SOFTWARE RELEASE NOTICE

1. SRN Number: GHGC-SRN-261

2. Project Title:
Evolution of the Near-Field Environment KTI

Project No. 20.01402.561

3. SRN Title: SOLCALC Version 1.0

4. Originator/Requestor: Roberto T. Pabalan

Date: July 13, 2001

5. Summary of Actions

- ■ Release of new software
- □ Release of modified software:
  - □ Enhancements made
  - □ Corrections made
- □ Change of access software
- □ Software Retirement

6. Persons Authorized Access

Name	Read Only/Read-Write	Addition/Change/Delete
All	Read Only	

7. Element Manager Approval: [signature] Date: 7/31/2001

8. Remarks:

CNWRA Form TOP-6 (05/98)

SOFTWARE SUMMARY FORM

1. Summary Date: July 13, 2001	2. Summary prepared by (Name and phone) Roberto T. Pabalan (x5304)	3. Summary Action: New
4. Software Date: June 18, 2001	5. Short Title: SOLCALC	
6. Software Title: SOLCALC, Version 1.0		07. Internal Software ID: None

08. Software Type: ☐ Automated Data System ■ Computer Program ☐ Subroutine/Module	09. Processing Mode: ■ Interactive ☐ Batch ☐ Combination	10. Application Area a. General: ☐ Scientific/Engineering ■ Auxiliary Analyses ☐ Total System PA ☐ Subsystem PA ☐ Other b. Specific: Salt precipitate analysis; chemistry on surfaces of drip shields and waste packages
11. Submitting Organization and Address: CNWRA/SwRI 6220 Culebra Road San Antonio, TX 78228		12. Technical Contact(s) and Phone: Roberto T. Pabalan (x5304)
13. Software Application: Calculations of vapor pressures and mineral solubilities in electrolyte solutions up to elevated temperatures and pressures.		

14. Computer Platform IBM PC compatible	15. Computer Operating System: Windows NT	16. Programming Language(s): Fortran 77	17. Number of Source Program Statements: 8,087
18. Computer Memory Requirements: 64 Mb	19. Tape Drives: 0	20. Disk Units: 1	21. Graphics: none
22. Other Operational Requirements			

23. Software Availability: ☐ Available ☐ Limited ■ In-House ONLY	24. Documentation Availability: ☐ Available ☐ Preliminary ■ In-House ONLY
25. Software Developer: R T Pabalan Date: 7/31/01	

CNWRA Form TOP-4-1 (05/98)

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→*ACQUIRED SOFTWARE NOT TO BE MODIFIED*←

Software Title/Name: SOLCALC

Version: 1.0

Demonstration workstation: Excalibur

Operating System: MS-DOS/NT 4.0

User: R. T. Pabalan

NOTE: Acquired software may or may not meet all requirements and will be evaluated on a case-by-case basis.

Installation Testing [TOP-018, Section 5.6]

Has *installation testing* been conducted for each intended computer platform and operating system?

Yes: ☑ No: ☐ N/A: ☐

Computer Platforms: P.C. Compatible Operating Systems: MS-DOS/NT 4.0

Location of Acceptance Test Results: S. Notebook #185

Comments:.

Software Output [TOP-018, Section 5.5.4]

Is software designed so that individual runs are uniquely identified by date, time, name of software and version?

Yes: ☐ No: ☑ N/A: ☐

Date and Time Displayed: N/A

Name/Version Displayed: N/A

Comments:

NOTE: Output identification content and format is typically taken as is.

Medium Documentation [TOP-018, Section 5.5.6]

The physical labeling of software medium (tapes, disks, etc.) contains: Program Name, Module/Name/Title, Module Revision, File type (ASCII, OBJ, EXE), Recording Date, and Operating System(s)?

Yes: ☑ No: ☐ N/A: ☐

Comments: Disk located in QA Records Room

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
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User Documentation [TOP-018, Section 5.5.7]

Is there a Users' Manual for the software and is it up-to-date?

Yes: ☐ No: ☐ N/A: ☑

User's Manual Version and Date: N/A
Comments:

Are there basic instructions for the *installation* and *use* of the software?

Yes: ☑ No: ☐ N/A: ☐

Location of Instructions: 3½ "Diskette in QA records file - Readme txt
Comments:

Configuration Control [TOP-018, Section 5.7, 5.9.3]

Is the Software Summary Form (Form TOP-4-1) completed and signed?

Yes: ☑ No: ☐ N/A: ☐

Date of Approval: July 31, 2001

Is the list of files attached to the Software Summary Form complete and accurate?

Yes: ☐ No: ☐ N/A: ☑

Comments:

Is the source code available or, is the executable code available in the case of (acquired/commercial codes)?

Yes: ☑ No: ☐ N/A: ☐

Location of Source Code: 3½ Diskette in QA file.
Comments:

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Have all the script/make files and executable files been submitted to the Software Custodian?

Only the executable files are being submitted.

Yes: ☑ No: ☐ N/A: ☐

Location of executable files: 3½ "Diskette in QA file.
Comments:

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES
QA VERIFICATION REPORT
FOR
→ *ACQUIRED SOFTWARE NOT TO BE MODIFIED* ←

Software Release [TOP-018, Section 5.9]

Upon acceptance of the software as verified above, has a Software Release Notice (SRN), Form TOP-6 been issued and does the version number of the software match the documentation?

Yes: ☑ No: ☐ N/A: ☐

SRN Number: GHGC-SWR-261

Comments:

Software Validation [TOP-018, Section 5.10]

Has a Software Validation Test Plan (SVTP) been prepared for the ***range of application*** of the software?

Yes: ☑ No: ☐ N/A: ☐

Version and Date of SVTP: 11/8/2001

Date Reviewed and Approved via QAP-002: 11/8/2001

Comments:

Has a Software Validation Test Report (SVTR) been prepared that documents the results of the validation cases, interpretation of the results, and determination if the software has been validated?

Yes: ☑ No: ☐ N/A: ☐

Version and Date of SVTR: 01/24/02

Date Reviewed and Approved via QAP-002: 01/30/02

Comments.:

Additional Comments:

N Mabalen 4/9/02 — Software Evaluator/User/Date

Susan Mahrer 4/9/2002 — Software Custodian/Date

Software Validation Test Report

SOFTWARE VALIDATION TEST PLAN FOR SOLCALC, VERSION 1.0

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–97–009

Prepared by

Roberto T. Pabalan

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

Approved by:

English C. Pearcy, Manager
Geohydrology and Geochemistry

11/8/2001
Date

CONTENTS

1 SCOPE OF THE VALIDATION

This document establishes the Software Validation Test Plan for validating the functionality of the code SOLCALC, Version 1.0, through comparisons of calculated results with experimental data available in the literature. SOLCALC, Version 1.0, is a program that calculates the solubility of mineral salts in mixed electrolyte systems using a matrix inversion technique for solving a series of mass-action and mass-balance equations. Activity coefficients are calculated using the Pitzer equations (1973, 1991). The program also calculates osmotic coefficients and vapor pressures of aqueous salt mixtures. The code was originally developed by R.T. Pabalan at the Department of Chemistry, University of California at Berkeley.

2 REFERENCES

The following documents are referenced in this Software Validation Test Plan.

Boecke, H.E. Ein Schlussel zur Beurtelung des Kristallisationsverlaufes der bei der Kalisalzverarbeitung vorkommenden Losungen. *Kali* 4: 271–300. 1910.

Harvie, C.E., N. Moller, and J.H. Weare. The Prediction of Mineral Solubilities in Natural Waters: The Na–K–Mg–Ca–Cl–SO_4–OH–HCO_3–CO_3–CO_2–H_2O System to High Ionic Strengths at 25 °C. *Geochimica et Cosmochimica Acta* 48(4): 723–751. 1984.

Linke, W.F. *Solubilities of Inorganic and Metal Organic Compounds.* Volumes 1 and 2. American Chemical Society. 1965.

Liu, C. and W.T.J. Lindsay. Thermodynamics of Sodium Chloride Solutions at High Temperatures. *Journal of Solution Chemistry.* 1: 45–69. 1972.

Liu, C. and W.T. J. Lindsay. Thermodynamic Properties of Aqueous Solutions at High Temperatures. Research and Development Program Report No. 722. Washington, DC. Office of Saline Water of the U.S. Department of Interior. 1971.

Pabalan, R.T. and K.S. Pitzer. Thermodynamics of Concentrated Electrolyte Mixtures and the Prediction of Mineral Solubilities to High Temperatures for Mixtures in the System Na–K–Mg–Cl–SO_4–OH–H_2O. *Geochimica et Cosmochimica Acta* 5l: 2,429–2,443. 1987.

Pabalan, R.T. and K.S. Pitzer. Mineral Solubilities in Electrolyte Solutions. In: K.S. Pitzer (Editor). *Activity Coefficients in Electrolyte Solutions.* Boca Raton, FL. CRC Press. pp. 435–490. 1991.

Pitzer, K.S. Thermodynamics of Electrolytes, 1. Theoretical Basis and General Equations. *Journal of Physical Chemistry* 77: 268–277. 1973.

