

Project: Project Name Here
 Client: Client Name Here
 Stream (Case):

Analyst: Analyst
 Revision: A
 Date: 1/1/2000

pH Calculation

Calculating pH for CO₂ / H₂S Systems and Partitioning of H₂S into Oil and Water

KNOWN:

$T := 250$	F	Operating Temperature
$P := 1000$	psia	Operating Pressure
$\text{GasMole\%}_{\text{CO}_2} := 4$	%	% Molarity of CO ₂
$\text{GasMole\%}_{\text{H}_2\text{S}} := .1$	%	% Molarity of H ₂ S
$\text{Bicarbonate} := 1000$	mg/l	
$\text{Chlorides} := 12000$	mg/l	Brine Salinity

SOLUTION:

$$\text{GasOilkValue} := 12.03 \cdot T^{.79} P^{-.97} \quad \text{GasOilkValue} = 1.16$$

$$\text{IonicStrength} := \frac{\text{Chlorides}}{32460} \quad \text{IonicStrength} = 0.37$$

$$T_c := \frac{(T - 32)}{1.8} \quad T_c = 121.111$$

$$T_k := T_c + 273.15 \quad T_k = 394.261$$

$$A := 1408 \quad B := -4001 \quad C := 34.51$$

$$A_x := \frac{-A}{298.15 \times 1.987} \quad A_x = -2.377$$

$$B_x := \frac{-B \cdot \left(\frac{1}{T_k} - \frac{1}{298.15} \right)}{1.987} \quad B_x = -1.646$$

$$C_x := C \cdot \frac{\left(\frac{298.15}{T_k} - 1 - \ln\left(\frac{298.15}{T_k} \right) \right)}{1.987} \quad C_x = 0.619$$

$$H2SHenryK := \exp(Ax + Bx + Cx) \quad H2SHenryK = 0.033$$

$$H2SpKHenry := -\log(H2SHenryK, 10) \quad H2SpKHenry = 1.478$$

$$FugacityCoefficientH2S := 1 - [.00025 - (T - 75).000001] \cdot P \quad FugacityCoefficientH2S = 0.925$$

$$ActivityCoefficientH2Saq := .93 + .33 \cdot \text{IonicStrength} \quad ActivityCoefficientH2Saq = 1.052$$

$$\text{molarH2Saq} := H2SHenryK \cdot \frac{P}{14.7} \cdot \frac{\text{GasMole\%}_{H2S}}{100} \cdot \frac{FugacityCoefficientH2S}{ActivityCoefficientH2Saq} \quad \text{molarH2Saq} = 1.988 \times 10^{-3}$$

$$H2Saq := \text{molarH2Saq} \cdot 34000 \quad H2Saq = 67.599 \text{ mg/l}$$

$$pKprime := 7.646 - 0.01054 \cdot T + .00002579 \cdot T^2 - .293 \cdot \text{IonicStrength}^{.5} + .04214 \cdot \text{IonicStrength}$$

$$pKprime = 6.46$$

$$Kprime := 10^{-pKprime} \quad Kprime = 3.465 \times 10^{-7}$$

$$\text{Beta} := H2SHenryK \cdot Kprime \cdot P \cdot \frac{(\text{GasMole\%}_{H2S})}{100} \cdot \frac{FugacityCoefficientH2S}{14.7 \cdot ActivityCoefficientH2Saq} \quad \text{Beta} = 6.889 \times 10^{-10}$$

$$CO2pKHenry := 2.27 + 0.00565 \cdot T - .00000806 \cdot T^2 + .075 \cdot \text{IonicStrength} \quad CO2pKHenry = 3.206$$

$$CO2KHenry := 10^{-CO2pKHenry} \quad CO2KHenry = 6.216 \times 10^{-4}$$

$$\text{molarCO2aq} := P \cdot \left(\frac{\text{GasMole\%}_{CO2}}{100} \right) \cdot CO2KHenry \quad \text{molarCO2aq} = 0.025$$

$$CO2aq := \text{molarCO2aq} \cdot 44000 \quad CO2aq = 1.094 \times 10^3 \text{ mg/l}$$

$$CO2pK1st := 6.41 - .001594 \cdot T + .00000852 \cdot T^2 - .0000307 \cdot P - .4772 \cdot \text{IonicStrength}^{.5} + .118 \cdot \text{IonicStrength}$$

$$CO2pK1st = 6.267$$

$$CO2K1st := 10^{-CO2pK1st} \quad CO2K1st = 5.41 \times 10^{-7}$$

$$\text{Alpha} := CO2KHenry \cdot CO2K1st \cdot P \cdot \frac{\text{GasMole\%}_{CO2}}{100} \quad \text{Alpha} = 1.345 \times 10^{-8}$$

$$H_{ion} := \frac{\left[\frac{-Bicarbonate}{61000} + \left[\left(\frac{Bicarbonate}{61000} \right)^2 + 4 \cdot (\alpha + \beta) \right]^{.5} \right]}{2}$$

$$H_{ion} = 8.626 \times 10^{-7}$$

$$pH := -\log(H_{ion}, 10)$$

$$pH = 6.064$$

$$molarHS_{neg} := K_{prime} \cdot \frac{molarH2S_{aq}}{10^{-pH}}$$

$$molarHS_{neg} = 7.986 \times 10^{-4}$$

$$HS_{neg} := molarHS_{neg} \cdot 31000$$

$$HS_{neg} = 24.758 \quad \text{mg/l}$$

$$TotalH2S_{inWater} := H2S_{aq} + HS_{neg}$$

$$TotalH2S_{inWater} = 92.357 \quad \text{mg/l}$$

$$molarHCO3_{neg} := CO2K1st \cdot \frac{molarCO2_{aq}}{10^{-pH}}$$

$$molarHCO3_{neg} = 0.016$$

$$HCO3_{neg} := molarHCO3_{neg} \cdot 61000$$

$$HCO3_{neg} = 951.335 \quad \text{mg/l}$$

$$H2S_{inOil} := \frac{GasMole\%_{H2S}}{GasOilkValue}$$

$$H2S_{inOil} = 0.086 \quad (\text{mole } \%)$$

$$H2S_{Total} := H2S_{aq} + HS_{neg}$$

$$H2S_{Total} = 92.357 \quad (\text{mg/l})$$

RESULTS:

For the following conditions: $T = 250 \text{ F}$ & $P = 1000 \text{ psia}$

The calculated pH for (accurate for pressures less than 3000 psia and temperatures less than 350 F) is:

$$pH = 6.064$$

The total H2S in Oil (accurate for pressures less than 750 psia) is:

$$H2S_{inOil} = 0.086 \quad (\text{mole } \%)$$

The total H2S is:

$$H2S_{Total} = 92.357 \quad (\text{mg/l})$$