(Cat-[An])/(Cat+[An]))         -0.60           Total C = 5.550622e+01		Mass	s of water (k	a) = 1.0	00e+00				
Total carbon (mol/kg) = 0.000+00 Total CO2 (mol/kg) = 25.00 Electrical balance (eg) = -1.217e-09 Percent error, 100*(Cat+lAn]) / (Cat+lAn]) Total H = 1.110124e+02 Total H = 1.110124e+02 Total G = 5.550622e+01 Distribution of species Distribution of species Distribution of species Distribution of species O Recent error, 100*Cat+lAn]) / (Cat+lAn]) OH- 1.013e-07 1.012e-07 -6.995 -6.995 -0.000 -4. H+ 1.001e-07 1.000e+00 1.744 0.000 0.000 18. H(0) 1.416e-25 H22 0.551e+01 1.000e+00 1.744 0.000 0.000 18. H(0) 1.416e-25 H2 0.079e-26 7.079e-26 -25.150 -25.150 0.000 28. O(0) 0.000e+00 0.000e+00 -42.080 -42.080 0.000 30. 	Total alkalinity (eq/kg) = 1.217e-09								
Total CO2 (mol/kg) = 0.000e+00 Temperature (*C) = 25.00 Electrical balance (eq) = -1.217e-09 Percent error, 100*(Cat- An])/(Cat+ An]) = -0.60 Total A = 0.60 Total A = 0.00 Total A = 1.110124e+02 Total O = 5.550E2e+01 		Total d	arbon (mol/k	(a) = 0.0	00e+00				
Temperature (*C)         25.00           Blectrical balance (eg)         -1.217e-09           Percent error, 100*(Cat-[An])/(Cat+[An])         -0.60           Iterations         0           Total H         1.110124e+02           Total O         = 5.350622e+01		Tota	al CO2 (mol/k	(a) = 0.0	00e+00				
Electrical balance [eq] = -1.217e-09 Percent error, 100*(Cat- An )/(Cat+ An ) = -0.60 Iterations = 0 Total G = 5.55022e+01 		Te	emperature (°	C) = 25.0	0				
Percent error, 100*(Cat-[An])/(Cat+[An]) = -0.60 Iterations = 0 Total H = 1.110124e+02 Total O = 5.550622e+01		Electrica	al balance (e	a) = -1.2	17e-09				
Iterations         0           Total H = 1.110124e+02 Total O = 5.550622e+01          Distribution of species	Percent	error, 100*(Cat- ]	An )/(Cat+ An	) = -0.6	0				
Total H = 1.110124e+02 Total O = 5.550622e+01          Distribution of species			Iteratio	ns = 0					
Total O = 5.550622e+01           Distribution of species           Log Log Log mole           Species           Molality         Activity         Molality         Activity         Gamma         cm²/m           OH         1.013e-07         1.012e-07         -6.955         -6.955         -0.000         -4.           H+         1.010e-07         -7.000         -7.000         -0.000         0.000           H20         5.551e+01         1.000e+00         1.744         0.000         0.000         18.           H20         1.416e-25         -25.150         -25.150         0.000         28.         0.000         0.000         30.           O(0)         0.000e+00         0.000e+00         -42.080         -42.080         0.000         30.			Total	H = 1.110	124e+02				
Distribution of species           Log         Log         Log         Log         Log         mole           Species         Molality         Activity         Molality         Activity         Gamma         cm*/m           OH-         1.013e-07         1.012e-07         -6.995         -6.995         -0.000         -4.           H+         1.001e-07         1.000e-07         -7.000         -7.000         -0.000         0.           H2         5.551e+01         1.000e+00         1.744         0.000         0.000         28.           O(0)         0.000e+00         -42.080         -42.080         0.000         28.           O(1)         0.000e+00         -42.080         -42.080         0.000         30.			Total	0 = 5.550	622e+01				
Distribution of species         Log Log Log mole           Species         Molality Activity Molality Activity Gamma cm³/m           OH-         1.013e-07         1.012e-07         -6.995         -0.000         -4.           H+         1.001e-07         1.000e-07         -7.000         -7.000         -0.000         0.           H20         5.551e+01         1.000e+00         1.744         0.000         0.000         18.           H2         7.079e-26         7.079e-26         -25.150         -25.150         0.000         28.           0(0)         0.000e+00         0.000e+00         -42.080         -42.080         0.000         30.									
Log         Log         Log         mole           OH-         1.013e-07         1.012e-07         -6.995         -0.000         -4.           H+         1.001e-07         1.000e-07         -7.000         -0.000         0.           H20         5.551e+01         1.000e+00         1.744         0.000         18.           H(0)         1.416e-25         1.7079e-26         -25.150         0.000         28.           O(1)         0.000e+00         0.000e+00         -42.080         -42.080         0.000         30.			Distributio	n of specie	s				
Log         Log         Log         Log         Log         mole           OH-         1.013e-07         1.012e-07         -6.995         -0.000         -4.           H+         1.001e-07         1.000e-07         -7.000         -7.000         -0.000         0.           H2         5.551e+01         1.000e+00         1.744         0.000         0.000         18.           H2         7.079e-26         7.079e-26         -25.150         -25.150         0.000         28.           0(0)         0.000e+00         0.000e+00         -42.080         -42.080         0.000         30.									
Species         Molality         Activity         Molality         Activity         Gamma         cm <sup>3</sup> /m           OH-         1.013e-07         1.012e-07         -6.995         -0.000         -4.           H+         1.001e-07         1.000e-07         -7.000         -0.000         0.01           H(0)         1.416e-25         1.000e+00         1.744         0.000         0.000         18.           H(0)         1.416e-25         7.079e-26         -25.150         -25.150         0.000         28.           O(0)         0.000e+00         0.000e+00         -42.080         -42.080         0.000         30.	<b>C</b>			Log	Log	Log	mole		
OH-       1.013e-07       1.012e-07       -6.995       -0.000       -4.         H+       1.001e-07       1.000e-07       -7.000       -7.000       0.000       0.000         H2O       5.551e+01       1.000e+00       1.744       0.000       0.000       18.         H2O       7.079e-26       7.079e-26       -25.150       -25.150       0.000       28.         0(0)       0.000e+00       0.000e+00       -42.080       -42.080       0.000       30.	Specie	s Molalit	y Activit	y Molality	Activity	Gamma	Cm <sup>3</sup> /m		
0n-       1.013e-0/7       1.012e-0/7       -6.995       -6.995       -0.000       -4.         H4       1.001e-0/7       1.000e+00       1.744       0.000       0.000       18.         H20       5.551e+01       1.000e+00       1.744       0.000       0.000       18.         H41       7.079e-26       7.079e-26       -25.150       -25.150       0.000       28.         0(0)       0.000e+00       0.000e+00       -42.080       -42.080       0.000       30.	017	1 010	1 010 -						
HT       1.000e-07       -7.000       -7.000       -0.000       0.000         H20       5.551e-01       1.000e+00       1.744       0.000       0.000       18.4         H(0)       1.416e-25       7.079e-26       7.079e-26       -25.150       -25.150       0.000       28.0         0(0)       0.000e+00       0.000e+00       -42.080       -42.080       0.000       30.         02       0.000e+00       0.000e+00       -42.080       -42.080       0.000       30.	UH-	1.013e-0	1.012e-0	/ -6.995	-6.995	-0.000	-4.		
hcc       1.0000000       1.744       0.000       0.000       18.         H(0)       1.416=25       7.079e-26       7.079e-26       -25.150       -25.150       0.000       28.         0(0)       0.0000e+00       0.0000e+00       -42.080       -42.080       0.000       30.         02       0.000e+00       0.0000e+00       -42.080       -42.080       0.000       30.         Phase       SI** log IAP       log K(298 K, 1 atm)         H2(g)       -22.05       -25.15       -3.10 H2         H20(g)       -1.50       0.00       1.50 H20         O2(g)       -39.19       -42.08       -2.89 O2         **For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.         For ideal gases, phi = 1.         Moles in assemblage         Beginning of batch-reaction calculations.         **For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.         For ideal gases, phi = 1.         ***For ideal gases, phi = 1.         ***For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.         ***For ideal gases, phi = 1.         ***********************************	H100	1.001e-0	1.000e-0	7 -7.000	-7.000	-0.000	0.0		
H2       7.079e-26       7.079e-26       -25.150       0.000       28.0         0(0)       0.000e+00       0.000e+00       -42.080       -42.080       0.000       30.0	H20	5.551e+(	1.000e+0	0 1.744	0.000	0.000	18.0		
number 20       7.075e-20       -25.150       -25.150       0.000       28.         02       0.000e+00       0.000e+00       -42.080       -42.080       0.000       30.	H2	7 0700-1	6 7 070- 0	6 _25 150	05 150	0 000	~~		
Oldstart	0(0)	0 0000+00	.0 /.0/9e=2	0 -25.150	-25.150	0.000	28.		
