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Verification Testing of OLI Systems Mixed Solvent Electrolyte Model for the Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O System to High Ionic Strength at 25^oC

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EXECUTIVE SUMMARY

This technical report summarizes model verification results and summary statistics for 41 evaporite mineral solubility cases evaluated by Savannah River National Laboratory using OLI Systems' aqueous electrolyte thermodynamic modeling software. The 41 verification cases containing a total of 60 solubility curves comprise mineral solubility data from low to high ionic strength at 25°C for the eight-component system $Na\text{-}K\text{-}Mg\text{-}Ca\text{-}H\text{-}Cl\text{-}SO_4\text{-}OH\text{-}HCO_3\text{-}CO_3\text{-}CO_2\text{-}H_2O$ as reported by Harvie et al. (1984).

Thermodynamic calculations were executed using OLI Systems' Stream Analyzer computation module within the OLI Studio software platform (Ver. 11.0, Rev. 11.0.1.9). The Mixed Solvent Electrolyte (MSE) thermodynamic framework was chosen for this investigation because of its superiority in modeling high-ionic-strength inorganic salt solutions and actinide redox chemistry and solubility, both of which are relevant to the geological repository conditions at the Waste Isolation Pilot Plant in Carlsbad, New Mexico.

Mineral solubility data in various inorganic salt solutions were digitized and extracted from figures generated by Harvie et al. (1984). For each of the 60 solubility curves, a case-specific chemistry model and input file were generated in OLI Studio using OLI Stream Analyzer and the MSE (H_3O^+ ion) public databank provided by OLI Systems. Model simulation results were exported to Microsoft Excel to calculate summary statistics and to generate graphs comparing the OLI model predictions to the solubility data. Summary statistics include residuals (model – data) and concordance (accuracy × precision, where precision is indicated by the Pearson correlation coefficient and accuracy accounts for bias and scale differential). Private databanks were not developed, and activity coefficient model regressions were not performed to improve OLI model fits to the data.

Of the 41 model verification plots, 83% have a mean of the percent residuals less than or equal to 25%. Similarly, 75% display a concordance greater than or equal to 0.75. Only seven of the 41 verification plots fail to show good agreement between the model and data. Of these seven, three are relevant to the WIPP repository because they involve the $Mg\text{-}OH\text{-}Cl\text{-}SO_4\text{-}CO_3$ aqueous system. The remaining four address salt solubilities at the pH extremes (strong acid and strong base). It should be noted that in two of the three $Mg\text{-}OH\text{-}Cl\text{-}SO_4\text{-}CO_3$ system cases, the regressed Harvie et al. (1984) solubility curve also deviated from the data.

Lack of agreement between the OLI model-predicted solubility curves and the data is attributable to one or more of the following: specific solid species are not included in the OLI MSE databank; there is significant variation among the different solubility datasets chosen by Harvie et al. (1984); the OLI MSE model's thermodynamic parameters were determined using different solubility datasets; and the activity coefficient parameters for certain relevant ion-ion and ion-molecule pairs have not been optimized via data regression.

Two recommendations for future work are to (1) evaluate solubility data for the $Mg\text{-}OH\text{-}Cl\text{-}SO_4\text{-}CO_3$ system at high ionic strength and, if necessary, develop a private OLI MSE database that includes missing species and, where necessary, regressed standard state properties and interaction parameters; (2) perform similar verification testing of the OLI model for actinide solubility data.

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LIST OF ABBREVIATIONS

AQ	Aqueous
CBFO	Carlsbad Field Office
MBG	Material Balance Group
MSE	Mixed Solvent Electrolyte
SRNL	Savannah River National Laboratory
U.S. DOE	United States Department of Energy
WIPP	Waste Isolation Pilot Plant

1.0 Introduction

This technical report summarizes model verification results and summary statistics for 41 evaporite mineral solubility cases evaluated by Savannah River National Laboratory (SRNL) using OLI Systems' aqueous electrolyte thermodynamic modeling software. The 41 verification cases comprise mineral solubility data from low to high ionic strength at 25°C for the eight-component system Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O as reported by Harvie et al. (1984). Verification testing of the OLI software is a key work activity listed in Section V (Description of Planned Activities), Subsection A (Unclassified Level of Effort Work Activities), of the Fiscal Year 2023 Work Authorization "SRNL Support for WIPP" (FY2023-SPD; B&R No. EY9009801) between United States Department of Energy (U.S. DOE) Carlsbad Field Office (CBFO) and SRNL. The specific unclassified level of effort work activity addressed by this report is "Comparison of OLI-MSE predictions of mineral solubility against Pitzer-based models of relevant systems including, but not limited to, the model of Harvie et al. (*Geochimica et Cosmochimica Acta*, 48(4):723-751) for the eight-component system Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O at 25°C and high ionic strength."

