SCIENTIFIC NOTEBOOK 817E

Alka Jain

SCIENTIFIC NOTEBOOK

Alka Jain

Center for Nuclear Waste Regulatory Analyses
Southwest Research Institute
San Antonio, Texas

Phone: (210) 522 5051
ajain@swri.org

06/16/05
AJ

INITIAL ENTRIES

Scientific Notebook 817E, issued to Alka Jain

Issue Date: May 27, 2005

Title: Software Validation Report for Stream Analyzer Version 2.0

Objective: The overall objective of the project is to document the validation of the recent version of OLI simulation software package, Stream Analyzer Version 2.0 and its new chemistry model MSE (Mixed Solvent Electrolyte). The validation involves comparing of calculated results with experimental data available in the literature.

Software: Stream Analyzer Version 2.0 is one of several software packages of the simulation family developed by OLI Systems, Inc. (Morris Plains, New Jersey). Stream Analyzer is used for evaluating the thermodynamic behavior of components of a single or of multiple aqueous streams. In contrast to previous versions of StreamAnalyzer, Version 2.0 has a new chemistry model, referred to as the Mixed Solvent Electrolyte (MSE) model, and associated thermodynamic parameters. The standard chemistry model of StreamAnalyzer is applicable to aqueous systems with ionic strengths up to 30 molal, temperatures up to -50 to 300 °C, and pressures up to 0 to 1,500 atm. The new MSE model is capable of calculating speciation, chemical, and phase equilibria, applicable to water-organic-salt systems in the full range of concentrations as well as aqueous electrolytes from dilute solutions to the fused salt limit.

Equipment:

- OLI simulation software package StreamAnalyzer Version 2.0
- Pentium III PC
- Windows 2000
- MS Excel

AJ
6/16/05, 6/17/05

Test Case 1: NaCl Solubility as a Function of Temperature

The solubility of NaCl was calculated from 25 to 300 °C (77 to 572 °F) to verify if StreamAnalyzer 2.0 can be used to accurately calculate the solubility of a single salt at different temperatures.

Input temperatures were 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, and 300 °C. Below 100 °C , the input pressure was 1.0 atm (14.7 psi). At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest.

The test was run by specifying the calculation types as constant pressure at temperatures below 100 °C and bubble point at temperatures equal to or above 100 °C.

The results of calculations with StreamAnalyzer 2.0 and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyzer2.0AQU_Case1.xls and StreamAnalyzer2.0MSE_Case1.xls, respectively (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and Cl^-.

AJ
06/18/05, 06/19/05

Test Case 2: NaCl and/or KCl Solubility in Mixed NaCl+KCl Solutions

The solubility of NaCl and/or KCl was calculated at different temperatures and compared with experimental data. The test was to determine the ability of the OLI software StreamAnalyzer 2.0 to accurately calculate the solubility of a mineral salt in a solution containing two types of dissolved salts and at different temperature conditions.

Input temperatures was 40, 100, and 150 °C [104, 212, and 302 °F]. Below 100 °C, the input pressure was1.0 atm [14.7 psi]. At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest. When the solubility of NaCl was calculated, a fixed value of K^+ concentration and an extra amount of NaCl were specified in the input stream. On the other hand, when the solubility of KCl was calculated, a fixed value of Na^+ concentration and an extra amount of KCl were specified in the input stream. The solubilities of the two salts in the eutonic solution of NaCl and KCl were calculated by specifying extra amounts of both NaCl and KCl in the input stream.

The test was run by specifying the calculation types as constant pressure at temperatures lower than 100 °C and bubble point at temperatures equal or above 100 °C.
The results of calculations StreamAnalyzer 2.0, and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyser2.0AQU_Case2.xls, and StreamAnalyzer2.0MSE_Case2.xls, respectively (see attached CD). These files list the

temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ and Cl^-.

AJ
6/20/05, 6/21/03

Test Case 3: Solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl Solutions

The solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl solutions was calculated at 0 and 50 °C [32 and 122 °F] and compared with experimental data. The test was to determine the ability of the OLI package StreamAnalyzer 2.0 to accurately calculate the solubility of minerals in a solution containing multi-component dissolved salts.

The input temperature was 0 and 50 °C and the input pressure was 1.0 atm [14.7 psi]. The concentrations of Ca^{2+}, Na^+ and K^+ were varied, and the saturated concentration of Mg^{2+} was calculated with a slight excess of $MgCl_2$ in the solid phase. The test was run by specifying the calculation type as isothermal.

The results of calculations StreamAnalyzer 2.0, and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyser2.0AQU_Case3.xls, and StreamAnalyzer2.0MSE_Case3.xls, respectively (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ Mg^{2+}, and Cl^-.

AJ
6/22/05, 6/23/05

Test Case 4 : Vapor Pressure of KCl Solutions at 300 °C [572 °F] as a Function of Concentration

The vapor pressure of KCl solutions as a function of concentration was calculated and compared with experimental data. The test was to determine the ability of the OLI package StreamAnalyzer 2.0 to accurately calculate the vapor pressures of single alkaline-chloride solutions.

The input temperature was 300 °C and the input pressure was the vapor saturation pressure at the temperature of interest. The input KCl concentrations were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations StreamAnalyzer 2.0, and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyser2.0AQU_Case4.xls, and StreamAnalyzer2.0MSE_Case4.xls, respectively (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of K^+ and Cl^-.

Test Case 5: Lowering of Vapor Pressure by $CaCl_2$ in Aqueous Solutions at 100 °C [212 °F] as a Function of Concentration

The vapor pressures of $CaCl_2$ solutions as a function of concentration were calculated and compared with experimental data. The test was to determine the ability of the OLI package StreamAnalyzer 2.0 to accurately calculate the vapor pressures of alkaline-earth-metal chloride solutions.

The input temperature was 100 °C [212 °F] and the input pressure was the vapor saturation pressure. The input $CaCl_2$ concentrations were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations StreamAnalyzer 2.0, and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyser2.0AQU_Case5.xls, and StreamAnalyzer2.0MSE_Case5.xls, respectively (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Ca^{2+} and Cl^-.

AJ
6/24/05, 6/27/05, 6/28/05

Test Case 6: Lowering of Vapor Pressure by $NaNO_3$, NaOH, and $NaHSO_4$ in Aqueous Solutions at 100 °C [212 °F]

The vapor pressures of $NaNO_3$, NaOH, and $NaHSO_4$ solutions were calculated and compared with the experimental data.

The input temperature was 100 °C and the input pressure was the vapor saturation pressure. The input concentrations of $NaNO_3$, NaOH and $NaHSO_4$ were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations StreamAnalyzer 2.0, and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyser2.0AQU_Case6.xls, and StreamAnalyzer2.0MSE_Case6.xls, respectively (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of cations and anions.

Test Case 7: Deliquescence Point of Mixed NaCl-$NaNO_3$-KNO_3 Salts

The mutual deliquescence point of mixed NaCl-$NaNO_3$-KNO_3 salts was calculated and compared with experimental data. The test was to determine the ability of the OLI Packages StreamAnalyzer 2.0 to accurately calculate the mutual deliquescence point of mixed salts.

The input temperature was 86 °C [186.8 °F]. The input concentrations of $NaNO_3$, NaCl, and KNO_3 were specified such that undissolved $NaNO_3$, NaCl, and KNO_3 were present in the output streams. The test was run by specifying the calculation type as bubble point.

The results of calculations StreamAnalyzer 2.0, and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyser2.0AQU_Case7.xls, and StreamAnalyzer2.0MSE_Case7.xls, respectively (see attached CD). These files list the

temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and NO_3^-, and Cl^-.

6/29/05, 6/30/05, 7/1/05

Test Case 8 (Note: Test case 9 in old validation report is renamed as Case 8) : Solubility of $NaNO_3$ and NaOH at Concentrations Beyond 30 M

The solubilities of $NaNO_3$ and NaOH salts were calculated and compared with experimental data. The test was to determine the ability of the OLI software StreamAnalyzer 2.0 with option MSE to accurately calculate the solution properties of extremely concentrated aqueous solutions.

The input temperature used was from 94 to 202 °C [201.2 to 395.6 °F]. The input concentrations of $NaNO_3$ and NaOH were specified such that undissolved $NaNO_3$ and NaOH were present in the output streams. The test was run by specifying the calculation type as bubble point with an exception of calculation for solubity of NaOH at 192°C. The test was run by specifying precipitation point calculation (with addition of NaOH and precipitation of NaOH solid) for solubity calculations of NaOH at 192°C

The results of calculations StreamAnalyzer 2.0, and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyser2.0AQU_Case8.xls, and StreamAnalyzer2.0MSE_Case8.xls, respectively (see attached CD). These files list the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, NO_3^-, and OH^-.

AJ
7/1/05, 7/5/05, 7/6/05

The output data from StreamAnalyzer 2.0 files for cases 1-8 was compared with data from literature.and saved to eight files named New Table_Case1.xls, New Table_Case2.xls, New Table_Case3.xls New Table_Case4.xls., New Table_Case5.xls, New Table_Case6.xls, New Table_Case7.xls, and New Table_Case8.xls respectively.