Saturation indices	02	0.00000000	0 000000	0 -42 080	-12 000	0 000	20		
Phase       SI** log IAP       log K(298 K, l atm)         H2(g)       -22.05       -25.15       -3.10 H2         H2O(g)       -1.50       0.00       1.50 H2O         O2(g)       -39.19       -42.08       -2.89 O2         **For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.         For ideal gases, phi = 1.         Beginning of batch-reaction calculations.	<u>v</u> 2	0.000000		-42.080	-42.080	0.000	30.		
Phase         SI** log IAP         log K(298 K, 1 atm)           H2(g)         -22.05         -25.15         -3.10         H2           H2O(g)         -1.50         0.00         1.50         H20           O2(g)         -39.19         -42.08         -2.89         O2           **For a gas, SI = logl0(fugacity). Fugacity = pressure * phi / 1 atm.           For ideal gases, phi = 1.			Saturatio	n indices					
Phase         SI** log IAP         log K(298 K, 1 atm)           H2(g)         -22.05         -25.15         -3.10         H2           H2O(g)         -1.50         0.00         1.50         H2O           O2(g)         -39.19         -42.08         -2.89         O2           ***For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.           For ideal gases, phi = 1.									
H2(g) -22.05 -25.15 -3.10 H2 H20(g) -1.50 0.00 1.50 H20 O2(g) -39.19 -42.08 -2.89 O2 **For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm. For ideal gases, phi = 1. 	Phase	SI**	log IAP lo	g K(298 K,	1 atm)				
H2(g) -22.05 -25.15 -3.10 H2 H2O(g) -1.50 0.00 1.50 H2O O2(g) -39.19 -42.08 -2.89 O2 **For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm. For ideal gases, phi = 1. 									
H2O(g)       -1.50       0.00       1.50       H2O         O2(g)       -39.19       -42.08       -2.89       O2         **For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.         For ideal gases, phi = 1.	H2(g)	-22.05	-25.15 -3	.10 H2					
O2(g)       -39.19       -42.08       -2.89       O2         **For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.         For ideal gases, phi = 1.	H2O(g)	-1.50	0.00 1	.50 H2O					
<pre>**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm. For ideal gases, phi = 1. </pre>				0.0 - 0					
<pre>**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm. For ideal gases, phi = 1. Beginning of batch-reaction calculations. Beginning of batch-reaction calculation. Below SI log IAP log K(T, P) Initial Final Delta Co2(g) -2.00 -3.47 -1.47 1.000e+01 9.998e+00 -1.646e-03 Below Below</pre>	02 (g)	-39.19	-42.08 -2	.89 02					
For ideal gases, phi = 1. Beginning of batch-reaction calculations. Reaction step 1. Using solution 2. water Using pure phase assemblage 1. Phase assemblage Phase SI log IAP log K(T, P) Initial Final Delta CO2(g) -2.00 -3.47 -1.47 1.000e+01 9.998e+00 -1.976e-03 Calcite 0.00 -8.48 -8.48 1.000e+01 9.998e+00 -1.646e-03 Solution composition Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03 Description of solution	02 (g)	-39.19	-42.08 -2	.89 02					
Beginning of batch-reaction calculations. Beaction step 1. Using solution 2. water Using pure phase assemblage 1. Phase assemblage Phase SI log IAP log K(T, P) Initial Final Delta CO2(g) -2.00 -3.47 -1.47 1.000e+01 9.998e+00 -1.976e-03 Calcite 0.00 -8.48 -8.48 1.000e+01 9.998e+00 -1.646e-03 Solution composition Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03 Description of solution	02(g) **For a g	-39.19 gas, SI = log10(fug	-42.08 -2 gacity). Fuga	.89 O2 city = pres:	sure * phi	/ 1 atm.			
Beginning of batch-reaction calculations. Reaction step 1. Using solution 2. water Using pure phase assemblage 1. Phase assemblage Phase assemblage Phase SI log IAP log K(T, P) Initial Final Delta CO2(g) -2.00 -3.47 -1.47 1.000e+01 9.998e+00 -1.976e-03 Calcite 0.00 -8.48 -8.48 1.000e+01 9.998e+00 -1.646e-03 Solution composition Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03 	O2(g) **For a g For ide	-39.19 mas, SI = log10(fug al gases, phi = 1.	-42.08 -2 Jacity). Fuga	.89 O2 city = pres:	sure * phi	/ 1 atm.			
Beginning of Datch-Feattion Calculations.         Reaction step 1.         Using solution 2. water         Using pure phase assemblage 1.	O2(g) **For a g For ide	-39.19 as, SI = log10(fug al gases, phi = 1.	-42.08 -2 gacity). Fuga	.89 O2 city = pres:	sure * phi	/ 1 atm.			
Reaction step 1. Using solution 2. water Using pure phase assemblage 1. Phase assemblage Moles in assemblage Phase SI log IAP log K(T, P) Initial Final Delta CO2(g) -2.00 -3.47 -1.47 1.000e+01 9.998e+00 -1.976e-03 Calcite 0.00 -8.48 -8.48 1.000e+01 9.998e+00 -1.646e-03 Solution composition Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03 Description of solution	O2(g) **For a g For ide	-39.19 as, SI = log10(fug al gases, phi = 1.	-42.08 -2	.89 O2 city = pres:	sure * phi	/ 1 atm.			
Reaction step 1. Using solution 2. water Using pure phase assemblage 1. Phase assemblage Moles in assemblage Phase SI log IAP log K(T, P) Initial Final Delta CO2(g) -2.00 -3.47 -1.47 1.000e+01 9.998e+00 -1.976e-03 Calcite 0.00 -8.48 -8.48 1.000e+01 9.998e+00 -1.646e-03 Solution composition Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03 Description of solution	O2(g) **For a g For ide Beginning	-39.19 mas, SI = log10(fug al gases, phi = 1.	-42.08 -2 yacity). Fuga	.89 O2 city = pres:  s.	sure * phi	/ 1 atm.			
Using solution 2. water Using pure phase assemblage 1. Phase assemblage Moles in assemblage Phase SI log IAP log K(T, P) Initial Final Delta CO2(g) -2.00 -3.47 -1.47 1.000e+01 9.998e+00 -1.976e-03 Calcite 0.00 -8.48 -8.48 1.000e+01 9.998e+00 -1.646e-03 Solution composition Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03 Description of solution	O2(g) **For a g For ide Beginning	-39.19 gas, SI = log10(fug al gases, phi = 1.	-42.08 -2 gacity). Fuga n calculation	.89 O2 city = pres: s. 	sure * phi	/ 1 atm.			