Zarembo, V.I., N.A. Antonov, V.N. Gilyarov, and M.K. Fedorov. Activity Coefficients of KCl in the System KCl–H_2O at temperatures of 150–350 °C and pressures up to 1,500 kg/cm^2. *Journal of Applied Chemistry USSR* 49: 1,259–1,263. 1976.

3 ENVIRONMENT

3.1 Software

SOLCALC (Version 0), was originally coded by R. Pabalan using FORTRAN 77 in a Digital Equipment Corporation VAX 8700 computer environment. The current version (Version 1.0) was recompiled and relinked by R. Pabalan using the Lahey FORTRAN 77, Version 5, compiler/linker. Version 1.0 currently runs in a DOS environment under either Windows 3.1 or Windows NT 4.0 operating systems. The following software items are required to perform the testing activities:

(i) SOLCALC, Version 1.0 executable code (SOLCALC.EXE)

(ii) DOS running under either Windows 3.1 or Windows NT 4.0 operating systems

(iii) Lahey FORTRAN 77 Version 5 compiler/linker

3.2 Hardware Requirements

SOLCALC, Version 1.0, runs on the IBM PC family of microcomputers or compatible systems. The program is interactive. Input information is entered using the keyboard, and output information is saved on the computer hard drive. No peripherals (e.g., tape drives, printers, plotters) are necessary to perform testing activities. However, comparison of calculated results and experimental data is facilitated through the use of graphical software such as Sigmaplot.

4 PREREQUISITES

Running SOLCALC, Version 1.0 requires the following Lahey FORTRAN 77 files be resident in the same directory as SOLCALC: (i) F77L3.eer, and (ii) run386.exe. Also, two files, solcalc.out and vpcalc.out, must already exist in the same directory. These files may be blank, and will be replaced with the output information after the program successfully runs.

5 ASSUMPTIONS AND CONSTRAINTS

The user of SOLCALC is assumed to be familiar with chemical thermodynamics and, specifically, with the Pitzer equations for calculating aqueous activity coefficients. The advantages and limitations of the Pitzer equations are discussed in several publications, including Pitzer (1973, 1991), Harvie et al. (1984), and Pabalan and Pitzer (1991).

6 TEST CASES

The test cases described in this section involve calculations of mineral solubilities and vapor pressures of salt solutions.

6.1 Test Case 1—NaCl(s) Solubility as a Function of Temperature

The solubility of NaCl(s) will be calculated from 25 to 300 °C and compared with experimental data. The test will determine the ability of SOLCALC, Version 1.0, to accurately calculate the solubility of a single salt at different temperature conditions.

6.1.1 Test Input

Input temperatures to be used are 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, and 300 °C. Below 100 °C, the input pressure will be 1.0 bar. At 100 °C and above, the input pressures will be the vapor saturation pressure at the temperature of interest. Saturation pressure condition is specified by inputting a value of (–1) when prompted by the program to input the pressure.

6.1.2 Test Procedure

The test is run by typing "solcalc," hitting return, and inputting the required information as prompted by the program.

6.1.3 Test Results

The results of the calculation are output to a file named SOLCALC.OUT. This file lists the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations, activities, and activity coefficients of Na^+ and Cl^-. The calculated Na^+ (or Cl^-) concentrations will be compared with experimental data given in Liu and Lindsay (1972) and Linke (1965). The test results will be considered acceptable if within ±10 percent of experimental data.

6.2 Test Case 2—NaCl(s) and/or KCl(s) Solubility in Mixed NaCl+KCl Solutions

The solubility of NaCl(s) and/or KCl(s) will be calculated at different temperatures and compared with experimental data. The test will determine the ability of SOLCALC, Version 1.0, to accurately calculate the solubility of a mineral salt in a solution containing two types of dissolved salts and at different temperature conditions.

6.2.1 Test Input

Input temperatures to be used are 40, 100, and 120 °C. Below 100 °C, the input pressure will be 1.0 bar. At 100 °C and above, the input pressures will be the vapor saturation pressure at the temperature of interest. Saturation pressure condition is specified by inputting a value of (–1) when prompted by the program. When the solubility of NaCl(s) is calculated, a fixed value of K^+ concentration will be input and the program will be told to constrain the Na^+ concentration with the NaCl(s) (or halite) solubility. On the other hand, when the solubility of KCl(s) is calculated, a fixed value of Na^+ concentration will be input and the program will be told to constrain the K^+ concentration with the KCl(s) (or sylvite) solubility. The solubilities when both

NaCl(s) and KCl(s) are present will be calculated by telling the program to constrain the Na^+ and K^+ with the solubility of halite and sylvite, respectively.

6.2.2 Test Procedure

The test is run by typing "solcalc," hitting return, and inputting the required information as prompted by the program.

6.2.3 Test Results

The results of the calculation are output to a file named SOLCALC.OUT. This file lists the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations, activities, and activity coefficients of Na^+, K^+, and Cl^-. The calculated Na^+ and K^+ concentrations will be compared with solubility data on NaCl(s) and KCl(s), respectively, given in Linke (1965). The test results will be considered acceptable if within ±10 percent of experimental data.

6.3 Test Case 3—Solubility in the System NaCl–KCl–$MgCl_2$

The solubility of NaCl(s) and KCl(s) in solutions containing Na^+, K^+, Mg^{2+}, and Cl^- will be calculated at a fixed temperature and compared with experimental data. The test will determine the ability of SOLCALC, Version 1.0, to accurately calculate the solubility of mineral in a solution containing three types of dissolved salts.

6.3.1 Test Input

The input temperature to be used is 90 °C and the input pressure will be 1.0 bar. The concentration of Mg^{2+} will be varied but fixed at specific input values. The Na^+ and K^+ concentrations will be constrained by the solubilities of halite and sylvite, respectively.

6.3.2 Test Procedure

The test is run by typing "solcalc," hitting return, and inputting the required information as prompted by the program.

6.3.3 Test Results

The results of the calculation are output to a file named SOLCALC.OUT. This file lists the temperature and pressure used in the calculation, the resulting ionic strength, and the calculated concentrations, activities, and activity coefficients of Na^+, K^+, Mg^{2+}, and Cl^-. The calculated Na^+ and K^+ concentrations will be compared with solubility data on NaCl(s) and KCl(s), respectively, given in Boecke (1910). The test results will be considered acceptable if within ±20 percent of experimental data. The tolerance limit is larger than for the other test cases because experimental measurements in ternary salt mixtures have larger uncertainties.

6.4 Test Case 4—Vapor Pressure of KCl Solutions as a Function of Temperature

The vapor pressure of KCl solutions as a function of concentration and at different temperatures will be calculated and compared with experimental data. The test will determine the ability of SOLCALC, Version 1.0, to accurately calculate the vapor pressures of single salt solutions.

6.4.1 Test Input

The input temperature to be used is 300 °C and the input pressure will be the vapor saturation pressure at the temperature of interest. Saturation pressure condition is specified by inputting a value of (-1) when prompted by the program. The input KCl concentrations will be varied.

6.4.2 Test Procedure

The test is run by typing "solcalc," hitting return, and inputting the required information as prompted by the program.

6.4.3 Test Results

The results of the calculation are output to a file named VPCALC.OUT. This file lists the temperature used in the calculation and the resulting osmotic coefficients and vapor pressures of the salt solution. The calculated KCl solution vapor pressure will be compared with vapor pressure data from Zarembo et al. (1976). The test results will be considered acceptable if within ±10 percent of experimental data.

6.5 Test Case 5—Vapor Pressure of Mixed NaCl–KCl–$MgCl_2$ Solutions as a Function of Temperature

The vapor pressure of simulated seawater, which is comprised of Na^+, K^+, Mg^{2+}, Cl^-, and SO_4^{2-} ions, as a function of total concentration and temperature will be calculated and compared with experimental data. The test will determine the ability of SOLCALC, Version 1.0, to accurately calculate the vapor pressures of multicomponent salt solutions over a wide range of temperature conditions.

6.5.1 Test Input

The input temperatures to be used are 75, 100, 106, 125, 150, 175, 200, 225, 250, 275, and 300 °C. The input pressure will be 1.0 bar below 100 °C and the vapor saturation pressure at the temperature of interest. Saturation pressure condition is specified by inputting a value of (–1) when prompted by the program. The input compositions of the simulated seawater will be varied.

6.5.2 Test Procedure

The test is run by typing "solcalc," hitting return, and inputting the required information as prompted by the program.

6.5.3 Test Results

The results of the calculation are output to a file named VPCALC.OUT. This file lists the temperature used in the calculation and the resulting osmotic coefficients and vapor pressures of the salt solution. The calculated KCl solution vapor pressure will be compared with vapor pressure data from Liu and Lindsay (1971). The test results will be considered acceptable if within ±10 percent of experimental data.

SOFTWARE VALIDATION REPORT FOR SOLCALC, VERSION 1.0

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC-02-97-009

Prepared by

Roberto T. Pabalan

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

Approved by:

E. C. P

English C. Pearcy
Manager, Geohydrology and Geochemistry

1/30/2002

Date

CONTENTS

1 SCOPE OF THE VALIDATION

This report documents the validation of the code SOLCALC, Version 1.0, as described in its software validation test plan (SVTP) (Pabalan, 2001). The validation involved comparisons of calculated results with experimental data available in the literature. SOLCALC, Version 1.0, is a program that calculates the solubility of mineral salts in mixed electrolyte systems using a matrix inversion technique for solving a series of mass-action and mass-balance equations. Activity coefficients are calculated using the Pitzer equations (1973, 1991). The program also calculates osmotic coefficients and vapor pressures of aqueous salt mixtures. The code was originally developed by R.T. Pabalan at the Department of Chemistry, University of California at Berkeley.