07/07/05
AJ

Test Case 6: Lowering of Vapor Pressure by $NaHCO_3$ in Aqueous Solutions at 100 °C [212 °F]

The vapor pressures of $NaHCO_3$ solutions were calculated and compared with the experimental data.

The input temperature was 100 °C and the input pressure was the vapor saturation pressure. The input concentrations of $NaHCO_3$ were varied.
The test was run by specifying the calculation type as bubble point.

The results of calculations StreamAnalyzer 2.0, and StreamAnalyzer 2.0 with option MSE were saved to two files named StreamAnalyser2.0AQU_Case6.xls, and StreamAnalyzer2.0MSE_Case6.xls, respectively (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of cations and anions.

07/11/05
AJ

Title: Thermodynamic Modeling of Brine Chemistry in the In-drift Environment of a Potential High Level Nuclear Waste Repository at Yucca Mountain, Nevada (OLI 23rd Users Conference Oct. 5 – 6, 2005).

Objective: The overall objective of this project is to document the results of thermodynamic modeling conducted to understand changes in chemistry of water contacting engineered materials of a potential high- level nuclear waste repository at the Yucca Mountain, Nevada. OLI simulation software package, Stream Analyzer Version 2.0 and LabAnalyzer Version 2.0 were used to conduct thermodynamic modeling.

Software: Stream Analyzer Version 2.0 and LabAnalyzer Version 2.0 are software packages of the simulation family developed by OLI Systems, Inc. (Morris Plains, New Jersey).
Stream Analyzer is used for evaluating the thermodynamic behavior of components of a single or of multiple aqueous streams. StreamAnalyzer, Version 2.0 has two chemistry models, Standard and Mixed Solvent Electrolyte (MSE) model. The standard chemistry model of StreamAnalyzer is applicable to aqueous systems with ionic strengths up to 30 molal, temperatures up to -50 to 300 °C, and pressures up to 0 to 1,500 atm. The MSE model is capable of calculating speciation, chemical, and phase equilibria, applicable to water-organic-salt systems in the full range of concentrations as well as aqueous electrolytes from dilute solutions to the fused salt limit.
Note: Validation of LabAnalyzer 2.0 is not required for this particular study as it was used to only generate the input streams for StreamAnalyzer 2.0

Equipment:

- OLI simulation software package StreamAnalyzer Version 2.0
- OLI simulation software package StreamAnalyzer Version 2.0
- Pentium III PC
- Windows 2000
- MS Excel

OLI calculations for water compositions NRG-6/ 158.2, NRG-6/ 160.8, NRG-6/171.0, and NRG-6/175.6 were conducted using LabAnalyzer 2.0 and StreamAnalyzer 2.0. The data was saved to file named "YM Pore Waters with Br&F.xls".

07/12/05
AJ

OLI calculations for water compositions NRG-6/219.9, NRG-6/244.6, NRG-6/255.9, NRG-7a/460.25, and SD-12/1495.5 were conducted using LabAnalyzer 2.0 and StreamAnalyzer 2.0. The data was saved to file named "YM Pore Waters with Br&F.xls".

07/13/05
AJ
An error in calculations of Test Case 3 (solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl solutions) observed by technical reviewer. The error was corrected and resulted changes to StreamAnalyzer2.0AQU_Case3.xls and StreamAnalyzer2.0MSE_Case3.xls files. The corrected data was saved to two files named as Revised StreamAnalyzer2.0AQU_Case3.xls and Revised StreamAnalyzer2.0MSE_Case3.xls. The corrected output data from StreamAnalyzer 2.0 and data from literature was compared and saved to file named Revised New Table_Case3.xls.

07/18/05
AJ

OLI calculations for water compositions SD-12/ 296.1, SD-6/ 509.9, SD-6/412.2, SD-6/443.5, SD-6/471.3 and SD-6/507.5 are conducted using LabAnalyzer 2.0 and StreamAnalyzer 2.0. The data is saved to file named "YM Pore Waters with Br&F.xls".

07/19/05
AJ

OLI calculations for water compositions SD-6/522.5, SD-6/370.3, SD-6/114.1, SD-9/135.1, SD-9/176.2, SD-9/ 94.2, UZ-14/1258.5, UZ-14/1277.7, UZ-14/ 1409.4,and UZ-14/1542.3 are conducted using LabAnalyzer 2.0 and StreamAnalyzer 2.0. The data is saved to file named "YM Pore Waters with Br&F.xls".

07/20/05
AJ

OLI calculations for water compositions, UZ-14/178.1, UZ-14/1825.8, UZ-14/2014.7, UZ-14/85.2-85.6, UZ-14/14C, UZ-16/1343.7, UZ-16/1643.4 and WT-24/1937.0 are conducted using LabAnalyzer 2.0 and StreamAnalyzer 2.0. The data is saved to file named "YM Pore Waters with Br&F.xls".

07/21/05 – 07/22 /05
AJ

Data from StreamAnalyzer 2.0 files is copied and saved to excel file "YM Pore Waters with BR&F.xls". Copied data from "YM Pore Waters with BR&F.xls" is reorganized in preferred format and saved to file "Additional YM Pore Waters with BR&F.xls".

07/25/05 – 07/29 /05
AJ

OLI calculations for compositions NRG-6/ 158.2, UZ-14/1277.7, NRG-6/244.6, SD-6/412.2, UZ-14/85.2-85.6, NRG-7a/460.25, UZ-14/1542.3 with fixed CO2 concentrations were computed using StreamAnalyzer 2.0. The data was saved to file named "YM Pore Waters with Br&F.xls".
Data from StreamAnalyzer 2.0 files is copied and saved to excel file "YM Pore Waters with BR&F.xls". Copied data from "YM Pore Waters with BR&F.xls" is reorganized in preferred format and saved to file "Additional YM Pore Waters with BR&F.xls".

08/2/05 – 08/8/05
AJ

Data from StreamAnalyzer 2.0 files "YM Pore Waters with BR&F.xls" is copied, reorganized in preferred format and saved to file "Additional YM Pore Waters with BR&F.xls".

08/09/05, 8/10/05
AJ

Title: Software Validation Report for LabAnalyzer Version 2.0

Objective: The overall objective of the project is to document the validation of the recent version of OLI simulation software package, LabAnalyzer Version 2.0. The validation involves comparing of calculated results with experimental data available in the literature.

Software: LabAnalyzer Version 2.0 is one of several software packages of the simulation family developed by OLI Systems, Inc. (Morris Plains, New Jersey). LabAnalyzer is used for evaluating the thermodynamic behavior of components of a single or of multiple aqueous streams. The standard chemistry model of LabAnalyzer is applicable to aqueous systems with ionic strengths up to 30 molal, temperatures up to -50 to 300 °C, and pressures up to 0 to 1,500 atm.

Equipment:

- OLI simulation software package LabAnalyzer Version 2.0
- Pentium III PC
- Windows 2000
- MS Excel

Test Case 1: NaCl Solubility as a Function of Temperature

The solubility of NaCl was calculated from 25 to 300 °C (77 to 572 °F) to verify if LabAnalyzer 2.0 can be used to accurately calculate the solubility of a single salt at different temperatures.

Input temperatures were 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, and 300 °C. Below 100 °C , the input pressure was 1.0 atm (14.7 psi). At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest.

The test was run by specifying the calculation types as constant pressure at temperatures below 100 °C and bubble point at temperatures equal to or above 100 °C.

The results of calculations with LabAnalyzer 2.0 were saved to a file named LabAnalyzer2.0_Case1.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and Cl^-.

08/11/05, 8/12/05, 08/15/05, 08/16/05, 08/17/05
AJ

Test Case 2: NaCl and/or KCl Solubility in Mixed NaCl+KCl Solutions

The solubility of NaCl and/or KCl was calculated at different temperatures and compared with experimental data. The test was to determine the ability of the OLI software LabAnalyzer 2.0 to accurately calculate the solubility of a mineral salt in a solution containing two types of dissolved salts and at different temperature conditions.

Input temperatures was 40, 100, and 150 °C [104, 212, and 302 °F]. Below 100 °C, the input pressure was1.0 atm [14.7 psi]. At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest. When the solubility of NaCl was calculated, a fixed value of K^+ concentration and an extra amount of NaCl were specified in the input stream. On the other hand, when the solubility of KCl was calculated, a fixed value of Na^+ concentration and an extra amount of KCl were specified in the input stream. The solubilities of the two salts in the eutonic solution of NaCl and KCl were calculated by specifying extra amounts of both NaCl and KCl in the input stream.

The test was run by specifying the calculation types as constant pressure at temperatures lower than 100 °C and bubble point at temperatures equal or above 100 °C.
The results of calculations LabAnalyzer 2.0 were saved to a file named LabAnalyzer2.0_Case2.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ and Cl^-.

AJ
08/18/05, 08/19/05

Test Case 3: Solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl Solutions

The solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl solutions was calculated at 0 and 50 °C [32 and 122 °F] and compared with experimental data. The test was to determine the ability of the OLI package LabAnalyzer 2.0 to accurately calculate the solubility of minerals in a solution containing multi-component dissolved salts.