Using solution 2. water Using pure phase assemblage 1. Phase assemblage Moles in assemblage Phase SI log IAP log K(T, P) Initial Final Delta CO2(g) -2.00 -3.47 -1.47 1.000e+01 9.998e+00 -1.976e-03 Calcite 0.00 -8.48 -8.48 1.000e+01 9.998e+00 -1.646e-03 Solution composition Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03 	O2(g) **For a g For ide Beginning	-39.19 (as, SI = log10(fuc al gases, phi = 1. of batch-reaction step 1.	-42.08 -2 gacity). Fuga	.89 02 city = pres:  s. 	sure * phi	/ 1 atm.			
Using pure phase assemblage 1. 	O2(g) **For a g For ide Beginning  Reaction	-39.19 (as, SI = log10(fug cal gases, phi = 1. () of batch-reaction () step 1.	-42.08 -2 gacity). Fuga	.89 02 city = pres:  s. 	sure * phi	/ 1 atm.			
Phase       SI       log IAP       log K(T, P)       Initial       Final       Delta         CO2(g)       -2.00       -3.47       -1.47       1.000e+01       9.998e+00       -1.976e-03         Calcite       0.00       -8.48       -8.48       1.000e+01       9.998e+00       -1.646e-03         Elements       Molality       Moles         C       3.622e-03       3.622e-03         Ca       1.646e-03       1.646e-03	O2(g) **For a g For ide Beginning Reaction Using sol	-39.19 (as, SI = log10(fug (al gases, phi = 1. () of batch-reaction () step 1. () ution 2. water	-42.08 -2 gacity). Fuga	.89 02 city = pres:  s. 	sure * phi	/ 1 atm.			
Moles in assemblage           Phase         SI log IAP log K(T, P)         Initial         Final         Delta           CO2(g)         -2.00         -3.47         -1.47         1.000e+01         9.998e+00         -1.976e-03           Calcite         0.00         -8.48         -8.48         1.000e+01         9.998e+00         -1.646e-03           Elements         Molality         Moles         Moles         C         3.622e-03         3.622e-03           Ca         1.646e-03         1.646e-03        Description of solution	O2(g) **For a g For ide Beginning  Reaction Using sol Using pur	-39.19 as, SI = log10(fug al gases, phi = 1. of batch-reaction step 1. ution 2. water re phase assemblage	-42.08 -2 yacity). Fuga calculation	.89 02 city = pres:  s. 	sure * phi	/ 1 atm.			
Moles in assemblage           Phase         SI log IAP log K(T, P)         Initial         Final         Delta           CO2(g)         -2.00         -3.47         -1.47         1.000e+01         9.998e+00         -1.976e-03           Calcite         0.00         -8.48         -8.48         1.000e+01         9.998e+00         -1.646e-03	O2(g) **For a g For ide Beginning Reaction Using sol Using pur	-39.19 (as, SI = log10(fug eal gases, phi = 1. () of batch-reaction () step 1. () ution 2. water () e phase assemblage	-42.08 -2 yacity). Fuga n calculation 	.89 02 city = pres:  s. 	sure * phi	/ 1 atm.			
Moles in assemblage           Phase         SI log IAP log K(T, P) Initial         Final         Delta           CO2(g)         -2.00         -3.47         -1.47         1.000e+01         9.998e+00         -1.976e-03           Calcite         0.00         -8.48         -8.48         1.000e+01         9.998e+00         -1.646e-03          Solution composition        Solution composition	O2(g) **For a g For ide Beginning Reaction Using sol Using pur	-39.19 (as, SI = log10(fug cal gases, phi = 1. ) of batch-reaction step 1. ution 2. water re phase assemblage	-42.08 -2 gacity). Fuga calculation 	.89 02 city = pres:  s.  semblage	sure * phi	/ 1 atm.			
Phase         SI log IAP log K(T, P) Initial         Final         Delta           CO2(g)         -2.00         -3.47         -1.47         1.000e+01         9.998e+00         -1.976e-03           Calcite         0.00         -8.48         -8.48         1.000e+01         9.998e+00         -1.646e-03          Solution composition        Solution composition	O2(g) **For a g For ide Beginning Reaction Using sol Using pur	-39.19 (as, SI = log10(fug al gases, phi = 1. ) of batch-reaction step 1. ution 2. water re phase assemblage	-42.08 -2 gacity). Fuga calculation = 1.	.89 O2 city = pres:  s.  semblage	sure * phi	/ 1 atm.			
CO2(g)       -2.00       -3.47       -1.47       1.000e+01       9.998e+00       -1.976e-03         Calcite       0.00       -8.48       -8.48       1.000e+01       9.998e+00       -1.646e-03        Solution composition      Solution composition	O2(g) **For a g For ide Beginning Reaction Using sol Using pur	-39.19 (as, SI = log10(fuc (al gases, phi = 1. ( of batch-reaction step 1. ution 2. water re phase assemblage	-42.08 -2 gacity). Fuga calculation = 1.	.89 O2 city = pres:  s.  semblage	sure * phi Moles	/ l atm.  in assembla	age		
CU2(g)       -2.00       -3.47       -1.47       1.000e+01       9.998e+00       -1.976e-03         Calcite       0.00       -8.48       -8.48       1.000e+01       9.998e+00       -1.646e-03        Solution composition	O2(g) **For a g For ide Beginning Reaction Using sol Using pur  Phase	-39.19 (as, SI = log10(fuc cal gases, phi = 1. (of batch-reaction step 1. (ution 2. water re phase assemblage SI log	-42.08 -2 gacity). Fuga calculation Phase as g IAP log K(	.89 O2 city = pres:  s.  semblage T, P) Init	sure * phi Moles tial	/ l atm. in assembla Final	age Delta		
Calcite         0.00         -8.48         -8.48         1.000e+01         9.998e+00         -1.646e-03          Solution composition        Solution composition	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase	-39.19 (as, SI = log10(fuc cal gases, phi = 1. (of batch-reaction step 1. (ution 2. water re phase assemblage SI log	-42.08 -2 yacity). Fuga calculation Phase as y IAP log K(	.89 O2 city = press  s.  s. T, P) Init	sure * phi Moles tial	/ l atm. in assembla Final	age Delta		
Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g)	-39.19 (as, SI = log10(fuc eal gases, phi = 1. (of batch-reaction step 1. (ution 2. water re phase assemblage SI log -2.00 -	-42.08 -2 yacity). Fuga in calculation a 1. Phase as y IAP log K( -3.47 -1.	.89 02 city = pres:  s.  T, P) Init 47 1.0004	Moles tial 9.9	/ 1 atm. in assembla Final 98e+00 -1	age Delta .976e-03		
Elements Molality Moles C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite	-39.19 (as, SI = log10(fug eal gases, phi = 1. (of batch-reaction step 1. (ution 2. water re phase assemblage SI log -2.00 - 0.00 -	-42.08 -2 gacity). Fuga 	.89 02 city = pres:  s.  T, P) Init 47 1.000 48 1.000	Moles tial e+01 9.9 e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		