2.0 OLI Thermodynamic Model

Thermodynamic calculations for this verification study were executed using OLI Systems' Stream Analyzer computation module within the OLI Studio software platform (Ver. 11.0, Rev. 11.0.1.9). SRNL maintains an annual multi-seat license for OLI Studio (single- and multiple-case batch equilibrium computations and real-solution Pourbaix diagrams), OLI Databook (private database development), and OLI Flowsheet (development of chemical process flowsheets for flowing systems). The Stream Analyzer module is typically employed to predict the chemical speciation of dissolved components and precipitates; saturation tendencies and activity coefficients; and equilibrium conditions including pH, E_h, temperature, pressure, ionic strength, total dissolved solids, specific conductance, and solution density. In addition, OLI Studio includes a Water Analyzer module that facilitates the input of water analysis data (cations, anions, pH, alkalinity, etc.) for reconciliation of pH and electroneutrality. Finally, the Corrosion Analyzer module will generate real-solution Pourbaix diagrams (i.e., E_h-pH diagrams) for the solution composition and ionic strength conditions of interest. The aqueous electrolyte thermodynamic frameworks implemented within the OLI code have been specifically developed and refined over the past 50 years for modeling aqueous systems under nonideal conditions (i.e., ionic strengths up to 30 molal, temperatures up to 300°C, and/or pressures up to 100 atm). The complete suite of OLI aqueous modeling tools has been successfully used at SRNL in numerous applications, including simulations involving high-ionic-strength tank waste.

The OLI software platform offers access to two aqueous electrolyte thermodynamic frameworks: (1) the original AQ (Aqueous) framework for aqueous-only systems up to 30 molal ionic strength; and (2) the more recently developed and supported MSE (Mixed Solvent Electrolyte) framework for mixed solvent electrolyte systems spanning 100% aqueous to 100% nonaqueous. The MSE framework was chosen for this investigation because of its superiority in modeling high-ionic-strength inorganic salt solutions and actinide redox chemistry and solubility, both of which are relevant to WIPP (Waste Isolation Pilot Plant) geological repository conditions. Wang et al. (2017) describe the MSE thermodynamic framework as well as recent improvements to the MSE thermodynamic database for U(IV, VI), Np(IV, V, VI), Pu(III, IV, V, VI), Am(III), and Cm(III) over the pH range 0 to 14. The MSE framework has been parameterized for actinide systems based on an analysis of extensive literature data on solubility, speciation, and vapor–liquid equilibrium, and it reproduces the complexities of the solubility behavior as a function of critical factors including pH, CO_2 partial pressure, concentration of carbonates, and the presence of other salt components. In addition, redox effects on solubility and speciation have also been considered, as demonstrated by the reductive and oxidative dissolutions of Np(VI) and Pu(IV) solids, respectively (Wang et al., 2017). In general, the MSE thermodynamic framework predicts solubility and speciation as a function of pH (from concentrated acids through moderate pH to concentrated alkaline solutions) at temperatures up to 573 K.

However, as noted by Wang et al. (2017), confidence in model predictions varies for different systems depending on the availability of underlying experimental data. Extensive documentation of the development and implementation of the OLI MSE thermodynamic framework over the last 20 years is available in the public domain (Anderko et al., 2007; Anderko et al., 2002; Anderko et al., 2003; Gruszkiewicz et al., 2007; Kosinski et al., 2007; Springer et al., 2014; 2015; Wang and Anderko, 2003; 2008; 2013; Wang et al., 2017; Wang et al., 2006; Wang et al., 2010; Wang et al., 2008; Wang et al., 2002; 2004a; 2011; Wang et al., 2013a; Wang et al., 2013b; Wang et al., 2004b)

3.0 Verification Testing Approach

Harvie et al. (1984) extended the mineral solubility model developed by Harvie and Weare (1980) to the eight-component system, Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O, at 25°C and from zero to high ionic strength. The Harvie et al. (1984) model was based on semi-empirical Pitzer equations (Pitzer, 1973) for aqueous electrolyte solutions and was parameterized using available isobaric, electromotive force, and solubility data available for many of the subsystems. The predictive abilities of the Harvie et al. (1984) model were further demonstrated through comparison to experimental data for systems more complex than those used in parameterization.