The input temperature was 0 and 50 °C and the input pressure was 1.0 atm [14.7 psi]. The concentrations of Ca^{2+}, Na^+ and K^+ were varied, and the saturated concentration of Mg^{2+} was calculated with a slight excess of $MgCl_2$ in the solid phase. The test was run by specifying the calculation type as isothermal.

The results of calculations LabAnalyzer 2.0 were saved to a file named LabAnalyzer2.0_Case3.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ Mg^{2+}, and Cl^-.

AJ
08/22/05

Test Case 4 : Vapor Pressure of KCl Solutions at 300 °C [572 °F] as a Function of Concentration

The vapor pressure of KCl solutions as a function of concentration was calculated and compared with experimental data. The test was to determine the ability of the OLI package LabAnalyzer 2.0 to accurately calculate the vapor pressures of single alkaline-chloride solutions.

The input temperature was 300 °C and the input pressure was the vapor saturation pressure at the temperature of interest. The input KCl concentrations were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations LabAnalyzer 2.0 were saved to a file named LabAnalyzer2.0_Case4.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of K^+ and Cl^-.

AJ
08/23/05

Test Case 5: Lowering of Vapor Pressure by $CaCl_2$ in Aqueous Solutions at 100 °C [212 °F] as a Function of Concentration

The vapor pressures of $CaCl_2$ solutions as a function of concentration were calculated and compared with experimental data. The test was to determine the ability of the OLI package LabAnalyzer 2.0 to accurately calculate the vapor pressures of alkaline-earth-metal chloride solutions.

The input temperature was 100 °C [212 °F] and the input pressure was the vapor saturation pressure. The input $CaCl_2$ concentrations were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations LabAnalyzer 2.0 were saved to a file named LabAnalyzer2.0_Case5.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Ca^{2+} and Cl^-.

AJ
08/24/05, 08/25/05

Test Case 6: Lowering of Vapor Pressure by $NaNO_3$, NaOH, and $NaHSO_4$ in Aqueous Solutions at 100 °C [212 °F]

The vapor pressures of $NaNO_3$, NaOH, and $NaHSO_4$ solutions were calculated and compared with the experimental data.

The input temperature was 100 °C and the input pressure was the vapor saturation pressure. The input concentrations of $NaNO_3$, NaOH and $NaHSO_4$ were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations LabAnalyzer 2.0, were saved to a file named LabAnalyzer2.0_Case6.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of cations and anions.

AJ
08/26/05, 08/29/05, 08/30/05, 08/31/05

Test Case 7: Deliquescence Point of Mixed NaCl-$NaNO_3$-KNO_3 Salts

The mutual deliquescence point of mixed NaCl-$NaNO_3$-KNO_3 salts was calculated and compared with experimental data. The test was to determine the ability of the OLI Packages LabAnalyzer 2.0 to accurately calculate the mutual deliquescence point of mixed salts.

The input temperature was 86 °C [186.8 °F]. The input concentrations of $NaNO_3$, NaCl, and KNO_3 were specified such that undissolved $NaNO_3$, NaCl, and KNO_3 were present in the output streams. The test was run by specifying the calculation type as bubble point.

The results of calculations LabAnalyzer 2.0 were saved to a file named LabAnalyzer2.0_Case7.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and NO_3^-, and Cl^-.

The output data from LabAnalyzer 2.0 files for cases 1-7 was compared with data from literature and saved to seven files named ESP7.0LabAnalyzer2.0New Table_Case1.xls,

ESP7.0LabAnalyzer2.0New Table_Case2.xls, ESP7.0LabAnalyzer2.0New Table_Case3.xls, ESP7.0LabAnalyzer2.0New Table_Case4.xls., ESP7.0LabAnalyzer2.0New Table_Case5.xls, ESP7.0LabAnalyzer2.0New Table_Case6.xls, ESP7.0LabAnalyzer2.0New Table_Case7.xls.

09/01/05, 09/02/05, 09/06/05
AJ

Title: Software Validation Report for ESP Version 7.0

Objective: The overall objective of the project is to document the validation of the recent version of OLI simulation software package ESP Version 7.0. The validation involves comparing of calculated results with experimental data available in the literature.

Software: ESP Version 7.0 is one of several software packages of the simulation family developed by OLI Systems, Inc. (Morris Plains, New Jersey). ESP is used for evaluating the thermodynamic behavior of components of a single or of multiple aqueous streams. The standard chemistry model of ESP is applicable to aqueous systems with ionic strengths up to 30 molal, temperatures up to -50 to 300 °C, and pressures up to 0 to 1,500 atm.

Equipment:

- OLI simulation software package ESP Version 7.0
- Pentium III PC
- Windows 2000
- MS Excel

Test Case 1: NaCl Solubility as a Function of Temperature

The solubility of NaCl was calculated from 25 to 300 °C (77 to 572 °F) to verify if ESP 7.0 can be used to accurately calculate the solubility of a single salt at different temperatures.

Input temperatures were 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, and 300 °C. Below 100 °C , the input pressure was 1.0 atm (14.7 psi). At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest.

The test was run by specifying the calculation types as constant pressure at temperatures below 100 °C and bubble point at temperatures equal to or above 100 °C.

The results of calculations with ESP 7.0 were saved to a file named ESP7.0_Case1.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and Cl^-.

09/07/05, 09/08/05, 09/09/05, 09/12/05, 09/13/05, 09/14/05
AJ

Test Case 2: NaCl and/or KCl Solubility in Mixed NaCl+KCl Solutions

The solubility of NaCl and/or KCl was calculated at different temperatures and compared with experimental data. The test was to determine the ability of the OLI software ESP 7.0 to accurately calculate the solubility of a mineral salt in a solution containing two types of dissolved salts and at different temperature conditions.

Input temperatures was 40, 100, and 150 °C [104, 212, and 302 °F]. Below 100 °C, the input pressure was1.0 atm [14.7 psi]. At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest. When the solubility of NaCl was calculated, a fixed value of K^+ concentration and an extra amount of NaCl were specified in the input stream. On the other hand, when the solubility of KCl was calculated, a fixed value of Na^+ concentration and an extra amount of KCl were specified in the input stream. The solubilities of the two salts in the eutonic solution of NaCl and KCl were calculated by specifying extra amounts of both NaCl and KCl in the input stream.

The test was run by specifying the calculation types as constant pressure at temperatures lower than 100 °C and bubble point at temperatures equal or above 100 °C.
The results of calculations ESP 7.0 were saved to a file named ESP7.0_Case2.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ and Cl^-.

AJ
09/15/05, 09/16/05, 09/19/05

Test Case 3: Solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl Solutions

The solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl solutions was calculated at 0 and 50 °C [32 and 122 °F] and compared with experimental data. The test was to determine the ability of the OLI package ESP 2.0 to accurately calculate the solubility of minerals in a solution containing multi-component dissolved salts.

The input temperature was 0 and 50 °C and the input pressure was 1.0 atm [14.7 psi]. The concentrations of Ca^{2+}, Na^+ and K^+ were varied, and the saturated concentration of Mg^{2+} was calculated with a slight excess of $MgCl_2$ in the solid phase. The test was run by specifying the calculation type as isothermal.

The results of calculations ESP 2.0 were saved to a file named ESP7.0 _Case3.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ Mg^{2+}, and Cl^-.

AJ
09/20/05

Test Case 4 : Vapor Pressure of KCl Solutions at 300 °C [572 °F] as a Function of Concentration

The vapor pressure of KCl solutions as a function of concentration was calculated and compared with experimental data. The test was to determine the ability of the OLI package ESP 7.0 to accurately calculate the vapor pressures of single alkaline-chloride solutions.

The input temperature was 300 °C and the input pressure was the vapor saturation pressure at the temperature of interest. The input KCl concentrations were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations ESP 7.0 were saved to file named ESP7.0_Case4.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of K^+ and Cl^-.

AJ
09/21/05

Test Case 5: Lowering of Vapor Pressure by $CaCl_2$ in Aqueous Solutions at 100 °C [212 °F] as a Function of Concentration

The vapor pressures of $CaCl_2$ solutions as a function of concentration were calculated and compared with experimental data. The test was to determine the ability of the OLI package ESP 7.0 to accurately calculate the vapor pressures of alkaline-earth-metal chloride solutions.

The input temperature was 100 °C [212 °F] and the input pressure was the vapor saturation pressure. The input $CaCl_2$ concentrations were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations ESP 7.0 were saved to a file named ESP7.0_Case5.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Ca^{2+} and Cl^-.

AJ
09/22/05, 09/23/05

Test Case 6: Lowering of Vapor Pressure by $NaNO_3$, NaOH, and $NaHSO_4$ in Aqueous Solutions at 100 °C [212 °F]

The vapor pressures of $NaNO_3$, NaOH, and $NaHSO_4$ solutions were calculated and compared with the experimental data.

The input temperature was 100 °C and the input pressure was the vapor saturation pressure. The input concentrations of $NaNO_3$, NaOH and $NaHSO_4$ were varied.
The test was run by specifying the calculation type as bubble point.