Elements         Molality         Moles           C         3.622e-03         3.622e-03           Ca         1.646e-03         1.646e-03	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite	-39.19 (as, SI = log10(fug (al gases, phi = 1. ( of batch-reaction ( step 1. (ution 2. water ( phase assemblage SI log -2.00 0.00	-42.08 -2 yacity). Fuga 	.89 02 city = pres:  s.  T, P) Init 47 1.000 48 1.000	Moles tial e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		
C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite	-39.19 (as, SI = log10(fuc (al gases, phi = 1. ( of batch-reaction step 1. ution 2. water re phase assemblage SI log -2.00 - 0.00 -	-42.08 -2 yacity). Fuga calculation Phase as y IAP log K( -3.47 -1. 8.48 -8. Solution c	.89 02 city = pres:  s.  T, P) Init 47 1.000 48 1.000 omposition	Moles tial e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		
C 3.622e-03 3.622e-03 Ca 1.646e-03 1.646e-03	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite	-39.19 (as, SI = log10(fuc (al gases, phi = 1. ( of batch-reaction step 1. ution 2. water re phase assemblage SI log -2.00 0.00	-42.08 -2 yacity). Fuga Phase as y IAP log K( -3.47 -1. -8.48 -8. Solution c	.89 02 city = pres:  s.  T, P) Init 47 1.0004 48 1.0004 omposition	Moles tial e+01 9.9 e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		
Ca 1.646e-03 1.646e-03	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite Eleme	-39.19 (as, SI = log10(fuc (al gases, phi = 1. ( of batch-reaction ( step 1. ( ution 2. water ( phase assemblage SI log -2.00 0.00 -2.00 -2.00 0.00 -2	-42.08 -2 yacity). Fuga 	.89 02 city = pres:  s.  T, P) Init 47 1.0006 48 1.0006 omposition oles	Moles tial e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		
Description of solution	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite Eleme	-39.19 (as, SI = log10(fuc (al gases, phi = 1. ( of batch-reaction step 1. ( ution 2. water re phase assemblage SI log -2.00 - 0.00 - mts Mola	-42.08 -2 yacity). Fuga calculation Phase as y IAP log K(' -3.47 -1. -8.48 -8. Solution co lity M	.89 02 city = pres:  s.  T, P) Init 47 1.0004 48 1.0000 omposition oles	Moles tial e+01 9.9 e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		
Description of solution	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite Eleme C	-39.19 (as, SI = log10(fug (al gases, phi = 1. ( of batch-reaction step 1. ( ution 2. water re phase assemblage SI log -2.00 0.00 -2.00 -0.00	-42.08 -2 yacity). Fuga 	.89 02 city = pres:  s.  T, P) Init 47 1.000 48 1.000 omposition oles e-03 	Moles tial e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		
	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite Eleme C Ca	-39.19 (as, SI = log10(fug (al gases, phi = 1. ( of batch-reaction step 1. ( ution 2. water re phase assemblage SI log -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 0.00 -2.00 -2.00 0.00 -2.	-42.08 -2 yacity). Fuga 	.89 02 city = pres:  s.  T, P) Init 47 1.000 48 1.000 omposition oles e-03 e-03	Moles tial e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		
	O2(g) **For a g For ide Beginning Reaction Using sol Using pur Phase CO2(g) Calcite Eleme C Ca	-39.19 (as, SI = log10(fuc (al gases, phi = 1. ( of batch-reaction step 1. ution 2. water re phase assemblage SI log -2.00 - 0.00 - mts Mola 3.622 1.646	-42.08 -2 yacity). Fuga 	.89 02 city = pres:  s.  T, P) Init 47 1.000 48 1.000 omposition cles e-03 e-03 of solution	Moles tial e+01 9.9	/ 1 atm. in assembla Final 98e+00 -1 98e+00 -1	age Delta .976e-03 .646e-03		

		r	H = 7.29	7 Cł	harge balance	
		r	e = -1.57	15 Ac	diusted to re	dox
		P	quilibrium	0 A	Jubieu to re	JUUN
Specifi	c Conductance (u	S/cm, 25°C	= 306			
	Den	sity (g/cm <sup>3</sup>	) = 0.99	726		
	0011	Volume (I	) = 1.00	300		
	Activ	ity of wate	r = 1.00	0		
	To	nic strengt	h = 4.82	6-03		
	Massio	f water (kc	1 = 1.02	00+00		
	Total alkali	nity (eg/kg	) = 3.20	10-03		
	Total	CO2 (mol/kg	) = 3.23	20-03		
	Tomo	erature (°C	) = 3.02	220-03		
	Electrical	balance ( c	1.21	70-09		
Percent erro	r 100*/CatalAni	)//Cattland	) = -1.21	1/6-09		
Lercenc erro	1, 100 (Cat- AII)	Ttoration		)		
		TLEFALION	$S = \pm 7$	240102		
		Total	H = 1.1101	240+02		
		Total	0 = 5.5515	bile+01		
	D	t a bard brock t an				
	D	istribution	or species	;======		
					T. C.	
Creation	Malaliter		Log	Log	g Log	mole
Species	Molality	Activity	Molality	Activity	y Gamma	cm <sup>3</sup> /mo
0.11	0 1 60 07	0 005 05	c . c . c . c	c		
OH-	2.162e-07	2.005e-07	-6.665	-6.698	-0.033	-4.0
H+	5.401e-08	5.048e-08	-7.268	-7.29	7 -0.029	0.0
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.0
C (-4)	1.401e-25					
CH4	1.401e-25	1.403e-25	-24.854	-24.853	3 0.000	35.
C(4)	3.622e-03					
HCO3-	3.224e-03	2.998e-03	-2.492	-2.523	3 -0.032	24.
C02	3.399e-04	3.403e-04	-3.469	-3.468	3 0.000	34.
CaHCO3+	4.887e-05	4.549e-05	-4.311	-4.342	2 -0.031	9.
CaCO3	5.559e-06	5.565e-06	-5.255	-5.255	5 0.000	-14.
CO3-2	3.724e-06	2.785e-06	-5.429	-5.555	5 -0.126	-5.2
(CO2)2	2.123e-09	2.125e-09	-8.673	-8.673	3 0.000	68.1
Ca	1.646e-03					
Ca+2	1.591e-03	1.189e-03	-2.798	-2.92	5 -0.126	-18.0
CaHCO3+	4.887e-05	4.549e-05	-4.311	-4.342	2 -0.031	9.
CaCO3	5.559e-06	5.565e-06	-5.255	-5.25	5 0.000	-14.6
CaOH+	4.213e-09	3.910e-09	-8.375	-8.40	8 -0.032	(0)
H(O)	5.090e-15					
H2	2.545e-15	2.548e-15	-14.594	-14.59	4 0.000	28.0
0(0)	0.000e+00					
02	0.000e+00	0.000e+00	-63.193	-63.19	2 0.000	30.4
		-Saturatior	indices			
Phase	SI** lo	g IAP loc	K(298 K,	1 atm)		
Aragonite	-0.14	-8.48 -8.	34 CaCO3			
0.1.11	0.00	-8.48 -8.	48 CaCO3			
Calcite	-22.05 -	24.85 -2.	80 CH4			
Calcite CH4(g)	-2.00	-3.47 -1	47 CO2 Pr	ressure	0.0 atm. phi	1.000
Calcite CH4 (g) CO2 (a)	-Z.UU		10 H2	COULC	c.o dem, pill	1.000
Calcite CH4 (g) CO2 (g) H2 (g)	-11.49 -	14.59 -3				
Calcite CH4 (g) CO2 (g) H2 (g) H2O (g)	-11.49 -	14.59 -3.	50 H20			
Calcite CH4 (g) CO2 (g) H2 (g) H2O (g) O2 (g)	-11.49 - -1.50	$ \begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	50 H20			
Calcite CH4 (g) CO2 (g) H2 (g) H2O (g) O2 (g)	-11.49 - -1.50 -60.30 -	14.59 -3. -0.00 1. 63.19 -2.	50 H20 89 O2			
Calcite CH4(g) CO2(g) H2(g) H2O(g) O2(g)	-11.49 - -1.50 -60.30 -	14.59 -3. -0.00 1. 63.19 -2.	50 H20 89 O2		. / 1 .t-	
Calcite CH4(g) CO2(g) H2(g) H2O(g) O2(g) **For a gas,	-2.00 -11.49 - -1.50 -60.30 - SI = log10(fugac	14.59 -3. -0.00 1. 63.19 -2. ity). Fugac	50 H20 89 O2 ity = press	sure * ph:	i / 1 atm.	
Calcite CH4(g) CO2(g) H2(g) H2O(g) O2(g) **For a gas, For ideal g	-11.49 - -11.50 -60.30 - SI = log10(fugac ases, phi = 1.	14.59 -3. -0.00 1. 63.19 -2. ity). Fugac	50 H20 89 O2 ity = press	sure * ph:	i / 1 atm.	