2 REFERENCES

The following documents are referenced in this validation report.

Boecke, H.E., 1910. Ein Schlussel zur Beurtelung des Kristallisationsverlaufes der bei der Kalisalzverarbeitung vorkommenden Losungen. Kali, 4: 271 and 300.

Linke, W.F., 1965. Solubilities of Inorganic and Metal Organic Compounds, Volumes 1 and 2. American Chemical Society.

Liu, C. and Lindsay, W.T.J., 1972. Thermodynamics of sodium chloride solutions at high temperatures. Journal of Solution Chemistry, 1: 45-69.

Liu, C. and Lindsay, W.T.J., 1971. Thermodynamic Properties of Aqueous Solutions at High Temperatures. Research and Development Program Report No. 722, Office of Saline Water of the U.S. Department of Interior, Washington, D.C.

Pabalan, R.T. 2001. Software Validation Test Plan for SOLCALC, Version 1.0. Center for Nuclear Waste Regulatory Analyses, San Antonio, Texas.

Pitzer, K.S., 1973. Thermodynamics of electrolytes, 1. Theoretical basis and general equations. Journal of Physical Chemistry, 77: 268-277.

Pitzer, K.S., 1991. Ion interaction approach: Theory and data correlation. In: K.S. Pitzer (Editor), Activity Coefficients in Electrolyte Solutions. CRC Press, Boca Raton, FL, pp. 75-153.

Zarembo, V.I., Antonov, N.A., Gilyarov, V.N. and Fedorov, M.K., 1976. Activity coefficients of KCl in the system KCl-H_2O at temperatures of 150-350 °C and pressures up to 1500 kg/cm^2. Journal of Applied Chemistry USSR, 49: 1259-1263.

3 ENVIRONMENT

The validation of SOLCALC, Version 1.0, was conducted using an IBM PC-compatible computer, specifically, the machine excalibur.cnwra.swri.edu located in Room A216 of Bldg. 189. The program is interactive. Input information was entered using the keyboard, and the program saved the output information to the computer hard drive.

4 TEST CASES

Several test cases, identified previously in the SVTP, were used to validate the code. The test cases involved calculations of mineral solubilities and vapor pressures of salt solutions.

4.1 Test Case 1—NaCl(s) solubility as a function of temperature

The solubility of NaCl(s) was calculated from 25 to 300 °C and compared with experimental data. The test was designed to determine the ability of SOLCALC, Version 1.0, to accurately calculate the solubility of a single salt at different temperature conditions.

Input temperatures used were 25, 50, 75, 100, 125, 150, 175, 200, 225, 250, 275, and 300 °C. Below 100 °C, the input pressure was specified as 1.0 bar. At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest. Saturation pressure condition was specified by inputting a value of (–1) when prompted by the program to input the pressure.

Comparisons of calculated results with experimental data are shown in Table 1 and Figure 1. The solubility data below 75 °C are from Linke (1965) and those above 75 °C are from Liu and Lindsay (1972). Table 1 shows that the calculated and experimental values all agree within ±10%. The validation test results are therefore acceptable.

4.2 Test Case 2—NaCl(s) and/or KCl(s) solubility in mixed NaCl+KCl solutions

The solubility of NaCl(s) and KCl(s) was calculated at different temperatures and compared with experimental data. The test was designed to determine the ability of SOLCALC, Version 1.0, 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 used were 40, 100, and 150 °C. Below 100 °C, the input pressure was 1.0 bar. At 100 °C and above, the input pressure was the vapor saturation pressure at the temperature of interest. Saturation pressure condition was specified by inputting a value of (–1) when prompted by the program. When the solubility of NaCl(s) was calculated, a fixed value of K^+ concentration was input and the Na^+ concentration was constrained by the NaCl(s) (or halite) solubility. On the other hand, when the solubility of KCl(s) was calculated, a fixed value of Na^+ concentration was input and the K^+ concentration was constrained with the KCl(s) (or sylvite) solubility. The solubilities when both NaCl(s) and KCl(s) are present were calculated by telling the program to constrain the Na^+ and K^+ with the solubility of halite and sylvite, respectively.

Table 1. Comparison of calculated and experimental solubility of NaCl(s).

Temp (°C)	Calculated values	Experimental data	% deviation
25	6.139	6.146	0.11
50	6.273	6.275	0.03
75	6.4480	6.46	0.19
100	6.660	6.68	0.30
125	6.910	6.935	0.36
150	7.201	7.198	-0.04
175	7.542	7.573	0.41
200	7.950	7.973	0.29
225	8.448	8.435	-0.15
250	9.062	8.989	-0.81
275	9.797	9.649	-1.54
300	10.535	10.413	-1.17

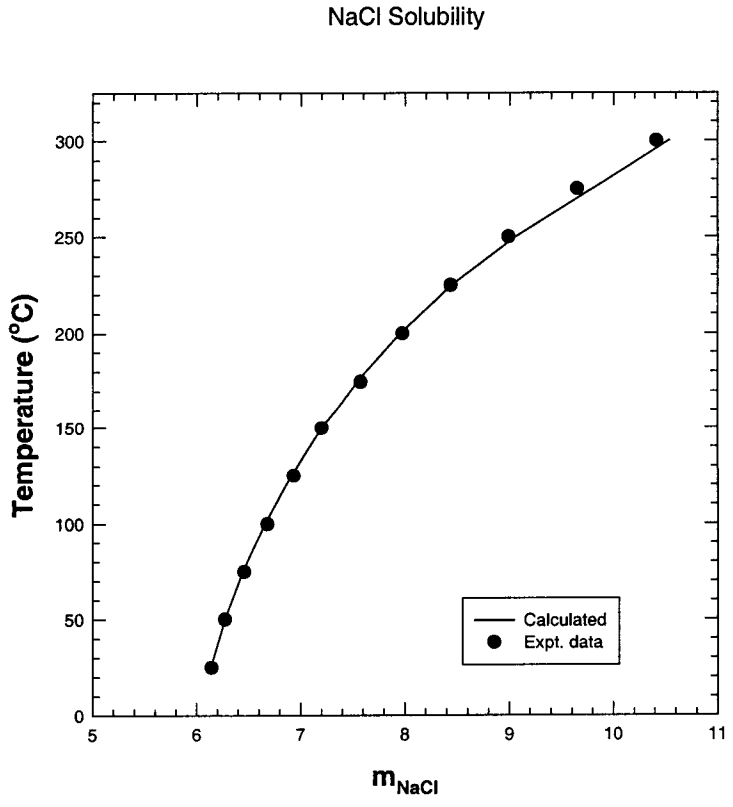

Figure 1. Comparison of calculated and experimental solubility of NaCl(s) as a function of temperature.

Comparisons of calculated results with experimental data are shown in Figure 2 and Table 2. The solubility data are from Linke (1965). Table 2 shows that the calculated and experimental values all agree within ±10%. The validation test results are therefore acceptable.

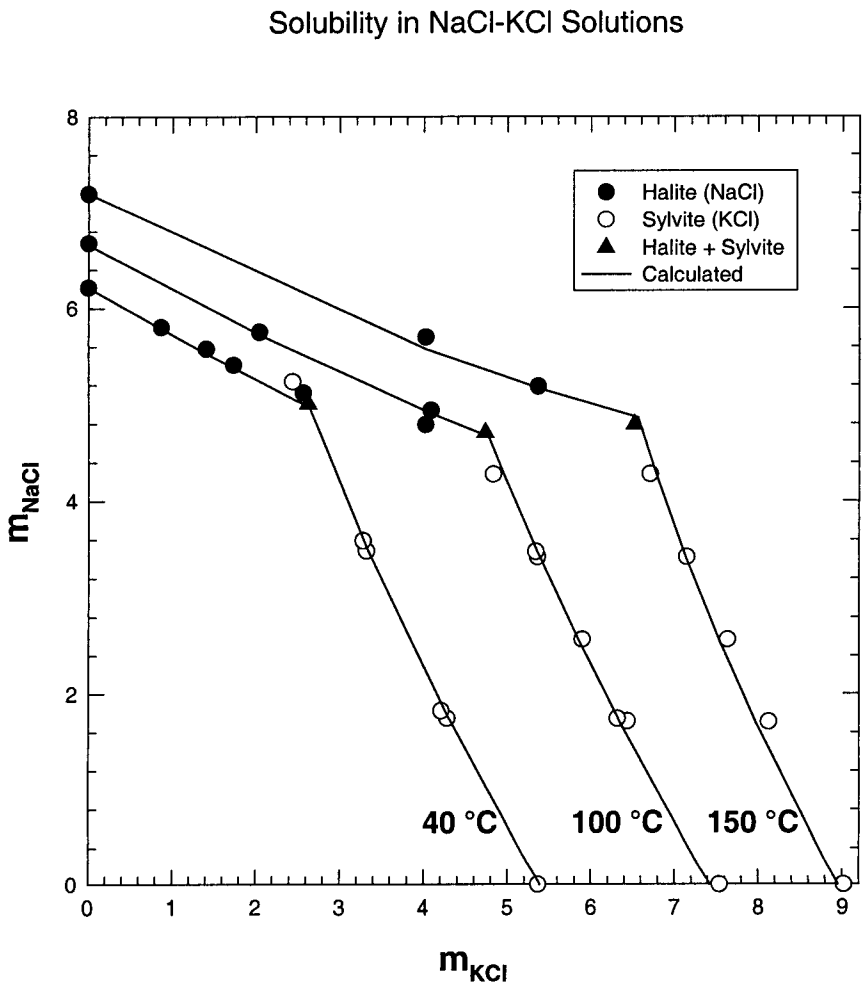

Figure 2. Comparison of calculated and experimental solubility of NaCl(s) and KCl(s) in mixed NaCl–KCl solutions.