The results of calculations ESP 7.0, were saved to two files named ESP7.0_Case6.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of cations and anions.

AJ
09/26/05, 09/27/05, 09/28/05, 09/29/05, 09/30/05

Test Case 7: Deliquescence Point of Mixed NaCl-$NaNO_3$-KNO_3 Salts

The mutual deliquescence point of mixed NaCl-$NaNO_3$-KNO_3 salts was calculated and compared with experimental data. The test was to determine the ability of the OLI Packages ESP 2.0 to accurately calculate the mutual deliquescence point of mixed salts.

The input temperature was 86 °C [186.8 °F]. The input concentrations of $NaNO_3$, NaCl, and KNO_3 were specified such that undissolved $NaNO_3$, NaCl, and KNO_3 were present in the output streams. The test was run by specifying the calculation type as bubble point.

The results of calculations ESP 7.0 were saved to a file named ESP7.0_Case7.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and NO_3^-, and Cl^-.

The output data from ESP 7.0 files for cases 1-8 was compared with data from literature and saved to seven files named ESP7.0LabAnalyzer2.0New Table_Case1.xls, ESP7.0LabAnalyzer2.0New Table_Case2.xls, ESP7.0LabAnalyzer2.0New Table_Case3.xls, ESP7.0LabAnalyzer2.0New Table_Case4.xls., ESP7.0LabAnalyzer2.0New Table_Case5.xls, ESP7.0LabAnalyzer2.0New Table_Case6.xls, and ESP7.0LabAnalyzer2.0New Table_Case7.xls respectively.

AJ
10/03/05, 10/04/05

Title: Software Validation Report for ESP Version 7.0 (Option MSE)

Objective: The overall objective of the project is to document the validation of recent version of OLI simulation software package, ESP Version 7.0 with its new chemistry model MSE (Mixed Solvent Electrolyte) only. The validation involves comparing of calculated results with experimental data available in the literature.

Software: ESP Version 7.0 is one of several software packages of the simulation family developed by OLI Systems, Inc. (Morris Plains, New Jersey). ESP Version 7.0 is used for evaluating the thermodynamic behavior of components of a single or of multiple aqueous streams. In contrast to previous versions of ESP Version 7.0 has a new chemistry model, referred to as the Mixed Solvent Electrolyte (MSE) model, and associated thermodynamic parameters. The new MSE model is capable of calculating speciation, chemical, and phase equilibria, applicable to water-organic-salt systems in the full range of concentrations as well as aqueous electrolytes from dilute solutions to the fused salt limit.

Equipment:

- OLI simulation software package ESP Version 7.0
- Pentium III PC

- Windows 2000
- MS Excel

Test Case 1: NaCl Solubility as a Function of Temperature

The solubility of NaCl was calculated from 25 to 300 °C (77 to 572 °F) to verify if ESP 7.0 (option MSE only) can be used to accurately calculate the solubility of a single salt at different temperatures.

Input temperatures were 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, and 300 °C. Below 100 °C , the input pressure was 1.0 atm (14.7 psi). At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest.

The test was run by specifying the calculation types as constant pressure at temperatures below 100 °C and bubble point at temperatures equal to or above 100 °C.

The results of calculations with ESP 7.0 (option MSE only) were saved to a file named ESP7.0-MSE_Case1.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and Cl^-.

10/05/05, 10/06/05, 10/07/05, 10/11/05, 10/12/05, 10/13/05
AJ

Test Case 2: NaCl and/or KCl Solubility in Mixed NaCl+KCl Solutions

The solubility of NaCl and/or KCl was calculated at different temperatures and compared with experimental data. The test was to determine the ability of the OLI software ESP 7.0 (option MSE only) to accurately calculate the solubility of a mineral salt in a solution containing two types of dissolved salts and at different temperature conditions.

Input temperatures was 40, 100, and 150 °C [104, 212, and 302 °F]. Below 100 °C, the input pressure was1.0 atm [14.7 psi]. At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest. When the solubility of NaCl was calculated, a fixed value of K^+ concentration and an extra amount of NaCl were specified in the input stream. On the other hand, when the solubility of KCl was calculated, a fixed value of Na^+ concentration and an extra amount of KCl were specified in the input stream. The solubilities of the two salts in the eutonic solution of NaCl and KCl were calculated by specifying extra amounts of both NaCl and KCl in the input stream.

The test was run by specifying the calculation types as constant pressure at temperatures lower than 100 °C and bubble point at temperatures equal or above 100 °C.
The results of calculations ESP 7.0 (option MSE only) were saved to a file named ESP 7.0-MSE_Case2.xls (see attached CD). These files list the temperatures and pressures

used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ and Cl^-.

AJ
10/14/05, 10/17/05, 10/18/05

Test Case 3: Solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl Solutions

The solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl solutions was calculated at 0 and 50 °C [32 and 122 °F] and compared with experimental data. The test was to determine the ability of the OLI package ESP 7.0 (option MSE only) to accurately calculate the solubility of minerals in a solution containing multi-component dissolved salts.

The input temperature was 0 and 50 °C and the input pressure was 1.0 atm [14.7 psi]. The concentrations of Ca^{2+}, Na^+ and K^+ were varied, and the saturated concentration of Mg^{2+} was calculated with a slight excess of $MgCl_2$ in the solid phase. The test was run by specifying the calculation type as isothermal.

The results of calculations ESP 7.0 (option MSE only) were saved to a file named ESP 7.0-MSE_Case3.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, K^+ Mg^{2+}, and Cl^-.

AJ
10/19/05

Test Case 4 : Vapor Pressure of KCl Solutions at 300 °C [572 °F] as a Function of Concentration

The vapor pressure of KCl solutions as a function of concentration was calculated and compared with experimental data. The test was to determine the ability of the OLI package ESP 7.0 (option MSE only) to accurately calculate the vapor pressures of single alkaline-chloride solutions.

The input temperature was 300 °C and the input pressure was the vapor saturation pressure at the temperature of interest. The input KCl concentrations were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations ESP 7.0 (option MSE only) were saved to a file named ESP 7.0-MSE_Case4.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of K^+ and Cl^-.

10/20/05
AJ

Test Case 5: Lowering of Vapor Pressure by $CaCl_2$ in Aqueous Solutions at 100 °C [212 °F] as a Function of Concentration

The vapor pressures of $CaCl_2$ solutions as a function of concentration were calculated and compared with experimental data. The test was to determine the ability of the OLI package ESP 7.0 (option MSE only) to accurately calculate the vapor pressures of alkaline-earth-metal chloride solutions.

The input temperature was 100 °C [212 °F] and the input pressure was the vapor saturation pressure. The input $CaCl_2$ concentrations were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations ESP 7.0 (option MSE only) were saved to a file named ESP 7.0-MSE_Case5.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of Ca^{2+} and Cl^-.

AJ
10/21/05, 10/24/05

Test Case 6: Lowering of Vapor Pressure by $NaNO_3$, NaOH, and $NaHSO_4$ in Aqueous Solutions at 100 °C [212 °F]

The vapor pressures of $NaNO_3$, NaOH, and $NaHSO_4$ solutions were calculated and compared with the experimental data.

The input temperature was 100 °C and the input pressure was the vapor saturation pressure. The input concentrations of $NaNO_3$, NaOH and $NaHSO_4$ were varied. The test was run by specifying the calculation type as bubble point.

The results of calculations ESP 7.0 (option MSE only) were saved to a file named ESP 7.0-MSE_Case6.xls (see attached CD). These files list the temperatures and pressures used in the calculation, the resulting ionic strength, and the calculated concentrations of cations and anions.

AJ
09/25/05

Test Case 7: Deliquescence Point of Mixed NaCl-$NaNO_3$-KNO_3 Salts

The mutual deliquescence point of mixed NaCl-$NaNO_3$-KNO_3 salts was calculated and compared with experimental data. The test was to determine the ability of the OLI Packages ESP 7.0 (option MSE only) to accurately calculate the mutual deliquescence point of mixed salts.

The input temperature was 86 °C [186.8 °F]. The input concentrations of $NaNO_3$, NaCl, and KNO_3 were specified such that undissolved $NaNO_3$, NaCl, and KNO_3 were present in the output streams. The test was run by specifying the calculation type as bubble point.

The results of calculations ESP 7.0 (option MSE only) were saved to a file named ESP 7.0-MSE_Case7.xls (see attached CD). These files list the temperatures and pressures

used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+ and NO_3^-, and Cl^-.

AJ
10/26/05

Test Case 8 (Note: Test case 9 in old validation report is renamed as Case 8) : Solubility of $NaNO_3$ and NaOH at Concentrations Beyond 30 M

The solubilities of $NaNO_3$ and NaOH salts were calculated and compared with experimental data. The test was to determine the ability of the OLI software ESP 7.0 (option MSE only) to accurately calculate the solution properties of extremely concentrated aqueous solutions.