Calcite CH4(g) CO2(g) H2(g) H2O(g) O2(g) **For a gas, For ideal g	-11.49 - -11.50 -60.30 - SI = log10(fugac ases, phi = 1.	14.59 -3. -0.00 1. 63.19 -2. ity). Fugac	50 H20 89 O2 ity = press	sure * ph	i / 1 atm.	
Calcite CH4 (g) CO2 (g) H2 (g) H2 (g) O2 (g) **For a gas, For ideal g	-2.00 -11.49 - -1.50 -60.30 - SI = log10(fugac ases, phi = 1.	14.59 -3. -0.00 1. 63.19 -2. ity). Fugac	50 H20 89 O2 ity = press	sure * ph:	i / 1 atm.	

3:57 PM

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C:\get\usgs\phreeqc\work\holden\nahs\nahs7_1e3.out
                                                                                     7
 383
      384
      Reading input data for simulation 3.
 385
       386
 387
          TITLE -- Part 3 mix the two
 388
          MIX 1
 389
                 0.001
          1 0.001
2 0.999
 390
          SAVE solution 3
 391
 392
          END
 393
 394
       TITLE
 395
       ____
 396
 397
        -- Part 3 mix the two
 398
 399
       Beginning of batch-reaction calculations.
 400
 401
       402
 403
       Reaction step 1.
 404
 405
       Using mix 1.
 406
 407
       Mixture 1.
 408
            1.000e-03 Solution 1 Solution after simulation 1.
9.990e-01 Solution 2 Solution after simulation 2.
 409
 410
 411
       -----Solution composition-----
 412
 413
 414
          Elements
                           Molality
                                          Moles
 415
                                     3.718e-03
          С
                           3.718e-03
 416
 417
          Ca
                           1.644e-03
                                      1.644e-03
 418
         Na
                           9.424e-03
                                      9.423e-03
 419
          S
                           7.950e-03
                                      7.950e-03
 420
 421
       -----Description of solution-----
 422
                                           pH = 9.515
pe = -6.726
 423
                                                           Charge balance
 424
                                                            Adjusted to redox
                                           equilibrium
            Specific Conductance (\muS/cm, 25°C) = 1217
 425
 426
                              Density (g/cm^3) = 0.99763
 427
                                   Volume (L) = 1.00312
                             Activity of water = 1.000
Ionic strength = 1.362e-02
 428
 429
                       Mass of water (kg) = 1.000e+00
Total alkalinity (eq/kg) = 1.235e-02
Total CO2 (mol/kg) = 3.536e-03
Temperature (°C) = 25.00
 430
 431
 432
 433
 434
                       Electrical balance (eq) = -1.215e-09
 435
        Percent error, 100*(Cat-|An|)/(Cat+|An|) = -0.00
                                    Iterations = 19
 436
 437
                                      Total H = 1.110191e+02
 438
                                      Total O = 5.551540e+01
 439
 440
       -----Distribution of species-----
 441
 442
                                                       Log
                                                  Log
                                                                   Log mole V
 443
         Species
                        Molality Activity Molality Activity Gamma cm3/mol
 444
 445
         OH-
                        3.738e-05 3.312e-05 -4.427 -4.480
                                                                  -0.052
                                                                            -4.01
```

gaphicedowo	k\holden\nahs\nahs7_1e3.out					
H+	3.382e-10	3.055e-10	-9.471	-9.515	-0.044	0.00
H20	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.07
C(-4)	1.818e-04					
CH4	1.818e-04	1.824e-04	-3.740	-3.739	0.001	35.46
C(4)	3.536e-03					
HCO	3- 2.480e-03	2.214e-03	-2.606	-2.655	-0.049	24.79
CO3	-2 5.353e-04	3.399e-04	-3.271	-3.469	-0.197	-4.9
CaC	03 4.262e-04	4.276e-04	-3.370	-3.369	0.001	-14.60
NaC	03- 5.929e-05	5.269e-05	-4.227	-4.278	-0.051	-0.8
CaH	2.364e-0	2.115e-05	-4.626	-4.675	-0.048	9.7
NaH	1.033e-05	1.037e-05	-4.986	-4.984	0.001	1.8
CO2	1.516e-0	5 1.521e-06	-5.819	-5.818	0.001	34.4
(CO	2)2 4.233e-1	4.247e-14	-13.373	-13.372	0.001	68.8
Ca	1.644e=03		20.070	10.072	0.001	00.0
Ca+	2 1.180e-0	3 7.488e-04	-2.928	-3.126	-0.198	-17.8
CaC	4 262e=0	4 276e=04	-3 370	-3 369	0.001	-14 6
Call	2 3640-0	2 1150-05	-1 626	-1 675	-0.049	9.7
Car	1 267~_0	1 3710-05	-4.020	-4.0/5	0.040	7.1
Cas	1.30/e-U	1.3/10-03	-4.804	-4.803	-0.001	1.5
Cao	4.5/60-0	4.06/e-0/	-0.340	-0.391	-0.051	(0)
CaH	504+ 3.098e-14	2.753e-14	-13.509	-13.560	-0.051	(0)
H(0)	3.730e-09	1 074 65				
H2	1.865e-0	1.871e-09	-8.729	-8.728	0.001	28.6
Na	9.424e-03					
Na+	9.349e-03	8.326e-03	-2.029	-2.080	-0.050	-1.3
NaC	03 5.929e-0	5.269e-05	-4.227	-4.278	-0.051	-0.8
NaH	CO3 1.033e-0	5 1.037e-05	-4.986	-4.984	0.001	1.8
NaS	04- 4.814e-0	6 4.297e-06	-5.318	-5.367	-0.049	14.4
NaC	H 2.749e-1	7 2.758e-17	-16.561	-16.559	0.001	(0)
0(0)	0.000e+00					
02	0.000e+0	0.000e+00	-74.926	-74.924	0.001	30.4
S(-2)	7.768e-03					
HS-	7.746e-0	6.864e-03	-2.111	-2.163	-0.052	20.6
H2S	1.828e-0	1.833e-05	-4.738	-4.737	0.001	37.1
S-2	4.299e-0	6 2.714e-06	-5.367	-5.566	-0.200	(0)
5(6)	1.818e-04		0.007	0.000	0.200	(0)
504	-2 1 633e=0	1 1 030e-04	-3 787	-3 987	-0.200	14 8
Cas	1.055c -0	5 1 3710-05	-4 864	-4 863	0.001	7 5
NaS	04- 4.814e-0	6 A 2970-06	-5 318	-5 367	-0.049	14 4
HQC HQC	A_ 3.441e_1	3 0586-12	-11 /63	-11 515	-0.051	10.3
Col	- 5.4416-1. COA: 2.000o-1	2 3.050e-12	-12 500	-12 560	-0.051	40.5
Can	504+ 5.098e-1	4 2.7558-14	-13.509	-13.560	-0.051	(0)
		Saturation	indices			
Dhee	0744	LOG TAD 100	V/200 V	1 ot=\		
Fnas	e 51**.	LOG TAP TOG	V(530 K'	1 acm)		
Anhy	drite -2.84	-7.11 -4.2	8 CaSO4			
Arad	onite 1.74	-6.59 -8.3	4 CaCO3			
Calc	ite 1.89	-6.59 -8.4	8 CaCO3			
CH4	a) -0.94	-3.74 -2.8	0 CH4			
CO2 /	a) -4.35	-5.82 -1 4	7 CO2			
Gune	um -2.53	-7.11 -4 9	8 CaS04 · 1	2820		
U2/0	-2.55	-8 73 -2 1	0 42	51120		
H20/	-5.63	-0.00 1 5	0 420			
1200	g) -1.50	-0.00 1.5	0 120			
HZS (	9) -3.69	-11.08 -/.5	HZS			
02 (g	-72.03	-/4.92 -2.8	9 02			
Sulf	ur -4.04	0.84 4.8	18 S			
**For	a gas, SI = log10(fug.	acity). Fugaci	tv = press	sure * phi	/ 1 atm.	
For	ideal gases, phi = 1.		-1 [01000	P		
De 1						
End of	simulation.					