For this evaluation of the OLI MSE thermodynamic model, mineral solubility data in various inorganic salt solutions were digitized and extracted from ten multiplot figures presented by Harvie et al. (1984). Appendix A, Page A-2, provides a list with titles of the resulting 41 model verification plots containing a total of 60 individual "solubility curves." Noted for each plot by yes or no is whether the mineral system and/or solution conditions (i.e., pH range, speciation, etc.) are relevant to the WIPP geological repository. Approximately 50% of the model verification plots are relevant to WIPP.

Verification testing proceeded as follows:

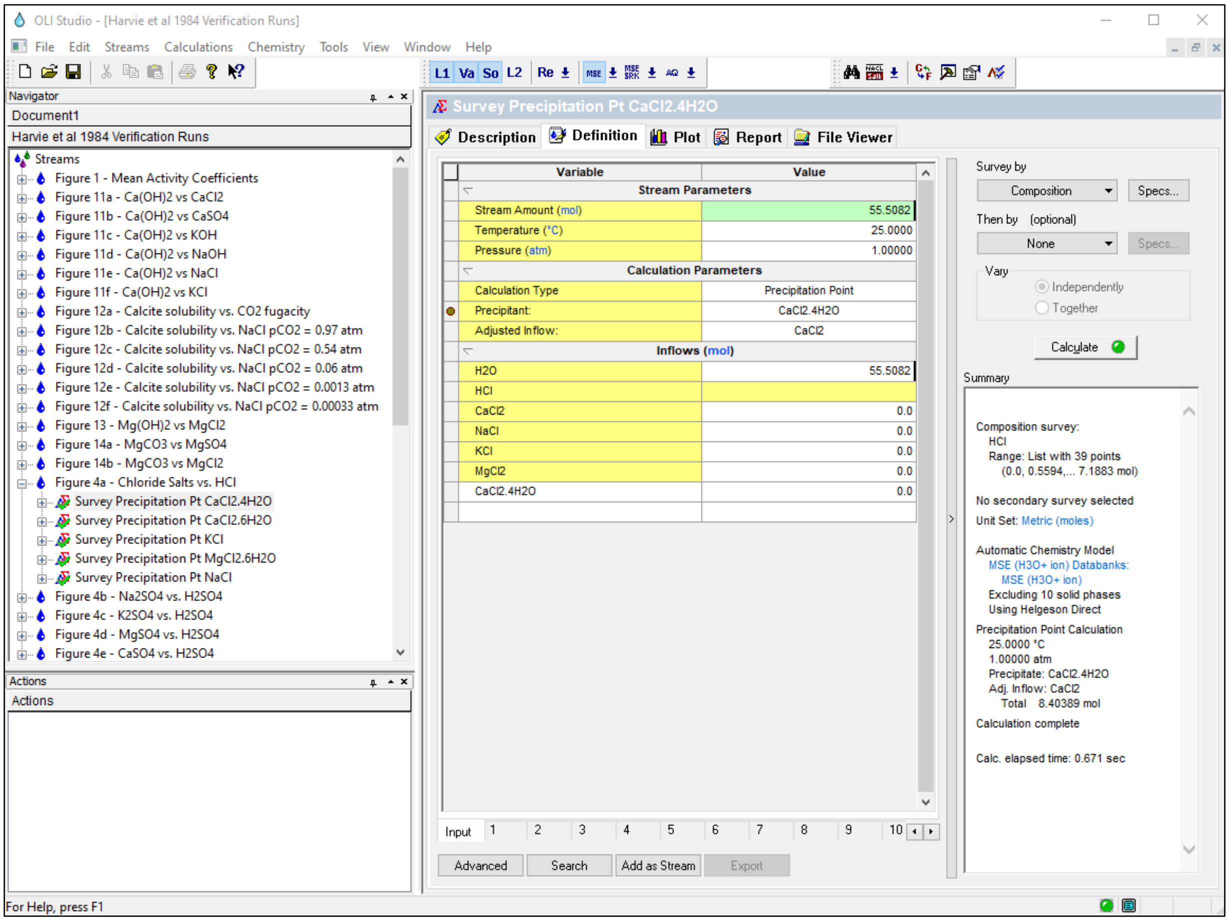
- For each of the 60 solubility curves, a case-specific chemistry model and input file were generated in OLI Studio using OLI Stream Analyzer and the MSE (H_3O^+ ion) public databank provided by OLI Systems. Figure 3-1 displays an example screen capture of the input file prepared for the $CaCl_2.4H_2O$ solubility data from Harvie et al. (1984; Figure 4a).
- All simulations were performed assuming 1 kg H_2O (55.5082 moles) at 25°C and 1 atm total pressure unless indicated otherwise.
- Various calculational approaches were utilized based on user experience to generate each solubility curve. In most situations, a "survey by composition" was performed where, for the case shown in Figure 3-1, the moles of HCl added were varied (surveyed) from 0.0 moles to 7.1883 moles in 39 points as shown in Figure 3-2. In tandem, the "Precipitation Point" calculation type was selected as displayed in Figure 3-3 to automatically adjust the molar inflow of $CaCl_2$ until the system reached saturation with respect to the specified precipitant (in this case, $CaCl_2.4H_2O$).
- Example output for the $CaCl_2.4H_2O$ solubility case using OLI Stream Analyzer's "Plot" postprocessor is shown in Figure 3-4. The solubility data for $CaCl_2.4H_2O$ are given in Column 2, labeled $CaCl_2$ (the adjusted inflow shown in Figure 3-3). The last five columns report scaling tendencies[1] for precipitates that could potentially form in the system. Note that the scaling tendency