Table 2. Comparison of calculated and experimental solubility of NaCl(s) and/or KCl(s) in mixed NaCl+KCl solutions.

Solubility of NaCl(s)				
Temp (°C)	fixed m_{KCl}	expt. m_{NaCl}	calc. m_{NaCl}	% deviation m_{NaCl}
40	0	6.217	6.214	0.05
	0.87	5.801	5.786	0.25
	1.407	5.577	5.531	0.82
	1.733	5.409	5.379	0.55
	2.566	5.12	5.003	2.29
100	0	6.68	6.660	0.30
	2.046	5.749	5.722	0.47
	4.024	4.791	4.933	-2.97
	4.086	4.94	4.911	0.59
150	0	7.198	7.201	-0.04
	4.024	5.698	5.576	2.15
	5.365	5.185	5.166	0.36
Solubility of KCl(s)				
Temp (°C)	fixed m_{NaCl}	expt. m_{KCl}	calc m_{KCl}	% deviation m_{KCl}
40	0	5.37	5.391	-0.39
	1.748	4.28	4.301	-0.49
	1.827	4.21	4.255	-1.06
	3.486	3.32	3.345	-0.75
	3.592	3.28	3.291	-0.31
100	0	7.54	7.426	1.52
	1.717	6.44	6.344	1.49
	1.744	6.32	6.328	-0.13
	2.567	5.9	5.852	0.82
	3.422	5.36	5.388	-0.51
	3.478	5.34	5.358	-0.34
	4.278	4.83	4.957	-2.62
150	0	9.02	8.953	0.74
	1.711	8.13	7.971	1.95
	2.567	7.64	7.534	1.39
	3.422	7.15	7.136	0.20
	4.278	6.71	6.781	-1.06

Solubility of NaCl(s) + KCl(s)						
Temp (°C)	expt. m_{KCl}	expt. m_{NaCl}	calc. m_{KCl}	calc. m_{NaCl}	% deviation m_{NaCl}	% deviation m_{KCl}
40	2.627	5.008	2.64	4.969	-0.61	0.78
100	4.734	4.708	4.77	4.668	-0.79	0.84
150	6.518	4.791	6.56	4.866	-0.71	-1.56

4.3 Test Case 3—Solubility in the system NaCl-KCl-$MgCl_2$

The solubility of NaCl(s) and KCl(s) in solutions containing Na^+, K^+, Mg^{2+}, and Cl^- were calculated at a fixed temperature and compared with experimental data. The test was designed to determine the ability of SOLCALC, Version 1.0, to accurately calculate the solubility of mineral in a solution containing three types of dissolved salts.

The input temperature used was 90 °C and the input pressure was 1.0 bar. The concentration of Mg^{2+} was varied. The Na^+ and K^+ concentrations were constrained by the solubilities of halite and sylvite, respectively.

Comparisons of calculated results with experimental data are shown in Table 3 and Figure 3. The solubility data are from Boecke (1910). Table 3 shows that the calculated and experimental values all agree within ±20%. The tolerance limit is larger than for the other test cases because experimental measurements in ternary salt mixtures have larger uncertainties. The validation test results are therefore acceptable.

Table 3. Comparison of calculated and experimental solubility at 90 °C of NaCl(s) + KCl(s) in mixed NaCl+KCl+$MgCl_2$ solutions.

expt. m_{MgCl2}	expt. m_{KCl}	expt. m_{NaCl}	fixed m_{MgCl2}	calc. m_{KCl}	calc. m_{NaCl}	% deviation m_{KCl}	% deviation m_{NaCl}
0	4.42	4.5	0	4.42	4.68	0.1	-4.1
0.13	4.35	4.33	0.13	4.35	4.50	0.1	-4.0
0.4	4.17	4.04	0.4	4.20	4.14	-0.7	-2.5
0.66	3.98	3.76	0.66	4.05	3.80	-1.7	-1.1
0.92	3.78	3.47	0.92	3.89	3.47	-3.0	-0.1
1.18	3.59	3.16	1.18	3.73	3.16	-3.8	0.0
1.44	3.38	2.85	1.44	3.56	2.86	-5.2	-0.4
1.67	3.15	2.56	1.67	3.40	2.61	-7.9	-1.9
1.93	3	2.29	1.93	3.22	2.34	-7.3	-2.0
2.18	2.8	2.05	2.18	3.04	2.09	-8.6	-1.9
2.43	2.63	1.81	2.43	2.86	1.86	-8.7	-2.5
2.67	2.46	1.57	2.67	2.68	1.65	-9.1	-4.9
2.9	2.29	1.36	2.9	2.52	1.46	-9.9	-7.4
3.12	2.13	1.17	3.12	2.36	1.30	-10.8	-10.7
3.39	1.97	1.02	3.39	2.17	1.11	-10.0	-8.7
3.64	1.83	0.87	3.64	1.99	0.95	-9.0	-9.5
3.88	1.71	0.71	3.88	1.83	0.82	-7.2	-15.2
4.16	1.65	0.58	4.16	1.65	0.68	-0.3	-17.2

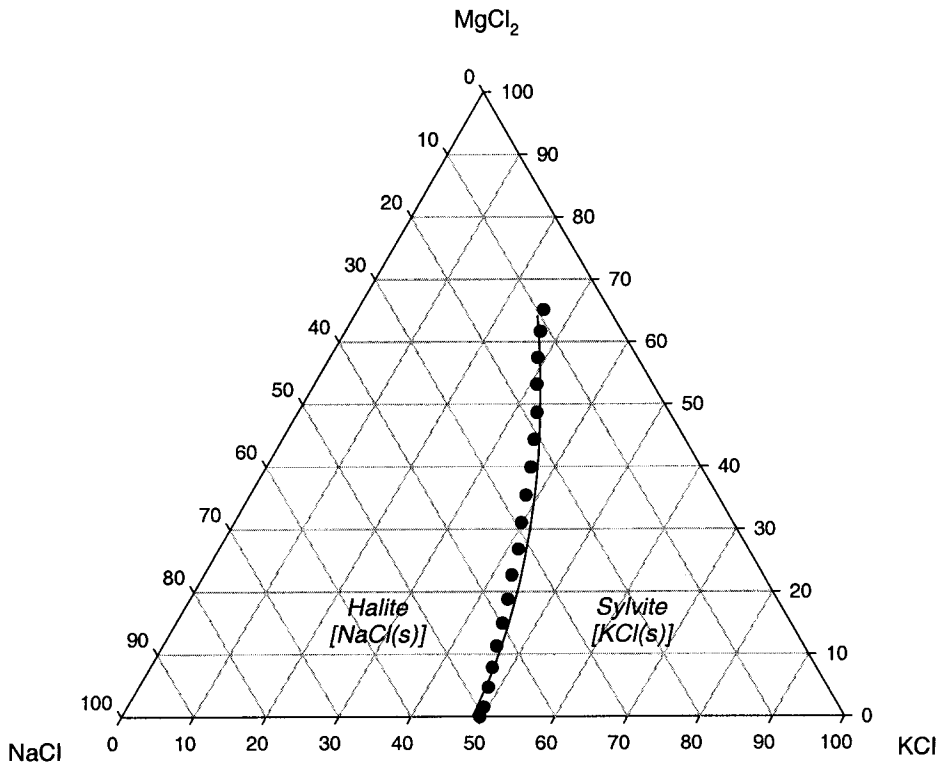

Figure 3. Comparison of calculated (solid line) and experimental (circles) solubility of NaCl(s) + KCl(s) in mixed NaCl+KCl+$MgCl_2$ solutions.

4.4 Test Case 4—Vapor pressure of KCl solutions 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 designed to determine the ability of SOLCALC, Version 1.0, to accurately calculate the vapor pressures of single salt solutions.

The input temperature used was 300 °C and the input pressure was the vapor saturation pressure at the temperature of interest. Saturation pressure condition was specified by inputting a value of (–1) when prompted by the program. The input KCl concentrations were varied.

Comparisons of calculated results with experimental data are shown in Table 4. The vapor pressure data are from Zarembo et al. (1976). Table 4 shows that the calculated and experimental values all agree within ±10%. The validation test results are therefore acceptable.