#### C:\get\usgs\phreeqc\work\holden\nahs\nahs7\_1e3.out

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#### Appendix C. Diffusion Models Script

```
C:\cygwin64\home\cwen461\work\octave\nahs\h2s_diff.m
```

```
# h2s_diff.m will calculate diffusion through liquid and gas phases along with
1
     volatilization fluc rate of hydrogen sulfide from water.
2
     clear all;
3
    t = [0:100]; #seconds
 4
     z = [0:200]; # cm
5
 6
     MW = 34.076; #g/mol
8
     sol = 5.66; # g/L
     Vp = 13376; # vapor pressure mmHg (17.6 atm)
9
     H1 = 9.8; # Henry's Law constant atm/mole/L
10
11
12
13
     diffw = 2e-5; # diffusion coefficient water (cm<sup>2</sup>/sec) 25C
14
     diffa = 0.166; # diffusion coefficient air (cm^2/sec) 25C
15
     volw = 3946.5; #volume of water (gallons)
volw = volw * 3.7854; # (L)
16
17
18
     #sa = 8*43; # water surface area in tank (ft^2)
19
     #sa = sa * 929.0304; # surface area (cm^2)
     sa = 7.6e4;
                        # (cm^2)
20
21
22
     conc = 8.88e-6; # (mole/L) calcluted with PHREEQC NaHS soln at pH = 11.5 25C
     concg = conc * MW; # g/L
tmass = conc*volw; # (grams)
23
24
25
26
27
     x = conc/55.55; # mole fraction (moles h2s / mole water)
28
     y = conc * H1; #mole fraction gas phase (equals partial pressure (atm))
29
30
     x1 = conc/1000; # mole/cm^3 liquid phase
31
     y1 = y/24400; # mole/cm^3 gas phase mole air = 24.4L at 25C 1000cm^3/L
32
33
     34
     # flux calculations in gas phase
35
     # t = 60 seconds flux at surface z=0
36
     jxt600 = (diffa/(pi*60))^(0.5)*y1  # flux mole/(cm^2 sec) at 60 seconds
jxt600 = (diffa/(pi*600))^(0.5)*y1  # flux mole/(cm^2 sec)

37
38
39
     jxt6000 = (diffa/(pi*6000))^(0.5)*y1
jxt60000 = (diffa/(pi*6000))^(0.5)*y1
                                                  # flux mole/(cm^2 sec) at 600 seconds
                                                     # flux mole/(cm^2 sec) at 6000 seconds
40
      jxt60000 = (diffa/(pi*60000))^(0.5)*y1
                                                     # flux mole/(cm^2 sec) at 60000 seconds
41
42
43
     # concentration calculations
44
     eta60 = (4*diffa*60)^{(-0.5)*z};
45
     eta600 = (4*diffa*600)^{(-0.5)*z};
46
      eta6000 = (4*diffa*6000)^(-0.5)*z;
47
48
      eta60000 = (4*diffa*60000)^(-0.5)*z;
     eta600000 = (4*diffa*600000)^{(-0.5)*z};
49
     eta6000000 = (4*diffa*6000000)^(-0.5)*z;
eta60000000 = (4*diffa*6000000)^(-0.5)*z;
50
51
52
53
54
     cz60 = y*ones(size(z)) - y * erf(eta60);
     cz600 = y*ones(size(z)) - y * erf(eta600);
cz6000 = y*ones(size(z)) - y * erf(eta6000);
cz60000 = y*ones(size(z)) - y * erf(eta60000);
55
56
57
     cz600000 = y*ones(size(z)) - y * erf(eta600000);
cz6000000 = y*ones(size(z)) - y * erf(eta6000000);
cz60000000 = y*ones(size(z)) - y * erf(eta60000000);
58
59
60
61
62
     figure(1)
63
```

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```
C:\cvgwin64\home\cwen461\work\octave\nahs\h2s diff.m
                                                                                                 2
        plot(z,cz60,z,cz600,z,cz6000,z,cz60000,z,cz600000,z,cz6000000,z,cz6000000), xlabel(
   64
         "Diffusion into Headspace (cm) "),...
ylabel("Gas Phase Mole Fraction H_2S "), title("Gas Phase Diffusion of H_2S
   65
         t=(1,10,100,1000,...1e6) minutes)")
   66
   67
       print -dpdf figl.pdf
   68
       print -dpng figl.png
   69
   70
   71
         72
        # consider constant liquid diffusion to ss
   73
   74
        t1 = 6*logspace(2,9);
   75
   76
        i=0;
   77
        for j = 1:length(t1);
   78
        i=i+1;
   70
        eta(i,:) = ((4*diffw*t1(j))^(-0.5))*z;
   80
        cz(i,:) = x*erfc(eta(i,:)); # x is mole fraction
   81
        end;
   82
   83
        figure(2)
   84
        mesh(cz), xlabel("Distance (cm)"), ylabel("Time (sec)"), zlabel("Liquid Phase Mole
        Fraction of H_2S"), title('Depth of H 2S Diffusion as t \rightarrow \infty')
   85
        print -dpdf fig2.pdf
       print -dpng fig2.png
   86
   87
   88
        figure (3)
        plot(z,cz),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"),
title('Depth of H 2S Diffusion as t \rightarrow \infty')
   89
   90
        print -dpdf fig3.pdf
   91
        print -dpng fig3.png
   92
   93
   94
        figure (4)
   95
        plot(z,cz(32,:),z,cz(33,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole
        Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days")
   96
   97
        print -dpdf fig4.pdf
   98
        print -dpng fig4.png
   99
  100
        front_speed1 = (90-77)/(t1(33)-t1(32))*(3600*24) # cm/day
  101
        cz (32,77)
  102
        cz (33,90)
  103
  104
        dist 180 1 = front speed1 * 180
  105
  106
        depth = 1000*volw/sa
  107
  108
        # check fourier number z^2/(diff*time)
  109
        # assume 100 cm
  110
        diff time = 100^{2}/diffw
                                    # 100cm time for 100cm saturation
        diff_depth_6_mo = (diffw*1.555e7)^(0.5) # diffusion depth in 6 months using
  112
        Fourier number
  113
  114
115
        ***********************************
        # consider pulse solution
  116
  117
        t2 = 6*logspace(1,8);
  118
        i=0;
  119
        for j = 1:length(t2);
  120
  121
        i=i+1;
```

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<pre>22 cl1;) = (tmass(t+p1*dirW+2(j))."(=0.3)).*exp(-2."2/(t*p1*dirW+2(j))); # (     grams/zm*3) 23 end; 24 25 figure(5) 26 mesh(c), xlabel("Distance (cm)"),ylabel("Time (sec)"), zlabel("Liquid Phase Mole Praction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 27 28 print -dpdf fig5.pdf 29 print -dpdf fig6.pdf 20 plot(z,c)(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Praction of H_2S"),     title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 30 31 figure(6) 32 plot(z,c)(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Praction of H_2S"),     title('Depth of H_2S Diffusion from 134 to 6944 days") 33 print -dpdf fig7.pdf 34 print -dpdf fig7.pdf 35 print -dpdf fig7.pdf 36 print -dpdf fig8.pdf 37 figure(6) 37 figure(6) 48 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Praction of H_2S"), 49 print -dpdf fig8.pdf 40 print -dpdf fig8.pdf 41 print -dpdf fig8.pdf 42 print -dpdf fig8.pdf 43 print -dpdf fig8.pdf 44 print -dpdf fig8.pdf 45 print -dpdf fig8.pdf 46 print -dpdf fig8.pdf 47 print -dpdf fig8.pdf 47 print -dpdf fig8.pdf 48 c(39,112) 40 c(39,112) 41 c(39,112)/(t2(40)-t2(39))*(3600*24)</pre>	0.0		- 2
<pre>23 end; 24 25 figure(5) 26 mesh(c), xlabel("Distance (cm)"),ylabel("Time (sec)"), zlabel("Liquid Phase Mole 27 28 print -dpdf fig5.pdf 29 print -dpdf fig5.pdf 20 plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), 30 title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 33 print -dpdf fig6.pdf 34 print -dpdf fig6.pdf 35 print -dpdf fig6.pdf 36 figure(7) 39 plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of 39 H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") 40 print -dpdf fig7.pdf 41 print -dpdf fig7.pdf 42 figure(8) 44 plot(z,c(39:), z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole 55 Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 45 Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 46 print -dpdf fig8.pdf 47 print -dpdf fig8.pdf 49 c(39,112) 49 c(40,130) 40 c(40,130) 51 t2(39)/2.592e6  # months 52 c(39,1) 53 c(39,1) 54 c(39,1) 55 c(39,1)</pre>	22	c(1,:) = (tmass*(4*p1*diffw*t2(j)).^(-0.5)).*exp(-z.^2/(4*p1*diffw*t2(j))); # ( grams/cm^3)	