The input temperature used was from 94 to 202 °C [201.2 to 395.6 °F]. The input concentrations of $NaNO_3$ and NaOH were specified such that undissolved $NaNO_3$ and NaOH were present in the output streams. The test was run by specifying the calculation type as bubble point with an exception of calculation for solubility of NaOH at 192°C. The test was run by specifying precipitation point calculation (with addition of NaOH and precipitation of NaOH solid) for solubility calculations of NaOH at 192°C

The results of calculations ESP 7.0 (option MSE only) were saved to a file named ESP 7.0-MSE_Case8.xls (see attached CD). These files list the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations of Na^+, NO_3^-, and OH^-.

AJ
10/27/05, 10/28/05, 10/31/05, 11/1/05

The output data from ESP 7.0 (option MSE only) files for cases 1-8 was compared with data from literature and saved to eight files named ESP7.0LabAnalyzer2.0New Table_Case1.xls, ESP7.0LabAnalyzer2.0New Table_Case2.xls, ESP7.0LabAnalyzer2.0New Table_Case3.xls, ESP7.0LabAnalyzer2.0New Table_Case4.xls., ESP7.0LabAnalyzer2.0New Table_Case5.xls, ESP7.0LabAnalyzer2.0New Table_Case6.xls, ESP7.0LabAnalyzer2.0New Table_Case7.xls, and ESP7.0MSENew Table_Case8.xls respectively.

AJ
11/21/05

Title: Software Validation Report for Corrosion Analyzer Version 2.0

Objective: The overall objective of the project is to document the validation of the recent version of OLI simulation software package Corrosion Analyzer Version 2.0. The validation involves comparing of the calculated stability diagram of the nickel-water system at 25 C with a published stability diagram.

Software: Corrosion Analyzer Version 2.0 is one of several software packages of the simulation family developed by OLI Systems, Inc. (Morris Plains, New Jersey). Corrosion

Analyzer is used for evaluating the thermodynamic properties that are related to the characteristics of corrosion and the corrosion rate of a metal in a given solution system. In contrast to previous version of Corrosion Analyzer Version 2.0 have a new chemistry model, referred to as the Mixed Solvent Electrolyte (MSE) model. The standard chemistry model of Corrosion Analyzer Version 2.0 is applicable to aqueous systems with ionic strengths up to 30 molal. The new MSE model is capable of calculating speciation, chemical, and phase equilibria, applicable to water-organic-salt systems in the full range of concentrations as well as aqueous electrolytes from dilute solutions to the fused salt limit. The standard chemistry model of Corrosion Analyzer Version 2.0 was tested.

Equipment:

- OLI simulation software package Corrosion Analyzer Version 2.0
- Pentium III PC
- Windows 2000
- MS Excel

AJ
11/28/05

Test Case 9—Stability Diagram for Nickel-Water System

The stability diagram of nickel-water system at 25 °C [77 °F] was calculated and compared with a published stability diagram. The test was to determine the ability of the Corrosion Analyzer 2.0 to accurately calculate the stability diagram of metals in solution.

The input temperature used was 25 C [77 F]. HCl and NaOH were used as the acid and base titrants, respectively, for pH adjustment. Only water was specified in the input stream. The concentration of Ni^{2+} was set at the trace species amount (1 molal), which is specified in the Option menu under Trace Species Amount submenu.

The test was run in the pH range of 0 to 14 and the potential range of 1.0 to 2.0 V. An E–pH diagram under standard state (1 M activity for dissolved species) was produced.

A hard copy of the output stability diagram (E–pH diagram) from the run with Corrosion Analyzer 2.0is shown in Figure 1. A published E-pH diagram for the same system is shown in Figure 2 (Pourbaix, 1974). The important lines (2, 3, 6, 7, 9, 11, and 14) in the two diagrams are close to each other. Detailed comparisons between the calculated and the published potential and pH values for selected points are presented in Table 1.

Table 1. Comparison of the Calculated pH and Potential Values with the Data from Published Literatures

	pH			Potential		
Data Point	Calculated	Reference*	Error	Calculated	Reference*	Error
B	5.39	6.03	-0.64	0.66	0.52	0.14
C	5.39	6.04	-0.65	-0.24	-0.24	0.00
D	14.00	14.01	-0.01	0.71	0.59	0.12
E	14.00	13.99	0.01	0.15	0.06	0.09
F	14.00	13.99	0.02	-0.74	-0.72	-0.02

*Pourbaix, M. "Reference: Atlas of Electrochemical Equilibriua in Aqueous Solutions." 2nd Edition. p. 333. Houston, Texas: NACE International. 1974.

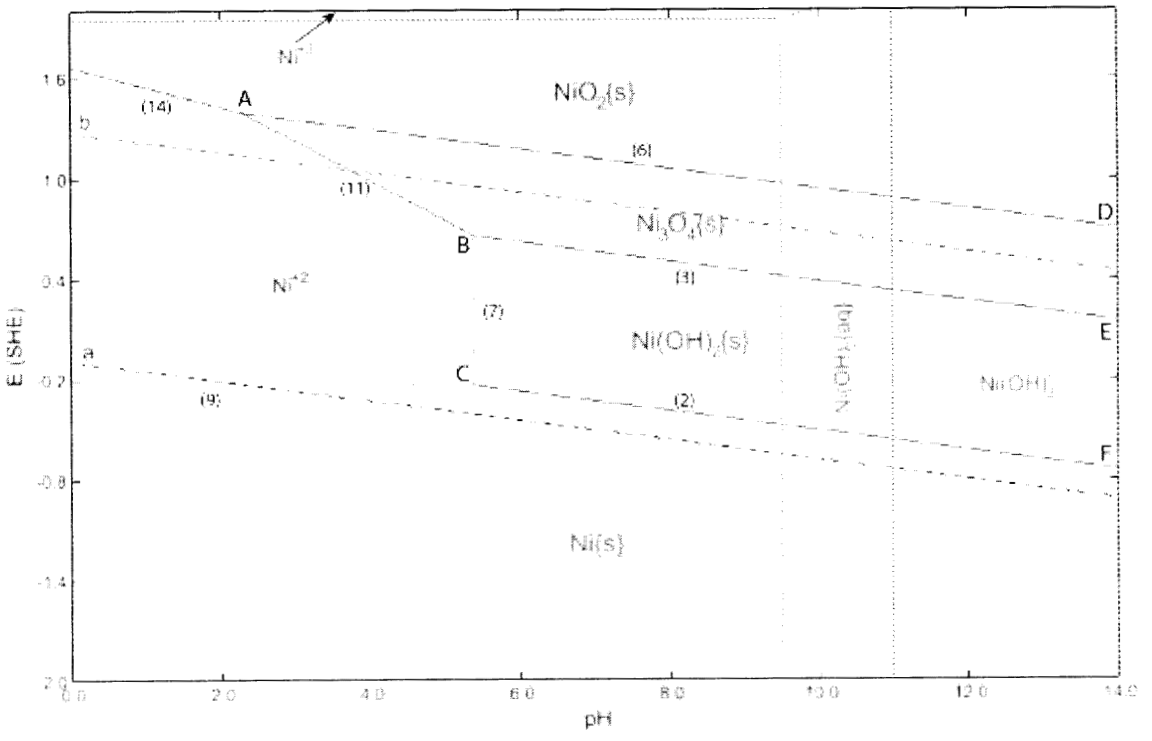


Figure 1. Calculated E-pH Diagram for Nickel-Water System.

AJ
12/19/05

An error in calculations of Test Case 3 (solubility of $MgCl_2$ in $CaCl_2$-NaCl-KCl solutions) was observed by technical reviewer. The error was corrected and resulted changes to files ESP7.0_Case3.xls, ESP7.0-MSE_Case3.xls and LabAnalyzer2.0_Case3 files. The corrected data was saved to files named as Revised ESP7.0_Case3.xls, Revised ESP7.0-MSE_Case3.xls and Revised LabAnalyzer2.0_Case3. The corrected output data from ESP 7.0, LabAnalyzer 2.0 and data from literature was compared and saved to file named Revised ESP7.0LanAnalyzer2.0New Table_Case3.xls.

AJ
02/22/06

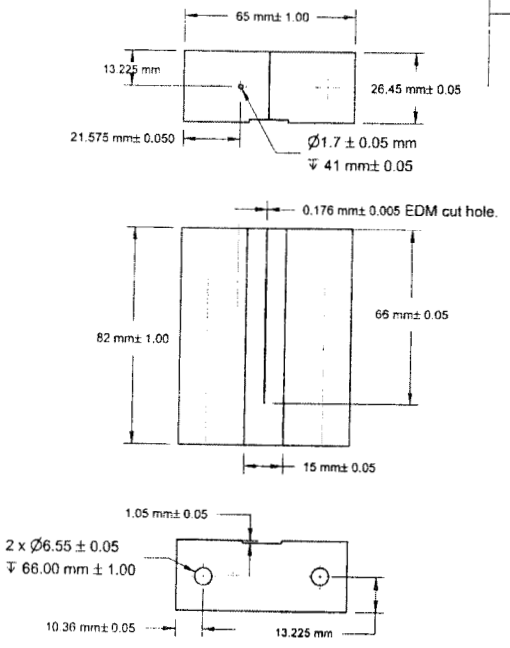
Title: Studies on Flow of In-Drift Water through Stress Corrosion Cracks

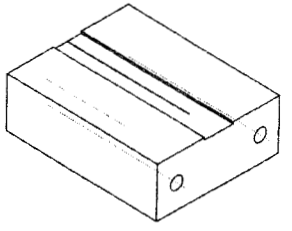
Objective: The overall objective of the project is to document the experimental studies on flow of in-drift water through stress corrosion cracks. The experimental studies include procedure, set-up, data collection and results.