Table 4. Comparison of calculated and experimental vapor pressure of

KCl solutions at 300 °C.

m_{KCl}	expt. vapor pressure (bar)	calc. vapor pressure (bar)	% deviation
0.549	85.7	84.01	1.97
0.966	84.78	82.78	2.36
1.392	83.32	81.57	2.10
1.904	81.78	80.16	1.98
2.954	79.02	77.3	2.18
3.388	77.62	76.13	1.92
4.283	75.26	73.72	2.05
4.528	74.56	73.06	2.01

4.5 Test Case 5—Vapor pressure of mixed NaCl-KCl-$MgCl_2$ solutions as a function of temperature

The vapor pressure of simulated seawater, which is comprised of Na^+, K^+, Mg^{2+}, Cl^-, and SO_4^{2-} ions, as a function of total concentration and temperature was calculated and compared with experimental data. The test was designed to determine the ability of SOLCALC, Version 1.0, to accurately calculate the vapor pressures of multicomponent salt solutions over a wide range of temperature conditions.

The input temperatures used were 75, 100, 106, 125, 150, 175, 200, 225, 250, 275, and 300 °C. The input pressure was 1.0 bar below 100 °C and the vapor saturation pressure at higher temperatures. Saturation pressure condition was specified by inputting a value of (–1) when prompted by the program. The input compositions of the simulated seawater were varied.

Comparisons of calculated results with experimental data are shown in Table 5. The vapor pressure data are from Liu and Lindsay (1971). The values in Table 5 are given in terms of vapor pressure depression, Δp, because that is how Liu and Lindsay (1971) reported their experimental data. Table 5 shows that the calculated and experimental values all agree within ±10%. The validation test results are therefore acceptable.

Table 5. Comparison of experimental and calculated vapor pressure depression for simulated seawater ($NaCl–Na_2SO_4–MgCl_2–H_2O$).

Temp (°C)	Concentrate Multiple of Simulated Seawater[#]	Vapor Pressure Lowering $\Delta p = p°–p$ (mm. Hg)		% deviation
		Expt.	Calc.	
75	2.8476	15.26	16.05	-5.18
75	5.8158	34.93	35.96	-2.95
100	1.4884	19.24	21.12	-9.77
100	2.8528	40.73	41.94	-2.97
100	5.8377	91.97	93.6	-1.77
106	1.4888	24.02	26.03	-8.37
125	1.4907	45.55	48.19	-5.80
125	2.8630	94.12	95.54	-1.51
125	5.8811	212.45	212.53	-0.04
150	1.4949	95.15	98.8	-3.84
150	2.8813	193.83	195.48	-0.85
150	5.9597	435.63	434.37	0.29
175	1.5018	181.03	186.07	-2.78
175	2.9128	366.74	367.9	-0.32
175	6.1004	823.97	820.34	0.44
200	1.5126	323.03	327.64	-1.43
200	2.9630	650.18	648.53	0.25
200	6.3279	1467.01	1460.07	0.47
225	1.5291	540.85	547.41	-1.21
225	3.0415	1098.26	1088.52	0.89
225	6.6980	2516.96	2497.72	0.76
250	3.1648	1782.33	1764.35	1.01
250	7.3078	4224.43	4186.03	0.91
275	3.3622	2843.63	2799.49	1.55
275	8.3482	7082.75	7018.41	0.91
300	3.6957	4569.66	4406.32	3.57
300	10.2027	12244.32	11971.52	2.23

[#]Actual compositions of the experimental solution are given by the concentrations listed below multiplied by the concentrate multiple of simulated seawater given in the second column of the table (data from Liu and Lindsay, 1971).

$NaCl = 0.42663$ m; $Na_2SO_4 = 0.02976$ m; $MgCl_2 = 0.06726$ m

January 22, 2002

The following pages document the results of calculations done to validate the acquired software SOLCALC Version 1.0, per the Software Validation Test Plan for SOLCALC Version 1.0 prepared by R.T. Pabalan.

1. SOLCALC Validation Test Case 1: NaCl(s) solubility as a function of temperature

The following is the "solcalc.out" output file of SOLCALC showing the calculated solubility of NaCl(s) (halite) from 25 to 300 °C. For each calculation, the temperature and pressure are input interactively, and saturation with halite is also specified interactively.

```
      SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

                TEMP(C) =   25.00     PRESS(BARS) =     1.00

     NUMBER CORRESPONDING TO SATURATED SOLID      20

                THE NUMBER OF ITERATIONS IS     6

                     EQUATION       LOG K

                        20          1.5810

                     IONIC STRENGTH =   6.1390

                 ACTIVITY         ACT.COEFF.         MOLALITY         %ERROR

  CATION #  1   0.61729E+01      0.10055E+01        0.61390E+01      0.0009
  ANION #   1   0.61729E+01      0.10055E+01        0.61390E+01      0.0009

    SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

                TEMP(C) =   50.00     PRESS(BARS) =     1.00

     NUMBER CORRESPONDING TO SATURATED SOLID      20

                THE NUMBER OF ITERATIONS IS     7

                     EQUATION       LOG K

                        20          1.6132

                     IONIC STRENGTH =   6.2732

                 ACTIVITY         ACT.COEFF.         MOLALITY         %ERROR

  CATION #  1   0.64061E+01      0.10212E+01        0.62732E+01      0.0009
  ANION #   1   0.64061E+01      0.10212E+01        0.62732E+01      0.0009

    SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

                TEMP(C) =   75.00     PRESS(BARS) =     1.00

     NUMBER CORRESPONDING TO SATURATED SOLID      20

                THE NUMBER OF ITERATIONS IS     8

                     EQUATION       LOG K
```

20 1.6074

IONIC STRENGTH = 6.4479

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.63637E+01	0.98694E+00	0.64479E+01	0.0009
ANION #	1	0.63637E+01	0.98694E+00	0.64479E+01	0.0009

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 9

EQUATION LOG K

20 1.5731

IONIC STRENGTH = 6.6601

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.61172E+01	0.91849E+00	0.66601E+01	0.0009
ANION #	1	0.61172E+01	0.91849E+00	0.66601E+01	0.0009

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 125.00 PRESS(BARS) = 2.33

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 11

EQUATION LOG K

20 1.5149

IONIC STRENGTH = 6.9099

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.57206E+01	0.82788E+00	0.69099E+01	0.0004
ANION #	1	0.57206E+01	0.82788E+00	0.69099E+01	0.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 12

EQUATION LOG K

20 1.4343

IONIC STRENGTH = 7.2007

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.52135E+01	0.72403E+00	0.72007E+01	0.0007
ANION #	1	0.52135E+01	0.72403E+00	0.72007E+01	0.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 175.00 PRESS(BARS) = 8.93

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
20	1.3312

IONIC STRENGTH = 7.5419

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.46304E+01	0.61395E+00	0.75419E+01	0.0006
ANION #	1	0.46304E+01	0.61395E+00	0.75419E+01	0.0006

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 200.00 PRESS(BARS) = 15.55

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 16

EQUATION	LOG K
20	1.2045

IONIC STRENGTH = 7.9500

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.40017E+01	0.50336E+00	0.79500E+01	0.0007
ANION #	1	0.40017E+01	0.50336E+00	0.79500E+01	0.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 225.00 PRESS(BARS) = 25.49

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 19

EQUATION	LOG K
20	1.0512

IONIC STRENGTH = 8.4480

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.33544E+01	0.39707E+00	0.84480E+01	0.0007
ANION #	1	0.33544E+01	0.39707E+00	0.84480E+01	0.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 250.00 PRESS(BARS) = 39.75

NUMBER CORRESPONDING TO SATURATED SOLID 20

```
            THE NUMBER OF ITERATIONS IS    23

                 EQUATION       LOG K

                    20          0.8666

                 IONIC STRENGTH =   9.0622

              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.27119E+01       0.29926E+00         0.90622E+01       0.0006
ANION #   1   0.27119E+01       0.29926E+00         0.90622E+01       0.0006

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =  275.00     PRESS(BARS) =    59.44

  NUMBER CORRESPONDING TO SATURATED SOLID      20

            THE NUMBER OF ITERATIONS IS    27

                 EQUATION       LOG K

                    20          0.6416

                 IONIC STRENGTH =   9.7972

              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.20932E+01       0.21366E+00         0.97972E+01       0.0010
ANION #   1   0.20932E+01       0.21366E+00         0.97972E+01       0.0010

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

            TEMP(C) =  300.00     PRESS(BARS) =    85.84

  NUMBER CORRESPONDING TO SATURATED SOLID      20

            THE NUMBER OF ITERATIONS IS    32

                 EQUATION       LOG K

                    20          0.3591

                 IONIC STRENGTH =  10.5346

              ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.15119E+01       0.14352E+00         0.10535E+02       0.0008
ANION #   1   0.15119E+01       0.14352E+00         0.10535E+02       0.0008
```

2. SOLCALC Validation Test Case 2: NaCl(s) and/or KCl(s) solubility in mixed NaCl+KCl solutions

The following is the "solcalc.out" output file of SOLCALC showing the calculated solubility of NaCl(s) (halite) and/or KCl(s) (sylvite) in mixed NaCl+KCl solutions. For each calculation, the temperature and pressure are input interactively. When calculating the solubility of NaCl, the concentration of K^+ is fixed at the experimentally measured value (listed in the output file) and saturation with halite is specified interactively. When calculating the solubility of KCl, the concentration of Na^+ is fixed at the experimentally measured value (listed in the output file) and saturation with sylvite is specified interactively. When calculating the solubility when the two solids are saturated, saturation with halite and sylvite is specified interactively.