---

[1] The scaling tendency for each solid species is equal to its ion activity product divided by its thermodynamic equilibrium constant. As a result, a scaling tendency equal to 1.0 signifies that the solid species is at saturation under the assumed conditions (temperature, pressure, composition, pH, and E_h) of the system and is "included" in the equilibrium calculations. A scaling tendency much less than 1.0 means that the solid is below saturation and is unlikely to form. Lastly, a scaling tendency much greater than 1.0 implies that the solid is above saturation but has been specifically excluded from the model based on expert judgment of its likelihood to form.

for $CaCl_2.4H_2O$ is equal to 1.0 because the model automatically adjusted the molar inflow of $CaCl_2$ until the system reached saturation with respect to $CaCl_2.4H_2O$.

- In some situations (e.g., CO_2 solubility in chloride and sulfate salt solutions at various CO_2 partial pressures), a fixed, excess quantity of the desired inflow species (e.g., CO_2) was specified in the inflows (i.e., input file). The solubility at each salt concentration point was obtained by choosing the liquid-phase Material Balance Group (MBG) output variable of interest (e.g., C(+4) Liq 1). The C(+4) Liq 1 MBG output variable equals the molar sum of all dissolved C(+4)-containing species in the liquid phase. As shown in Figure 3-5, MBG output variables are available for all elemental species in the model in each redox state in all phases (vapor, liquid, solid, and total).
- In many plots, two or three different minerals comprise the overall solubility curve because mineral stability will change as a function of the background salt concentration, pH, temperature, etc. In these instances, multiple input model cases were prepared and executed to generate an individual solubility curve for each mineral. The individual curves were then combined in Microsoft Excel to obtain the overall "minimum solubility" profile.
- Model simulation results were exported to Microsoft Excel to calculate summary statistics and to generate graphs comparing the OLI model predictions to the solubility data extracted from the paper by Harvie et al. (1984). Summary statistics include residuals (model – data) and concordance (accuracy × precision, where precision is indicated by the Pearson correlation coefficient and accuracy accounts for bias and scale differential). See Appendix B for a list of the statistical calculations performed, which are based on the approach described by van Belle (2008) for assessing agreement in terms of accuracy, scale differential, and precision.
- For the limited number of cases (seven in total) where agreement between the OLI MSE model and the raw solubility data was less than satisfactory, OLI's AQ thermodynamic model was also evaluated. AQ model results are also included for comparison. In some but not all cases, the older AQ model provides better agreement with the Harvie et al. (1984) data.
- Note that private databanks were not developed, and activity coefficient model regressions were not performed to improve model fits to the data. In other words, the verification runs are based on "out of the box" OLI model predictions. This should be considered when comparing OLI-predicted solubility curves to the model curves generated by Harvie et al. (1984), which are best-fit regressions to the data.