Equipment and Suplies:

- Agilent 1100 series isocratic pump
- Agilent handheld control module
- Machined Alloy 22 coupon with crack
- Electronic balance
- Glass beakers
- Plexiglass cylinder
- Microstop
- Plastic capillary tube
- Ultrasonic cleaner

Procedure and Experimental set-up: Alloy 22 coupons are prepared as per drawing shown in fig.1. Electric discharge machining (EDM) is used to create micron size crack in the coupon.



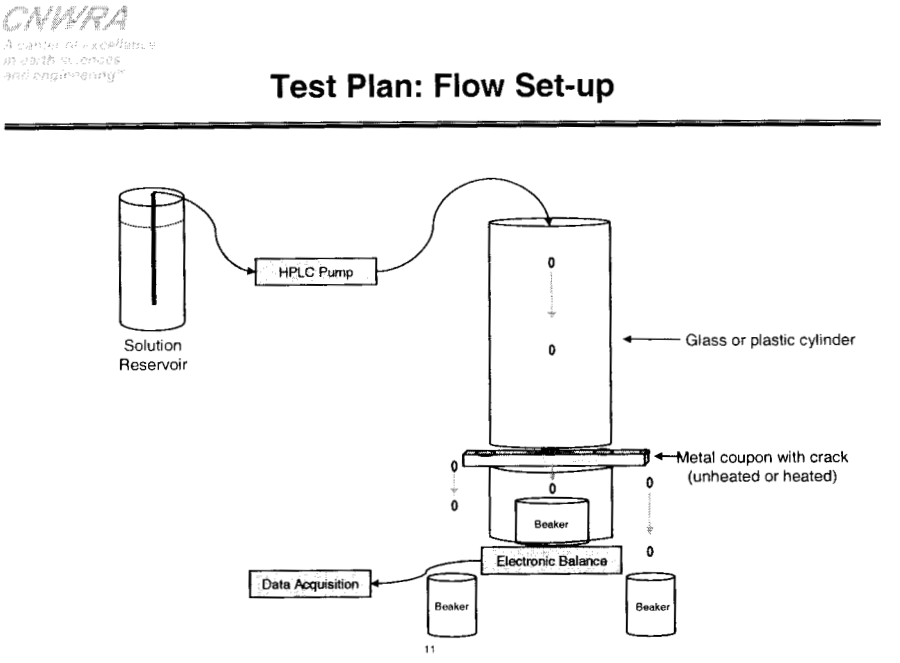


REVISIONS				
ZONE	REV	DESCRIPTION	DATE	APPROVED

Note: EDM cut hole which appears as line in center section breaks out on end and is through all material.

DRAWN JAIN / BANNON	DATE MARCH 22, 2006	SOUTHWEST RESEARCH INSTITUTE - CNWRA
CHECKED	CHECKED	ALLOY 22 COUPON WITH STRESS CORROSION CRACK
	3/22/06	
INITIATED BY: Alka Jain ajain@swri.org 3/22/06	MFG	SIZE A · FSCM NO. · DWG NO. 20.06002.212-001 · REV 0
PH. 210-522-5051 FAX 210-522-5184	APPROVED for EEP	SCALE · Alloy22Coupon032206DWG · SHEET 1 OF 1

The experimental set-up is as shown in the following figure.



4/27/06
AJ

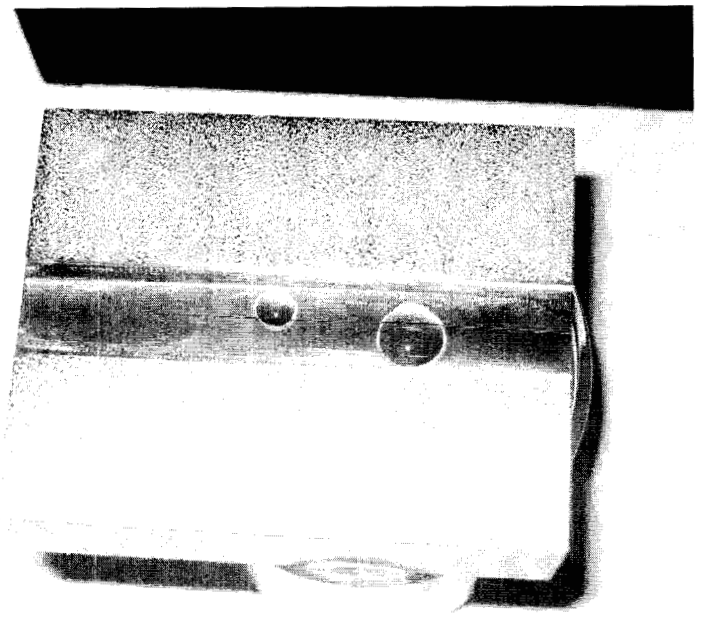


Figure 1: Alloy C-22 coupon with standing water droplets

AJ
05/01/06

Alloy-22 coupon is ultrasonically cleaned in acetone for 10 minutes and then followed by ultrasonic cleaning in de-ionized water. Coupon is dried with compressed air and placed over glass beaker. A few drops of DI water are placed over crack. No water flows through the crack as shown in pictures.

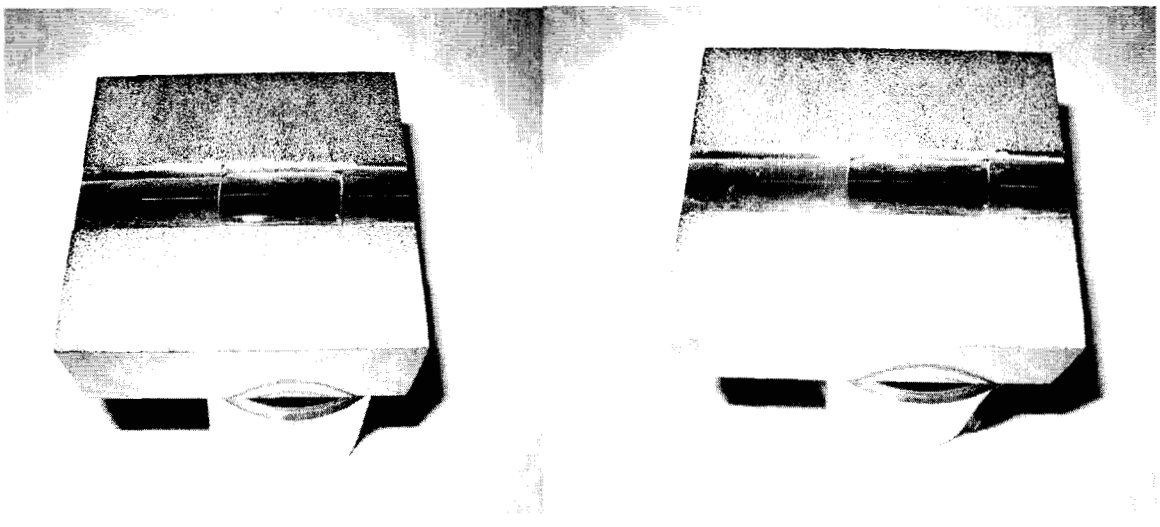


Figure 2: Alloy C22 coupon @ 0 hour and after 2hrs and 45 minutes

AJ
05/02/06

About 300ml of DI water is sonicated for 10 minutes to de-air the water. The bottle is covered with parafilm until ready to use. A setting of 2ml/min flow rate is used on isocratic pump for water flow over crack. Alloy-22 coupon is placed over glass beaker and water flow at the rate of 2ml/min is started over crack using isocratic pump. No water flows through the crack. The water flow is stopped and sample is dried. A mixture of hand soap and water is used to observe the flow through the crack. The soap water starts flowing through the crack within couple of minutes. The soap water is then switched with DI water through isocratic pump. The water flows through the crack at the rate of 2ml/min.

AJ
05/03/06
A small plastic capillary tube is sealed at one edge of crack using microstop as shown in the picture. Microstop is exposed to air for 5min. before sealing the capillary tube to coupon. The exposure of microstop to air allowed it to be more viscous and thus prevented the seepage of microstop inside the crack. The coupon is allowed to dry for I hour after sealing. The crack length outside the capillary tube is blocked using two layers of thin mylar sheet. The capillary is filled with DI water up to 1 cm. mark. No water flows through crack. The water level is slowly raised to 2 cm mark , no flow of water is

observed through crack. Then water level is slowly raised to 3 cm mark , no flow of water is observed through crack again. Finally, water level is slowly raised to 4.5 cm mark and the whole set up is left untouched for several minutes. After 20 minutes, 3.5 cm of water seeped through the crack as shown in pictures. After another 10 minutes all the flowed through the crack. The sample was left for drying overnight.