a) Solubility of two solids, NaCl + KCl:

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.6058
53	1.0420

IONIC STRENGTH = 7.6121

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.54722E+01	0.11013E+01	0.49691E+01	-.0002
CATION #	2	0.14940E+01	0.56527E+00	0.26430E+01	0.0006
ANION #	1	0.73727E+01	0.96854E+00	0.76121E+01	-.0002

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

THE NUMBER OF ITERATIONS IS 17

EQUATION	LOG K
20	1.5731
53	1.3272

IONIC STRENGTH = 9.4399

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.46882E+01	0.10043E+01	0.46683E+01	-.0003
CATION #	2	0.26612E+01	0.55771E+00	0.47716E+01	0.0007
ANION #	1	0.79820E+01	0.84556E+00	0.94399E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

THE NUMBER OF ITERATIONS IS 20

EQUATION	LOG K
20	1.4343
53	1.3524

IONIC STRENGTH = 11.4302

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.36768E+01	0.75567E+00	0.48656E+01	0.0001
CATION #	2	0.30454E+01	0.46392E+00	0.65646E+01	0.0009
ANION #	1	0.73924E+01	0.64674E+00	0.11430E+02	0.0001

b) NaCl solubility:

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 7

EQUATION LOG K

20 1.6058

IONIC STRENGTH = 6.2139

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.63517E+01	0.10222E+01	0.62139E+01	0.0005
ANION #	1	0.63517E+01	0.10222E+01	0.62139E+01	0.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 7

EQUATION LOG K

20 1.6058

CATION # TOTAL

2 0.8700

IONIC STRENGTH = 6.6563

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.60543E+01	0.10463E+01	0.57863E+01	-.0005
CATION #	2	0.46351E+00	0.53277E+00	0.87000E+00	0.0000
ANION #	1	0.66639E+01	0.10011E+01	0.66563E+01	-.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 8

EQUATION	LOG K
20	1.6058

CATION #	TOTAL
2	1.4070

IONIC STRENGTH = 6.9380

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.58744E+01	0.10621E+01	0.55310E+01	0.0006
CATION #	2	0.76311E+00	0.54236E+00	0.14070E+01	0.0000
ANION #	1	0.68678E+01	0.98989E+00	0.69380E+01	0.0006

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 7

EQUATION	LOG K
20	1.6058

CATION #	TOTAL
2	1.7330

IONIC STRENGTH = 7.1122

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.57667E+01	0.10720E+01	0.53792E+01	0.0009
CATION #	2	0.95020E+00	0.54830E+00	0.17330E+01	0.0000
ANION #	1	0.69960E+01	0.98366E+00	0.71122E+01	0.0009

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 7

EQUATION	LOG K
20	1.6058

CATION #	TOTAL
2	2.5660

IONIC STRENGTH = 7.5690

ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR

CATION #	1	0.54968E+01	0.10987E+01	0.50030E+01	-.0003
CATION #	2	0.14467E+01	0.56381E+00	0.25660E+01	0.0000
ANION #	1	0.73397E+01	0.96970E+00	0.75690E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 9

EQUATION	LOG K
20	1.5731

IONIC STRENGTH = 6.6601

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.61172E+01	0.91849E+00	0.66601E+01	0.0009
ANION #	1	0.61172E+01	0.91849E+00	0.66601E+01	0.0009

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 9

EQUATION	LOG K
20	1.5731

CATION #	TOTAL
2	2.0460

IONIC STRENGTH = 7.7679

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.54608E+01	0.95436E+00	0.57219E+01	-.0005
CATION #	2	0.10746E+01	0.52523E+00	0.20460E+01	0.0000
ANION #	1	0.68528E+01	0.88219E+00	0.77679E+01	-.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 8

EQUATION	LOG K
20	1.5731

CATION #	TOTAL

2	4.0240

IONIC STRENGTH = 8.9574

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.48878E+01	0.99074E+00	0.49334E+01	-.0007
CATION #	2	0.22114E+01	0.54954E+00	0.40240E+01	0.0000
ANION #	1	0.76562E+01	0.85473E+00	0.89574E+01	-.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 8

EQUATION	LOG K
20	1.5731

CATION #	TOTAL
2	4.0860

IONIC STRENGTH = 8.9967

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.48708E+01	0.99187E+00	0.49107E+01	-.0007
CATION #	2	0.22483E+01	0.55025E+00	0.40860E+01	0.0000
ANION #	1	0.76828E+01	0.85396E+00	0.89967E+01	-.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 20

THE NUMBER OF ITERATIONS IS 12

EQUATION	LOG K
20	1.4343

IONIC STRENGTH = 7.2007

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.52135E+01	0.72403E+00	0.72007E+01	0.0007
ANION #	1	0.52135E+01	0.72403E+00	0.72007E+01	0.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 12

EQUATION	LOG K
20	1.4343

CATION #	TOTAL
2	4.0240

IONIC STRENGTH = 9.5997

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.41787E+01	0.74945E+00	0.55757E+01	-.0007
CATION #	2	0.18438E+01	0.45820E+00	0.40240E+01	0.0000
ANION #	1	0.65047E+01	0.67759E+00	0.95997E+01	-.0007

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 2

THE NUMBER OF ITERATIONS IS 13

EQUATION	LOG K
20	1.4343

CATION #	TOTAL
2	5.3650

IONIC STRENGTH = 10.5313

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.38983E+01	0.75455E+00	0.51663E+01	0.0005
CATION #	2	0.24841E+01	0.46303E+00	0.53650E+01	0.0000
ANION #	1	0.69724E+01	0.66207E+00	0.10531E+02	0.0005

c) KCl solubility:

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 53

THE NUMBER OF ITERATIONS IS 13

EQUATION	LOG K
53	1.0420

IONIC STRENGTH = 5.3909

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	2	0.33189E+01	0.61564E+00	0.53909E+01	0.0008

ANION # 1 0.33189E+01 0.61564E+00 0.53909E+01 0.0008

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 17

EQUATION	LOG K
53	1.0420

CATION #	TOTAL
1	1.7480

IONIC STRENGTH = 6.0490

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.15105E+01	0.86412E+00	0.17480E+01	0.0000
CATION #	2	0.25588E+01	0.59492E+00	0.43010E+01	0.0005
ANION #	1	0.43048E+01	0.71165E+00	0.60490E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 13

EQUATION	LOG K
53	1.0420

CATION #	TOTAL
1	1.8270

IONIC STRENGTH = 6.0817

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.15869E+01	0.86859E+00	0.18270E+01	0.0000
CATION #	2	0.25275E+01	0.59406E+00	0.42547E+01	0.0005
ANION #	1	0.43580E+01	0.71658E+00	0.60817E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K

53 1.0420

CATION # TOTAL

1 3.4860

IONIC STRENGTH = 6.8308

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.34044E+01	0.97659E+00	0.34860E+01	0.0000
CATION #	2	0.19322E+01	0.57766E+00	0.33448E+01	0.0008
ANION #	1	0.57009E+01	0.83459E+00	0.68308E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 40.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION LOG K

53 1.0420

CATION # TOTAL

1 3.5920

IONIC STRENGTH = 6.8830

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.35364E+01	0.98452E+00	0.35920E+01	0.0000
CATION #	2	0.18980E+01	0.57671E+00	0.32910E+01	0.0009
ANION #	1	0.58036E+01	0.84318E+00	0.68830E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

THE NUMBER OF ITERATIONS IS 17

EQUATION LOG K

53 1.3272

IONIC STRENGTH = 7.4256

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	2	0.46088E+01	0.62067E+00	0.74256E+01	0.0008
ANION #	1	0.46088E+01	0.62067E+00	0.74256E+01	0.0008

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 13

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	1.7170

IONIC STRENGTH = 8.0612

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.14993E+01	0.87323E+00	0.17170E+01	0.0000
CATION #	2	0.37902E+01	0.59743E+00	0.63442E+01	0.0006
ANION #	1	0.56043E+01	0.69522E+00	0.80612E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 13

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	1.7440

IONIC STRENGTH = 8.0721

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.15248E+01	0.87431E+00	0.17440E+01	0.0000
CATION #	2	0.37783E+01	0.59706E+00	0.63281E+01	0.0006
ANION #	1	0.56219E+01	0.69646E+00	0.80721E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 12

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	2.5670

IONIC STRENGTH = 8.4187

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.23313E+01	0.90817E+00	0.25670E+01	0.0000
CATION #	2	0.34297E+01	0.58610E+00	0.58517E+01	0.0009
ANION #	1	0.61934E+01	0.73567E+00	0.84187E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	3.4220

IONIC STRENGTH = 8.8096

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.32359E+01	0.94561E+00	0.34220E+01	0.0000
CATION #	2	0.30962E+01	0.57469E+00	0.53876E+01	0.0010
ANION #	1	0.68604E+01	0.77874E+00	0.88096E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	3.4780