Document1

Harvie et al 1984 Verification Runs

- Streams
  - Figure 1 - Mean Activity Coefficients
  - Figure 11a - Ca(OH)2 vs CaCl2
  - Figure 11b - Ca(OH)2 vs CaSO4
  - Figure 11c - Ca(OH)2 vs KOH
  - Figure 11d - Ca(OH)2 vs NaOH
  - Figure 11e - Ca(OH)2 vs NaCl
  - Figure 11f - Ca(OH)2 vs KCl
  - Figure 12a - Calcite solubility vs. CO2 fugacity
  - Figure 12b - Calcite solubility vs. NaCl pCO2 = 0.97 atm
  - Figure 12c - Calcite solubility vs. NaCl pCO2 = 0.54 atm
  - Figure 12d - Calcite solubility vs. NaCl pCO2 = 0.06 atm
  - Figure 12e - Calcite solubility vs. NaCl pCO2 = 0.0013 atm
  - Figure 12f - Calcite solubility vs. NaCl pCO2 = 0.00033 atm
  - Figure 13 - Mg(OH)2 vs MgCl2
  - Figure 14a - MgCO3 vs MgSO4
  - Figure 14b - MgCO3 vs MgCl2
  - Figure 4a - Chloride Salts vs. HCl
    - Survey Precipitation Pt CaCl2.4H2O
    - Survey Precipitation Pt CaCl2.6H2O
    - Survey Precipitation Pt KCl
    - Survey Precipitation Pt MgCl2.6H2O
    - Survey Precipitation Pt NaCl
  - Figure 4b - Na2SO4 vs. H2SO4
  - Figure 4c - K2SO4 vs. H2SO4
  - Figure 4d - MgSO4 vs. H2SO4
  - Figure 4e - CaSO4 vs. H2SO4

Survey Precipitation Pt CaCl2.4H2O

Variable	Value
Stream Parameters	
Stream Amount (mol)	55.5082
Temperature (°C)	25.0000
Pressure (atm)	1.00000
Calculation Parameters	
Calculation Type	Precipitation Point
Precipitant:	CaCl2.4H2O
Adjusted Inflow:	CaCl2
Inflows (mol)	
H2O	55.5082
HCl	
CaCl2	0.0
NaCl	0.0
KCl	0.0
MgCl2	0.0
CaCl2.4H2O	0.0

Survey by: Composition

Then by (optional): None

Vary: ○ Independently ○ Together

Summary

Composition survey:
HCl
Range: List with 39 points
(0.0, 0.5594,... 7.1883 mol)

No secondary survey selected

Unit Set: Metric (moles)