<pre>figure(5) figure(5) figure(5) figure(5) figure(5) fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') figure(6) figure(6) figure(6) figure(6) figure(7) figure(7)</pre>	23	end;	
<pre>25 figure(5) 26 mesh(c), xlabel("Distance (cm)"),ylabel("Time (sec)"), zlabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 27 28 print -dpdf fig5.pdf 29 print -dpdf fig5.pdf 29 plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), 20 title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 39 print -dpdf fig6.pdf 30 figure(7) 39 plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of 39 H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") 40 print -dpdf fig7.pdf 41 print -dpdf fig7.pdf 42 figure(8) 44 plot(z,c(39):),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 45 print -dpdf fig8.pdf 47 print -dpdf fig8.pdf 48 c(39,112) 49 c(40,130) 49 c(39,112) 49 title(B) 49 c(39,112) 40 c(40,130) 50 fort_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	24		
<pre>26 mesh(c), xlabel("Distance (cm)"),ylabel("Time (sec)"), zlabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 27 27 30 31 figure(6) 32 plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), 33 34 title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 35 print -dpdf fig6.pdf 36 figure(7) 36 plot(z,c(26:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of 37 figure(7) 39 plot(z,c(26:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of 37 figure(7) 39 plot(z,c(26:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of 37 figure(8) 40 print -dpdf fig7.pdf 41 print -dpdf fig7.pdf 42 plot(z,c(26);), z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole 54 Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 55 er(39,112) 56 c(40,130) 51 front speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	25	figure (5)	
<pre>print -dpdf fig5.pdf print -dpdf fig5.png figure(6) plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') print -dpdf fig6.pdf print -dpdf fig6.pdf plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") print -dpdf fig7.pdf print -dpdf fig7.pdf print -dpdf fig8.pdf print -dpdf fig8.pdf print -dpdf fig8.pdf print -dpdf fig8.pdf print -dpdf fig8.pdf print -dpdf fig8.pdf f print -dpdf fig8.pdf print -dpdf fig8.pdf f print -d</pre>	26	<pre>mesh(c), xlabel("Distance (cm)"),ylabel("Time (sec)"), zlabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty')</pre>	
<pre>print -dpdf fiq5.pdf print -dpdf fiq5.png figure(6) plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') print -dpdf fiq6.pdf print -dpdf fiq6.pdf plot(z,c(36:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") print -dpdf fiq7.pdf print -dpdf fiq7.pdf print -dpdf fiq7.pdf figure(8) figure(8) print -dpdf fiq8.pdf print -dpdf fiq8.pdf print -dpdf fiq8.pdf print -dpdf fiq8.pdf front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	27		
<pre>print -qbqf fig5.png print -qbqf fig5.png figure(6) plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') print -dpdf fig6.pdf print -dpdf fig6.pdf figure(7) print -dpdf fig7.pdf print -dpdf fig7.pdf figure(8) plot(z,c(39.:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") print -dpdf fig7.pdf figure(6) plot(z,c(39.:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") print -dpng fig8.pdf print -dpng fig8.pdf fort speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	28	print _dndf fig5 ndf	
<pre>print = dping fig5.png figure(6) plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') print = dping fig6.pdf print = dping fig6.png figure(7) plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") print = dping fig7.pdf print = dping fig7.png figure(8) print = dping fig8.pdf print = dping fig8.pdf print = dping fig8.pdf sc (39,112) c (40,130) front speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	20	print doug figs.put	
<pre>30 figure(6) 31 figure(6) 32 plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), 33 34 print -dpdf fig6.pdf 35 print -dpng fig6.png 36 37 figure(7) 39 40 print -dpdf fig7.pdf 41 print -dpng fig7.pdf 42 43 figure(8) 44 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") 45 46 print -dpng fig7.png 47 48 figure(8) 49 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 45 46 print -dpdf fig8.pdf 47 print -dpng fig8.png 48 c (39,112) 51 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	22	princ -dpig rigs.pig	
<pre>31 Ingure(0) 32 plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 33 34 print -dpdf fig6.pdf 35 print -dpdf fig6.pdf 35 plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of 36 H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") 39 40 print -dpdf fig7.pdf 41 print -dpdf fig7.pdf 42 figure(8) 42 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole 43 Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 44 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole 45 Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 46 print -dpdf fig8.pdf 47 print -dpdf fig8.pdf 48 c(39,112) 50 c(40,130) 51 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	30		
<pre>32 plot(2,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_25"), 33 title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty') 34 print -dpdf fig6.pdf 35 print -dpng fig6.png 36 37 figure(7) 39 plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") 39 40 print -dpdf fig7.pdf 41 print -dpng fig7.png 42 42 figure(8) 44 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 45 46 print -dpdf fig8.pdf 47 print -dpng fig8.png 48 49 c(39,112) c(40,130) 51 front speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	31	figure (6)	
<pre>33 34 print -dpdf fig6.pdf 35 print -dpng fig6.png 35 36 36 37 38 plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of 39 40 print -dpdf fig7.pdf 41 print -dpng fig7.png 42 43 figure(8) 44 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole 55 Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 45 print -dpng fig8.pdf 46 print -dpdf fig8.pdf 47 print -dpng fig8.png 48 49 c(39,112) 50 c(40,130) 51 52 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	32	<pre>plot(z,c),xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title('Pulse Release Depth of H_2S Diffusion as t \rightarrow \infty')</pre>	
<pre>34 print -dpdf fig6.pdf 5 print -dpng fig6.png 37 figure(7) 38 plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") 39 40 print -dpdf fig7.pdf 41 print -dpng fig7.png 42 42 figure(8) 43 figure(8) 44 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole 54 Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 45 print -dpdf fig8.pdf 47 print -dpdf fig8.pdf 48 c(39,112) 50 c(40,130) 51 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	33		
<pre>35 print -dpng fig6.png 36 37 figure(7) 38 plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of 39 40 print -dpdf fig7.pdf 41 print -dpng fig7.png 42 43 figure(8) 44 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole 54 Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 45 print -dpdf fig8.pdf 46 print -dpdf fig8.pdf 47 print -dpng fig8.png 48 49 c(39,112) 50 c(40,130) 51 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	34	print -dpdf fig6.pdf	