IONIC STRENGTH = 8.8364

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.32976E+01	0.94814E+00	0.34780E+01	0.0000
CATION #	2	0.30754E+01	0.57394E+00	0.53584E+01	0.0010
ANION #	1	0.69069E+01	0.78164E+00	0.88364E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 100.00 PRESS(BARS) = 1.02

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 16

EQUATION	LOG K
53	1.3272

CATION #	TOTAL
1	4.2780

IONIC STRENGTH = 9.2346

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.42155E+01	0.98539E+00	0.42780E+01	0.0000
CATION #	2	0.27910E+01	0.56309E+00	0.49566E+01	0.0006
ANION #	1	0.76107E+01	0.82415E+00	0.92346E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

THE NUMBER OF ITERATIONS IS 10

EQUATION	LOG K
53	1.3524

IONIC STRENGTH = 8.9531

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	2	0.47449E+01	0.52997E+00	0.89531E+01	-.0009
ANION #	1	0.47449E+01	0.52997E+00	0.89531E+01	-.0009

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 13

EQUATION	LOG K
53	1.3524

CATION #	TOTAL
1	1.7110

IONIC STRENGTH = 9.6823

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.12096E+01	0.70698E+00	0.17110E+01	0.0000
CATION #	2	0.40507E+01	0.50816E+00	0.79713E+01	-.0007
ANION #	1	0.55579E+01	0.57403E+00	0.96823E+01	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
53	1.3524

CATION #	TOTAL
1	2.5670

IONIC STRENGTH = 10.1005

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.18525E+01	0.72167E+00	0.25670E+01	0.0000
CATION #	2	0.37433E+01	0.49689E+00	0.75335E+01	-.0009
ANION #	1	0.60143E+01	0.59545E+00	0.10100E+02	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 15

EQUATION	LOG K
53	1.3524

CATION #	TOTAL
1	3.4220

IONIC STRENGTH = 10.5576

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.25170E+01	0.73552E+00	0.34220E+01	0.0000
CATION #	2	0.34622E+01	0.48520E+00	0.71356E+01	0.0010
ANION #	1	0.65025E+01	0.61590E+00	0.10558E+02	0.0000

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 150.00 PRESS(BARS) = 4.77

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 1

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K

```
                53          1.3524

            CATION #        TOTAL

                1           4.2780

            IONIC STRENGTH =  11.0590

          ACTIVITY        ACT.COEFF.        MOLALITY        %ERROR

CATION #  1  0.32004E+01     0.74811E+00      0.42780E+01     0.0000
CATION #  2  0.32065E+01     0.47286E+00      0.67810E+01     -.0009
ANION #   1  0.70213E+01     0.63490E+00      0.11059E+02     0.0000
```

3. SOLCALC Validation Test Case 3: Solubility in the NaCl-KCl-$MgCl_2$ system

The following is the "solcalc.out" output file of SOLCALC for solubility calculations in the NaCl-KCl-$MgCl_2$ system [two solids saturated: NaCl(s) (halite) and KCl(s) (sylvite) in an aqueous solution containing K^+, Na^+, Mg^{2+}, and Cl^- ions]. For each calculation, the temperature, pressure, and experimentally measured Mg^{2+} concentration (listed in the output file) are input interactively, and saturation with both halite and sylvite are also specified interactively.

```
SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   90.00     PRESS(BARS) =     0.71

NUMBER CORRESPONDING TO SATURATED SOLID      20

NUMBER CORRESPONDING TO SATURATED SOLID      53

          THE NUMBER OF ITERATIONS IS    15

              EQUATION       LOG K

                 20          1.5899
                 53          1.3018

              IONIC STRENGTH =   9.0981

          ACTIVITY        ACT.COEFF.        MOLALITY        %ERROR

CATION #  1  0.48702E+01     0.10400E+01      0.46829E+01     -.0003
CATION #  2  0.25087E+01     0.56820E+00      0.44152E+01     0.0008
ANION #   1  0.79856E+01     0.87773E+00      0.90981E+01     -.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

          TEMP(C) =   90.00     PRESS(BARS) =     1.00

NUMBER CORRESPONDING TO SATURATED SOLID      20

NUMBER CORRESPONDING TO SATURATED SOLID      53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      3

          THE NUMBER OF ITERATIONS IS    13

              EQUATION       LOG K
```

20	1.5899
53	1.3018

CATION #	TOTAL
3	0.1300

IONIC STRENGTH = 9.2405

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.46471E+01	0.10319E+01	0.45034E+01	-.0004
CATION #	2	0.23935E+01	0.55060E+00	0.43471E+01	0.0010
CATION #	3	0.13625E+00	0.10481E+01	0.13000E+00	0.0000
ANION #	1	0.83699E+01	0.91871E+00	0.91105E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	0.4000

IONIC STRENGTH = 9.5389

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.42092E+01	0.10169E+01	0.41393E+01	-.0003
CATION #	2	0.21680E+01	0.51625E+00	0.41996E+01	0.0007
CATION #	3	0.40956E+00	0.10239E+01	0.40000E+00	0.0000
ANION #	1	0.92404E+01	0.10111E+01	0.91389E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 14

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	0.6600

IONIC STRENGTH = 9.8300

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.38188E+01	0.10048E+01	0.38005E+01	-.0004
CATION #	2	0.19669E+01	0.48572E+00	0.40495E+01	0.0009
CATION #	3	0.66427E+00	0.10065E+01	0.66000E+00	0.0000
ANION #	1	0.10185E+02	0.11107E+01	0.91700E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 15

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	0.9200

IONIC STRENGTH = 10.1259

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.34564E+01	0.99488E+00	0.34742E+01	-.0003
CATION #	2	0.17803E+01	0.45745E+00	0.38917E+01	0.0006
CATION #	3	0.91527E+00	0.99486E+00	0.92000E+00	0.0000
ANION #	1	0.11253E+02	0.12224E+01	0.92059E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	1.1800

IONIC STRENGTH = 10.4277

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.31201E+01	0.98712E+00	0.31608E+01	-.0003
CATION #	2	0.16071E+01	0.43121E+00	0.37268E+01	0.0006
CATION #	3	0.11674E+01	0.98932E+00	0.11800E+01	0.0000

ANION #	1	0.12466E+02	0.13480E+01	0.92477E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	1.4400

IONIC STRENGTH = 10.7366

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.28082E+01	0.98150E+00	0.28611E+01	-.0003
CATION #	2	0.14464E+01	0.40681E+00	0.35555E+01	0.0007
CATION #	3	0.14260E+01	0.99027E+00	0.14400E+01	0.0000
ANION #	1	0.13851E+02	0.14899E+01	0.92966E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	1.6700

IONIC STRENGTH = 11.0170

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.25513E+01	0.97833E+00	0.26079E+01	-.0004
CATION #	2	0.13141E+01	0.38660E+00	0.33991E+01	0.0007
CATION #	3	0.16650E+01	0.99703E+00	0.16700E+01	0.0000
ANION #	1	0.15245E+02	0.16310E+01	0.93470E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	1.9300

IONIC STRENGTH = 11.3433

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.22814E+01	0.97682E+00	0.23356E+01	-.0003
CATION #	2	0.11751E+01	0.36519E+00	0.32178E+01	0.0007
CATION #	3	0.19535E+01	0.10122E+01	0.19300E+01	0.0000
ANION #	1	0.17049E+02	0.18111E+01	0.94133E+01	-.0003

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 19

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	2.1800

IONIC STRENGTH = 11.6681

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.20414E+01	0.97750E+00	0.20884E+01	-.0004
CATION #	2	0.10514E+01	0.34590E+00	0.30397E+01	0.0008
CATION #	3	0.22569E+01	0.10353E+01	0.21800E+01	0.0000
ANION #	1	0.19053E+02	0.20081E+01	0.94881E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 19

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	2.4300

IONIC STRENGTH = 12.0052

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.18195E+01	0.98036E+00	0.18560E+01	-.0004
CATION #	2	0.93716E+00	0.32776E+00	0.28593E+01	0.0008
CATION #	3	0.25956E+01	0.10682E+01	0.24300E+01	0.0000
ANION #	1	0.21377E+02	0.22325E+01	0.95752E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 17

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	2.6700

IONIC STRENGTH = 12.3421

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.16229E+01	0.98523E+00	0.16472E+01	-.0005
CATION #	2	0.83589E+00	0.31133E+00	0.26849E+01	0.0010
CATION #	3	0.29655E+01	0.11107E+01	0.26700E+01	0.0000
ANION #	1	0.23967E+02	0.24779E+01	0.96721E+01	-.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	2.9000

IONIC STRENGTH = 12.6785

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.14489E+01	0.99194E+00	0.14607E+01	-.0005
CATION #	2	0.74630E+00	0.29641E+00	0.25178E+01	0.0009
CATION #	3	0.33739E+01	0.11634E+01	0.29000E+01	0.0000
ANION #	1	0.26844E+02	0.27452E+01	0.97785E+01	-.0005

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 18

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	3.1200

IONIC STRENGTH = 13.0140

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.12954E+01	0.10003E+01	0.12950E+01	-.0004
CATION #	2	0.66719E+00	0.28282E+00	0.23590E+01	0.0008
CATION #	3	0.38283E+01	0.12270E+01	0.31200E+01	0.0000
ANION #	1	0.30027E+02	0.30349E+01	0.98940E+01	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 20