AJ
05/05/06

The capillary is filled with DI water up to 1 cm. mark. No water flows through crack even after 1 hour. The water level is slowly raised to 2 cm mark. The set up is observed after 22 minutes and few drops of water have seeped through the crack as shown in pictures.

AJ
05/07/06

A larger plastic capillary (25 ml) tube is sealed at one edge of crack using microstop as shown in the picture. Microstop is exposed to air for 5min. before sealing the capillary tube to coupon. The exposure of microstop to air allowed it to be more viscous and thus prevented the seepage of microstop inside the crack. The coupon is allowed to dry for I hour after sealing. The crack length outside the capillary tube is blocked using 0.006" shim stock material. The capillary is filled with DI water up to 1 cm. mark. No water flows through crack even after 1 hour. The water level is slowly raised to 2 cm mark , no flow of water is observed through crack after 1 hour. Then water level is slowly raised to 3 cm mark , no flow of water is observed through crack again. Finally, water level is slowly raised to 4.0 cm mark and the whole set up is left untouched for two days.

AJ
05/10/06

No water flows though crack even after 2 days as shown in pictures .The water level is slowly raised to 5 cm mark . No water flow is observed through crack even after 1 hour. Water level was slowly raised to 5.5 cm and water flow starts through the crack. The time was recorded for water to flow through the crack and was 4 minutes and 32 seconds. Volume of total water flow from crack is measured and was 7.2 ml. The calculated flow rate is 1.6 ml/min.

AJ
05/15/06
The old capillary was removed from coupon 1 and coupon was soaked in acetone to dissolve residues of microstop. The coupon was then ultrasonically cleaned for 7 min and inspected visually and showed some more residue from microstop. Coupon was cleaned once more ultrasonically in acetone for 5 minutes. Coupon was then rinsed with DI water several times and then ultrasonically cleaned in DI water for 12 minutes.
A 60 ml plastic syringe was converted to a capillary tube by cutting the nozzle edge of the syringe. A new 60 ml capillary with **ID = 26.35 mm** was attached to coupon 1 using 5-minute epoxy. Crack length was set to about 15mm using 0.006" shim stock.
Crack Length for Capillary 1 was measured with Starrett vernier calipers = 15.14 mm
After dring for 10 minutes, water was added to the capillary to check for any leaks. Water oozed slowly from opening at the junction of shim material and capillary. Viscous microstop was used to seal this leak. After one hour, capillary was filled with 25.1 ml

water to test any leaks. No leak was observed. No flow was observed through the crack for 55 minutes. Another 10.1ml was added to the capillary and water started to flow through the crack.
Water from a 25 ml burette was added constantly to the capillary to maintain a constant head and the flow rate through the crack was measured by using a stop watch.
Constant head of 34-35 ml was maintained and flow rate was measured.
7 ml/ 2.45 min = 2.86 ml/min
15 ml/ 2.533 min = 5.92 ml/min
Constant head of 34-36 ml was maintained and flow rate was measured.
25 ml/ 4.77 min = 5.25 ml/min
20 ml/ 3.433 min = 5.83 ml/min
Constant head of 37-38 ml was maintained and flow rate was measured.
25 ml/ 2.62min = 9.55 ml/min
Flow through the crack was also measured without maintaining a constant head.
10 ml/ 1.3833 min = 7.23 ml/min

AJ
5/16/06

Capillary 1 was filled with 25 ml of DI water and no flow thru the crack was observed.
Another 8 ml of water was added and water started flowing through the crack.
Water from a 25 ml burette was added constantly to the capillary to maintain a constant head and the flow rate through the crack was measured by using a stop watch.
Constant head of 37-39 ml was maintained and flow rate was measured.
25 ml/ 4.573min = 5.24 ml/min
Constant head of 48-50 ml was maintained and flow rate was measured.
25 ml/ 5.467 min = 4.57 ml/min
Constant head of 24-26 ml was maintained and flow rate was measured.
25 ml/ 2.683 min = 9.32 ml/min

Flow through the crack was also measured without maintaining a constant head.
5 ml/ 0.65min = 7.69 ml/min
5 ml/0.717 min = 6.97 ml/min
5 ml/ 0.9 min = 5.56 ml/min
10 ml/1.95 min = 5.13 ml/min

AJ
05/17/06

Capillary 1 (15.14 mm crack length) was filled with DI water. No water flowed through crack from 20 ml to 28 ml. Water started flowing through the capillary at 29 ml level. The flow rate through the crack was measured.
5 ml/3.917min = 1.28 ml/min
10 ml/8.483 min = 1.18 ml/min
15 ml/ 13.833 min = 1.08 ml/min
Capillary 1 was dried thoroughly with compressed air and kim wipes. 25 ml DI water was added to capillary and water started flowing through the crack. The flow rate through the crack was measured.
5 ml/5.65min = 0.89 ml/min
10 ml/12.417 min = 0.81 ml/min

Capillary 1 was dried thoroughly with compressed air and kim wipes. 25 ml DI water was added to capillary and water started flowing through the crack. The flow rate through the crack was measured.
5 ml/3.65min = 1.37 ml/min
10 ml/8.017 min = 1.25 ml/min
Capillary 1 was dried thoroughly with compressed air and kim wipes. DI water was added to capillary and water started flowing through the crack at 23.5 ml. The flow rate through the crack was measured.
2 ml/ 9.083min = 0.22 ml/min
3 ml/13.5 min = 0.22 ml/min
4 ml/ 18.283min = 0.22 ml/min
5ml/23.567 min = 0.21 ml/min
Capillary 1 was dried thoroughly with compressed air and kim wipes. DI water was added to capillary and water started flowing through the crack at 25 ml.
Capillary 1 was dried thoroughly with compressed air and kim wipes. DI water was added to capillary and water started flowing through the crack at 25 ml within 12 sec. The flow rate through the crack was measured.
1 ml/ 1.1 min = 0.91 ml/min
2 ml/ 2.35min = 0.85 ml/min
3 ml/3.833 min = 0.78 ml/min
4 ml/5.2 min = 0.77ml/min
5 ml/6.517 min = 0.77 ml/min
6 ml/8.133 min = 0.74 ml/min
7 ml/9.783 min = 0.72 ml/min
8 ml/11.233 min = 0.71 ml/min
9 ml/12.9 min = 0.70 ml/min
10 ml/14.483 min = 0.69 ml/min
Capillary 1 was dried thoroughly with compressed air and kim wipes. 20 ml DI water was added to capillary and water column was left undisturbed overnight.

AJ
5/18/06

20 ml water column in capillary 1 was not stable overnight as water has flowed through the crack sometime during night time. Capillary and crack were visually inspected and were very dry. No water residues were observed inside the crack. This may indicate flow of water through crack after first few hours.
Capillary 1 was dried thoroughly with compressed air and kim wipes. 20 ml DI water was added to capillary and water column was left undisturbed. Water did not flow through the crack after 2 hrs, 3 hrs, 5 hrs, 8 hrs. so the standing water column was left undisturbed overnight.

AJ
05/19/06

20 ml water column in capillary 1 was stable overnight and even after 26 hours and 15 minutes. Water level in capillary 1 was then raised slowly to 22ml at 12:26 pm. Water started flowing through the crack(15.2mm) at 2:22pm, possibly due to the disturbance from closing the metal cabinet abruptly. The flow rate through the crack was measured as 22ml/23min = 0.96ml/min

Capillary1 is dried thoroughly with kim wipes and compressed air. At 3:30 pm, it is filled with 20ml of water using Agilent isocratic pump and left undisturbed overnight.

AJ
05/20/06

20 ml water in capillary 1 had flowed through ~ 15.2 mm length crack in alloy -22 coupon. Another coupon to which capillary 2 was glued using 5-minute epoxy and microstop was cured and ready to use.
20 ml of DI water was added to each capillary (1 and 2) @ 4:00pm and left undisturbed until next day morning to observe the stability of standing water column over crack.
Crack Length for Capillary 2 was measured with Starrett vernier calipers = 10.07 mm

AJ
05/22/06
A column of 20 ml water standing over ~ 15.2 mm cracks in capillary 1 and 10.1 mm crack in capillary 2 (attached to two alloy-22 coupons) was unstable overnight. Water had already flowed through the crack as observed in the morning.
Both the samples were dried thoroughly with compressed air and kim wipes.
Capillary 2 was filled with DI water using isocratic pump. Water does not flow through the crack from 20ml to 23 ml water column, but water starts flowing through the crack within few seconds at 24 ml. The flow rate of water through crack (10.1mm) was measured as follows:
11 ml/ 6min 6 sec = 1.8 ml/min
10 ml/ 5min 26 sec. = 1.84 ml/min
10 ml/ 5 min 29 sec. = 1.82 ml/min
Capillary 2 was dried thoroughly again with compressed air and flow through crack was measured again. It shows no flow through crack from 20 ml to 21 ml but water starts flowing through the crack at 22 ml within 3 minutes. May be sample did not dry well. The flow rate of water through crack was measured again.
10 ml/4min 54 sec = 2.04 ml/min
10 ml/ 4min 58 sec. = 2.01 ml/min
10 ml/ 4 min 52 sec. = 2.05 ml/min
Capillary 2 was dried thoroughly again with compressed air and stable water column was measured again. It shows no flow through crack up from 18 ml to 21 ml but water starts flowing through the crack at 22 ml immediately.
Capillary 2 was dried thoroughly again with compressed air and stable water column was measured again. It shows no flow through crack up to 18 ml but water starts flowing through the crack at 19 ml. May be sample requires longer drying.
Capillary 2 was dried thoroughly again with compressed air and stable water column was measured again. It shows no flow through crack up to 18 ml to 20 ml but water starts flowing through the crack at 21 ml immediately.
Capillary 2 was dried thoroughly again with compressed air and left for an hour for air dry. The level of stable water column was measured again. Water starts flowing through the crack at 21 ml again.
Capillary 2 was dried thoroughly again with compressed air and stable water column was measured again. It shows no flow through crack up to 18 ml to 20 ml but water starts flowing through the crack at 21 ml within 10 sec.