<pre>36 37 figure(7) 38 plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of     H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") 39 40 print -dpdf fig7.pdf 41 print -dpng fig7.png 42 43 figure(8) 44 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 45 print -dpdf fig8.pdf 47 print -dpng fig8.png 48 49 c(39,112) 50 c(40,130) 51 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	35	print -dpng fig6.png	
<pre>figure(7) plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") print -dpdf fig7.pdf print -dpng fig7.png figure(8) plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") print -dpdf fig8.pdf print -dpdf fig8.png (c(39,112)) c(40,130) front speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	36		
<pre>plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion from 134 to 6944 days") print -dpdf fig7.pdf print -dpng fig7.png figure(8) plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") print -dpdf fig8.pdf print -dpdf fig8.png c (39,112) c (40,130) front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	37	figure (7)	
<pre>print -dpdf fig7.pdf print -dpng fig7.png figure(8) plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") print -dpdf fig8.pdf print -dpng fig8.png c (39,112) c (40,130) front speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	88	<pre>plot(z,c(38:50,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H 2S"), title("Depth of H 2S Diffusion from 134 to 6944 days")</pre>	
<pre>print -dpdf fig7.pdf print -dpng fig7.png  figure(8) plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days")  print -dpdf fig8.pdf print -dpng fig8.png  c (39,112) c (40,130)  front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	39		
<pre>print -dpng fig7.png figure(8) plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") print -dpdf fig8.pdf print -dpng fig8.png (39,112) c (40,130) front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	0	print -dpdf fig7.pdf	
<pre>figure(8) figure(8) plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") print -dpdf fig8.pdf print -dpng fig8.png c(39,112) c(40,130) front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	1	print -dppg fig7 ppg	
<pre>figure(8) figure(8) f</pre>	2	France ober 3 173 ( ber 3	
<pre>1 Figure() 4 plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H_2S"), title("Depth of H_2S Diffusion at t = 186 and 259 days") 5 print -dpdf fig8.pdf 7 print -dpng fig8.png 9 c(39,112) 0 c(40,130) 1 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)</pre>	3	figure (2)	
<pre>5 print -dpdf fig8.pdf 7 print -dpng fig8.png 8 9 c (39,112) 0 c (40,130) 1 2 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day 3 dist_180_2 = front_speed2 * 180 4 5 t2(39)/2.592e6  # months 6 c (39,1) 9 0 1 2 3 3 4 </pre>	4	<pre>plot(z,c(39,:),z,c(40,:)), xlabel("Distance (cm)"), ylabel("Liquid Phase Mole Fraction of H 2S"), title("Depth of H 2S Diffusion at t = 186 and 259 days")</pre>	
<pre>6 print -dpdf fig8.pdf 7 print -dpng fig8.png 8 9 c (39,112) 0 c (40,130) 1 1 2 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day 3 dist_180_2 = front_speed2 * 180 4 5 t2(39)/2.592e6  # months 6 6 7 c (39,1) 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9</pre>	5		
<pre>print dpur ing0.pur print -dpng fig8.png 19 c (39,112) c (40,130) 11 12 front speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day dist_180_2 = front_speed2 * 180 14 15 t2(39)/2.592e6  # months 16 17 18 18 19 10 10 10 10 10 10 10 10 10 10 10 10 10</pre>	16	print -dodf fig8 odf	
<pre>print -dping rige.ping 49 c (39,112) 50 c (40,130) 51 52 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day 53 dist_I80_2 = front_speed2 * 180 54 55 t2(39)/2.592e6  # months 56 57 c (39,1) 58 59 50 51 52 53 54 55 55 55 55 55 55 55 55 55 55 55 55</pre>	17	nrint doug fig0 ng	
<pre>*** 49 c(39,112) c(40,130) 51 52 front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day 53 dist_180_2 = front_speed2 * 180 54 55 t2(39)/2.592e6  # months 56 57 c(39,1) 58 59 60 61 62 63 64 </pre>	10	prine -apila ride-bild	
<pre>dist_12) c (40,130) front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day dist_180_2 = front_speed2 * 180 t2(39)/2.592e6  # months c (39,1) c (39,1) </pre>	10		
<pre>c (40,130) front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day dist_180_2 = front_speed2 * 180 t2(39)/2.592e6  # months c (39,1) c (39,1) </pre>	E C	C (37,112)	
<pre>front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day dist_180_2 = front_speed2 * 180 t2(39)/2.592e6  # months c(39,1) c(39,1) d d d d d d d d d d d d d d d d d d d</pre>	50	c (40,130)	
<pre>front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)  # cm/day dist_180_2 = front_speed2 * 180 t2(39)/2.592e6  # months c(39,1) c(39,1) dist_12(30)/2.592e6  # months dist_12(30)/2.592</pre>	1		
<pre>dist_180_2 = front_speed2 * 180 t2(39)/2.592e6  # months c(39,1) c(39,1) define d</pre>	52	front_speed2 = (130-112)/(t2(40)-t2(39))*(3600*24)	
54 55 t2(39)/2.592e6 # months 56 57 c(39,1) 59 50 51 52 53 54	53	dist_180_2 = front_speed2 * 180	
55 t2(39)/2.592e6 # months 56 c(39,1) 58 59 50 50 51 52 52 53 54 55 55 55 55 55 55 55 55 55 55 55 55	54		
56 57 c(39,1) 58 59 60 61 62 63 64	55	t2(39)/2.592e6 # months	
57 c(39,1) 58 59 50 51 52 53 54	6		
59 50 51 52 53 54	7	c(39.1)	
59 50 51 52 53 54	58		
50 51 52 53	0		
50 51 52 53 54	20		
51 62 63 64	00		
62 63 64	01		
63 54	52		
54	63		
	54		
65	65		
66	66		
67			
	Y 1		

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#### Appendix D. Pulse Release Air Model Script

```
C:\cygwin64\home\cwen461\work\octave\nahs\air.m
```

```
% air.m
                air modeling for nahs release at holden
 1
       graphics_toolkit gnuplot
3
    clear all;
 4
    clf();
    s x=14.9; % dispersion coefficient (meters)
 6
     s_y = s_x; % table 8.8 s_x = 9.44*x/1000 + 1.5
s_z = 3.5; % at 1500 m table 8.9 for stable s_z = 3.2x/1000+0.75
 7
8
9
    u = 12; % wind speed (m/s)
10
    q m = 6000; % release mass (mg)
11
     x1 = 0;
12
       %for x=1:10:2000
13
       for x=1:1:2000
14
         x1 = x1+1;
15
          for t=1:200
16
                s_x = 9.44*x/1000+1.5;
17
18
                        s_y = s_x;
s_z = 3.2*x/1000+0.75;
19
20
                c(x1,t) = (q m/(2^{(0.5)}*pi^{(3/2)}*s x*s y*s z))*exp(-0.5*(((x-u*t)/s x)^2))
                )); % mg/m^3
21
22
     end:
23
     end;
24
25
     figure(1)
26
     plot(c(:,125),"linewidth",3), xlabel('Distance from Release (meters)'), ylabel(
'H_2S Concentration (mg/m^3)'), ...
27
28
      title ('Plume after 125 seconds with 12 m/s wind (IDLH 100 ppm)')
29
       grid
30
     print -dpdf air.pdf
print -dpng air.png
31
32
33
     %print -deps -color air.eps
34
35
      c max = max(c(:,125))
     c_max_ppm = c_max*24.4/29 % 24.4 L/mole at 25C and air 29 g/mole
36
37
38
     figure(2)
39
     plot(24.4/29*c(:,125),"linewidth",3), xlabel('Distance from Release (meters)'),
40
     ylabel('H_2S Concentration (ppm)'), ..
41
       title('Plume after 125 seconds with 12 m/s wind (IDLH 100 ppm)')
       grid
42
43
     print -dpdf air_ppm.pdf
44
     print -dpng air_ppm.png
45
46
     %print -deps -color air_ppm.eps
47
48
     figure(3)
49
     plot(24.4/29*c(:,9),"linewidth",3), xlabel('Distance from Release (meters)'), ylabel
50
     ('H_2S Concentration (ppm)'), ...
51
      title('Plume after 9 seconds with 12 m/s wind (IDLH 100 ppm)')
52
       grid
53
54
     print -dpdf air_ppm_nearby.pdf
     print -dpng air_ppm_nearby.png
56
     %print -deps -color air ppm nearby.eps
57
58
```

Monday, July 10, 2017

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