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	3.3900

IONIC STRENGTH = 13.4458

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.11233E+01	0.10133E+01	0.11086E+01	-.0004
CATION #	2	0.57857E+00	0.26696E+00	0.21672E+01	0.0007
CATION #	3	0.44975E+01	0.13267E+01	0.33900E+01	0.0000
ANION #	1	0.34626E+02	0.34434E+01	0.10056E+02	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 20

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	3.6400

IONIC STRENGTH = 13.8670

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.97950E+00	0.10280E+01	0.95279E+00	-.0004
CATION #	2	0.50451E+00	0.25299E+00	0.19942E+01	0.0007
CATION #	3	0.52612E+01	0.14454E+01	0.36400E+01	0.0000
ANION #	1	0.39709E+02	0.38828E+01	0.10227E+02	-.0004

SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

TEMP(C) = 90.00 PRESS(BARS) = 1.00

NUMBER CORRESPONDING TO SATURATED SOLID 20

NUMBER CORRESPONDING TO SATURATED SOLID 53

NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY 3

THE NUMBER OF ITERATIONS IS 20

EQUATION	LOG K
20	1.5899
53	1.3018

CATION #	TOTAL
3	3.8800

IONIC STRENGTH = 14.2919

		ACTIVITY	ACT.COEFF.	MOLALITY	%ERROR
CATION #	1	0.85489E+00	0.10448E+01	0.81827E+00	-.0004
CATION #	2	0.44033E+00	0.24014E+00	0.18336E+01	0.0008

```
CATION #  3   0.61668E+01      0.15894E+01        0.38800E+01      0.0000
ANION #   1   0.45497E+02      0.43697E+01        0.10412E+02      -.0004

  SOLUBILITY AND SPECIATION CALCULATION IN MIXED ELECTROLYTE SYSTEMS

           TEMP(C) =   90.00     PRESS(BARS) =     1.00

  NUMBER CORRESPONDING TO SATURATED SOLID      20

  NUMBER CORRESPONDING TO SATURATED SOLID      53

  NUMBER CORRESPONDING TO CATION WITH FIXED MOLALITY      3

           THE NUMBER OF ITERATIONS IS    20

                EQUATION       LOG K

                   20          1.5899
                   53          1.3018

                CATION #       TOTAL

                    3          4.1600

                IONIC STRENGTH =  14.8143

             ACTIVITY          ACT.COEFF.          MOLALITY          %ERROR

CATION #  1   0.72533E+00      0.10674E+01        0.67951E+00      -.0004
CATION #  2   0.37359E+00      0.22576E+00        0.16548E+01      0.0009
CATION #  3   0.75088E+01      0.18050E+01        0.41600E+01      0.0000
ANION #   1   0.53624E+02      0.50331E+01        0.10654E+02      -.0004
```

4. SOLCALC Validation Test Case 4: Vapor pressure of KCl solutions as a function of concentration

The following is the "vpcalc.out" output file of SOLCALC showing the results of calculating the vapor pressure (VP) of KCl solutions at 300 °C as a function of concentration. For each calculation, the temperature, pressure, and K^+ and Cl^- concentrations are input interactively. The following concentrations of K^+ and Cl^- are used (note: m_{K+} is equal to m_{Cl-}): 0.549, 0.966, 1.392, 1.904, 2.954, 3.388, 4.283, and 4.528. These concentration values are used because experimental vapor pressure data are available at these concentrations from Zarembo et al. (1976).

TEMP(C)	TOTMOL	OSMO	**VP bar**	P0-VP bar	VP/P0	(P0-VP) mm Hg
300.00	1.0980	0.7224	**84.01**	1.82	0.97875	1368.11
300.00	1.9320	0.6957	**82.78**	3.06	0.96440	2291.88
300.00	2.7840	0.6815	**81.57**	4.26	0.95034	3196.84
300.00	3.8080	0.6732	**80.16**	5.68	0.93388	4256.99
300.00	5.9080	0.6715	**77.30**	8.53	0.90066	6395.72
300.00	6.7760	0.6743	**76.13**	9.70	0.88699	7275.27
300.00	8.5660	0.6832	**73.72**	12.11	0.85887	9085.76
300.00	9.0560	0.6861	**73.06**	12.77	0.85121	9579.23

5. SOLCALC Validation Test Case 5: Vapor pressure of mixed NaCl-KCl-$MgCl_2$ solutions as a function of total concentration and temperature

The following is the "vpcalc.out" output file of SOLCALC showing the results of calculating the vapor pressure of mixed NaCl-KCl-$MgCl_2$ solutions as a function of total concentration and temperature. For each calculation, the temperature, pressure, and Na^+, Mg^{2+}, Cl^-, and SO_4^- concentrations are input interactively. The ion concentrations were calculated from the (i) simulated seawater composition and (ii) concentrate multiple of seawater composition given by Liu and Lindsay (1971). The ion concentrations used as input are as follows:

Temp (°C)	Concentrate multiple	m_{Na}	m_{Mg}	m_{Cl}	m_{SO4}
75	2.8476	1.384361	0.19153	1.597931	0.084745
75	5.8158	2.827351	0.391171	3.263536	0.173078
100	1.4884	0.723586	0.10011	0.835216	0.044295
100	2.8528	1.386889	0.191879	1.600849	0.084899
100	5.8377	2.837998	0.392644	3.275825	0.17373
106	1.4888	0.72378	0.100137	0.83544	0.044307
125	1.4907	0.724704	0.100264	0.836506	0.044363
125	2.863	1.391847	0.192565	1.606572	0.085203
125	5.8811	2.859097	0.395563	3.300179	0.175022
150	1.4949	0.726746	0.100547	0.838863	0.044488
150	2.8813	1.400744	0.193796	1.616841	0.085747
150	5.9597	2.897308	0.400849	3.344286	0.177361
175	1.5018	0.7301	0.101011	0.842735	0.044694
175	2.9128	1.416058	0.195915	1.634518	0.086685
175	6.1004	2.965709	0.410313	3.423239	0.181548
200	1.5126	0.73535	0.101737	0.848795	0.045015
200	2.963	1.440462	0.199291	1.662687	0.088179
200	6.3279	3.076309	0.425615	3.550901	0.188318
225	1.5291	0.743372	0.102847	0.858054	0.045506
225	3.0415	1.478625	0.204571	1.706738	0.090515
225	6.698	3.256233	0.450507	3.758583	0.199332
250	3.1648	1.538568	0.212864	1.775928	0.094184
250	7.3078	3.552687	0.491523	4.100772	0.21748
275	3.3622	1.634534	0.226142	1.886699	0.100059
275	8.3482	4.058477	0.5615	4.684592	0.248442
300	3.6957	1.796665	0.248573	2.073842	0.109984
300	10.2027	4.960043	0.686234	5.725245	0.303632

TEMP(C)	TOTMOL	OSMO	VP bar	P0-VP bar	VP/P0	**(P0-VP) mm Hg**
75.00	3.2586	0.9629	0.36	0.02	0.94452	**16.05**
75.00	6.6551	1.0979	0.34	0.05	0.87569	**35.96**
100.00	1.7032	0.9021	0.99	0.03	0.97221	**21.12**
100.00	3.2645	0.9493	0.96	0.06	0.94482	**41.94**
100.00	6.6802	1.0753	0.89	0.12	0.87685	**93.60**
106.00	1.7037	0.8990	1.22	0.03	0.97224	**26.03**
125.00	1.7058	0.8878	2.26	0.06	0.97231	**48.19**
125.00	3.2762	0.9302	2.19	0.13	0.94510	**95.54**

125.00	6.7299	1.0460	2.04	0.28	0.87788	**212.53**
150.00	1.7106	0.8698	4.63	0.13	0.97231	**98.80**
150.00	3.2971	0.9064	4.50	0.26	0.94522	**195.48**
150.00	6.8198	1.0114	4.18	0.58	0.87826	**434.37**
175.00	1.7185	0.8482	8.67	0.25	0.97218	**186.07**
175.00	3.3332	0.8780	8.43	0.49	0.94500	**367.90**
175.00	6.9808	0.9725	7.82	1.09	0.87736	**820.34**
200.00	1.7309	0.8226	15.10	0.44	0.97188	**327.64**
200.00	3.3906	0.8447	14.67	0.86	0.94435	**648.53**
200.00	7.2411	0.9289	13.59	1.95	0.87471	**1460.07**
225.00	1.7498	0.7921	24.75	0.73	0.97136	**547.41**
225.00	3.4804	0.8057	24.03	1.45	0.94304	**1088.52**
225.00	7.6647	0.8802	22.15	3.33	0.86930	**2497.72**
250.00	3.6215	0.7594	37.38	2.35	0.94080	**1764.35**
250.00	8.3625	0.8257	34.15	5.58	0.85955	**4186.03**
275.00	3.8474	0.7026	55.70	3.73	0.93720	**2799.49**
275.00	9.5530	0.7636	50.07	9.36	0.84255	**7018.41**
300.00	4.2291	0.6287	79.96	5.87	0.93156	**4406.32**
300.00	11.6752	0.6883	69.87	15.96	0.81405	**11971.52**