Capillary 1 shows no flow from 20ml to 22 ml. Capillary1 is left @ 22ml for 30 minutes and water starts flowing after 30 minutes. The flow rate of water through crack was measured as follows:
10 ml/ 14min 41 sec = 2.14 ml/min
5 ml/ 6min 50 sec. = 0.73 ml/min
10 ml/ 17 min 45 sec. = 0.56 ml/min
10 ml/ 17min 49 sec =0.56 ml/min
Capillary 1 was dried thoroughly again with compressed air and left for an hour for air dry. The level of stable water column was measured. Water starts to flow through the crack at 26 ml with in 30 sec.
Capillary 1 was dried thoroughly again with compressed air and stable water column was measured again. It shows no flow through crack up to 20 ml to 25 ml but water starts flowing through the crack at 26 ml within 30 sec.

Capillary 1 was dried thoroughly with compressed air and filled with 18 ml of DI water with isocratic pump. The sample was left undisturbed overnight.

Capillary 2 was dried thoroughly with compressed air and filled with 14 ml of DI water with isocratic pump. The sample was left undisturbed overnight.

AJ
5/23/06

Water column in capillary 1 and 2 did not stay stable overnight. Water has flowed through the crack in both ,capillary 1 and 2 by the morning. The visual inspection of the crack showed no retained water inside the crack for coupon 1 whereas the crack through coupon 2 was filled with water. This may indicate that the water through coupon 2 crack flowed earlier than coupon 1 crack.
Capillary 1 was dried thoroughly again with compressed air and stable water column was measured again. It shows no flow through crack up to 20 ml to 25 ml but water starts flowing through the crack at 26 ml within 30 sec.
Capillary 2 was dried thoroughly again with compressed air and stable water column was measured again. It shows no flow through crack up to 18 ml to 20 ml but water starts flowing through the crack at 21 ml within 60 sec.
Capillary 1 was dried thoroughly with compressed air and filled with 18 ml of DI water with isocratic pump. Water column was stable for 4hours and 45 minutes. So, it was left undisturbed overnight.
Capillary 2 was dried thoroughly with compressed air and filled with 14 ml of DI water with isocratic pump. The sample was left undisturbed for few hours and water starts flowing through the crack after 2 hrs and 43.75 sec.
Capillary 2 was dried thoroughly with compressed air and filled with 10 ml of DI water with isocratic pump. Water column was left undisturbed over night.

AJ
5/24/06

Water column in capillary 1 and 2 did not stay stable overnight. Water has flowed through the crack in both ,capillary 1 and 2 by the morning. The visual inspections of the cracks in coupon 1 and 2 showed no water residues inside the crack. This may indicate that the water flowed through the coupon 1 and 2 only after few hours and there was enough time for sample to dry in air.

Capillary 2 was dried thoroughly again with compressed air and stable water column was measured. It shows no flow through crack up to 18 ml to 20 ml but water starts flowing through the crack at 21 ml within 30 sec.

Capillary 1 was dried thoroughly again with compressed air and stable water column was measured. It shows no flow through crack up to 20 ml to 25 ml but water starts flowing through the crack at 26 ml within 80 sec.
The flow rate of water through crack was measured as follows:
10 ml/ 15min 38 sec = 0.64 ml/min
10 ml/ 15 min 35 sec. = 0.64 ml/min
10 ml/ 15min 52 sec =0.63 ml/min

Capillary 1 was dried thoroughly with compressed air and filled with 15 ml of DI water with isocratic pump. Water column was left undisturbed over night.
Capillary 2 was dried thoroughly with compressed air and filled with 7.5 ml of DI water with isocratic pump. Water column was.

AJ
5/26/06

15 ml water column in capillary 1 was stable for 21 hours. 7.5 ml water column was stable in capillary 2 for 21 hours also. Both capillaries were dried thoroughly with kim wipes and compressed air and left in air for 1.5 hours.
At 3:30 pm Capillary 1 was filled with 15 ml neutral brine and water column was left undisturbed over night.
Capillary 2 was filled with 7.5 ml neutral brine and water column was left undisturbed over night.

AJ
5/27/06

Water column in capillary 1 and 2 did not stay stable overnight. After 23.5 hrs (3:00pm), neutral brine in Capillary 1 and Capillary 2 has already flowed through the crack.

AJ
5/29/06
Capillary 2 was dried with compressed air and stable neutral brine column was measured. It shows no flow through crack up to 20 ml to 23 ml but neutral brine starts flowing through the crack at 24 ml within 30 sec.
The flow rate of neutral brine through crack was measured as follows:
10 ml/ 5min 45 sec = 1.74 ml/min
10 ml/ 5 min 38 sec. = 1.77 ml/min
10 ml/ 5min 35 sec = 1.79 ml/min
10 ml/ 5 min 35 sec. = 1.79 ml/min
10 ml/ 5min 41sec = 1.76 ml/min

Capillary 1 was dried with compressed air and stable neutral brine column was measured. It shows no flow through crack up to 20 ml to 25 ml but neutral brine starts flowing through the crack at 26 ml within 90 sec.
The flow rate of neutral brine through crack was measured as follows:
10 ml/ 6 min 33 sec = 1.53 ml/min

10 ml/ 6 min 28 sec. = 1.55 ml/min
10 ml/ 6 min 27 sec = 1.55 ml/min
10 ml/ 6 min 34 sec. = 1.52 ml/min
10 ml/ 7 min 16 sec = 1.38 ml/min
10 ml/ 7min 36 sec = 1.32 ml/min
Capillaries were cleaned, dried and left in air overnight.

AJ
5/31/06

Capillary 1 was filled with Ca-Cl brine and stable brine column was measured. It shows no flow through crack up to 20 ml to 25 ml but neutral brine starts flowing through the crack at 26 ml within 30 sec.
The flow rate of neutral brine through crack was measured as follows:
10 ml/ 5 min 19sec = 1.88 ml/min
10 ml/ 5 min 8 sec. = 1.95 ml/min
10 ml/ 5 min 2 sec = 1.99 ml/min
10 ml/ 4 min 56 sec. = 2.03 ml/min
10 ml/ 4 min 43 sec = 2.12 ml/min

Capillary 2 was filled with Ca-Cl brine and stable brine column was measured. It shows no flow through crack up to 20 ml to 21 ml but neutral brine starts flowing through the crack at 22 ml within 38 sec.
The flow rate of neutral brine through crack was measured as follows:
10 ml/ 4 min 15sec = 2.35 ml/min
10 ml/ 4 min 12 sec. = 2.38 ml/min
10 ml/ 4 min 7 sec = 2.43 ml/min
10 ml/ 4 min 4 sec. = 2.46 ml/min
10 ml/ 4 min 1 sec = 2.49 ml/min

Capillary 1 was filled with alkaline brine and stable brine column was measured. It shows no flow through crack up to 20 ml to 25 ml but neutral brine starts flowing through the crack at 26 ml within 30 sec.
The flow rate of neutral brine through crack was measured as follows:
10 ml/ 7 min 23sec = 1.35 ml/min
10 ml/ 7 min 33 sec. = 1.32 ml/min
10 ml/ 7 min 30 sec = 1.33 ml/min
10 ml/ 7 min 30 sec. = 1.33 ml/min
10 ml/ 7 min 30 sec = 1.33 ml/min

Capillary 2 was filled with alkaline brine and stable brine column was measured. It shows no flow through crack up to 20 ml to 23 ml but neutral brine starts flowing through the crack at 24 ml in < 30 sec.
The flow rate of neutral brine through crack was measured as follows:
10 ml/ 4 min 24sec = 2.27 ml/min
10 ml/ 4 min 20 sec. = 2.31 ml/min
10 ml/ 4 min 16 sec = 2.34 ml/min
10 ml/ 4 min 15 sec. = 2.35 ml/min
10 ml/ 4 min 14 sec = 2.36 ml/min

Entries into Scientific Notebook No. 817E for the period June 16, 2005, through May 31, 2006, have been made by

Alka 8/9/06

Alka Jain / Date

No original entry into this Scientific Notebook has been removed.

Alka 8/9/06

Alka Jain / Date

I have reviewed this scientific notebook and find it in agreement with QAP-001.

E.C. Pearcy 8/22/2006