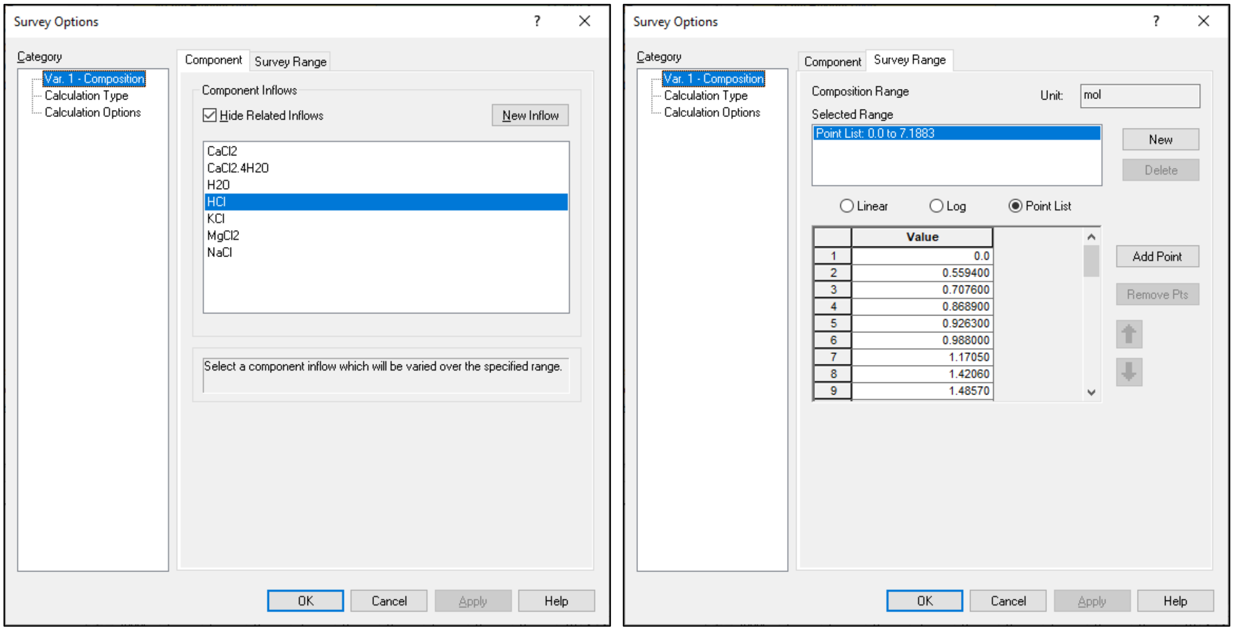
Automatic Chemistry Model
MSE (H3O+ ion) Databanks:
MSE (H3O+ ion)
Excluding 10 solid phases
Using Helgeson Direct

Precipitation Point Calculation
25.0000 °C
1.00000 atm
Precipitate: CaCl2.4H2O
Adj. Inflow: CaCl2
Total 8.40389 mol

Calculation complete

Calc. elapsed time: 0.671 sec

Figure 3-1. Example OLI Input File for $CaCl_2.4H_2O$ Solubility Case.



Component Inflows

☑ Hide Related Inflows

- CaCl2
- CaCl2.4H2O
- H2O
- HCl
- KCl
- MgCl2
- NaCl

Select a component inflow which will be varied over the specified range.

Composition Range

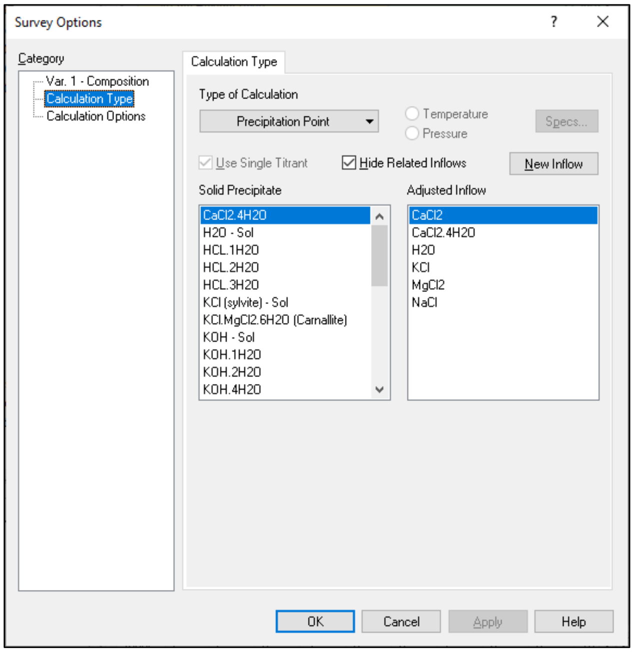
Unit: mol

Selected Range: Point List: 0.0 to 7.1883

○ Linear ○ Log ● Point List

	Value
1	0.0
2	0.559400
3	0.707600
4	0.868900
5	0.926300
6	0.988000
7	1.17050
8	1.42060
9	1.48570

Figure 3-2. Example HCl Composition Survey for $CaCl_2.4H_2O$ Solubility Case.



Type of Calculation: Precipitation Point

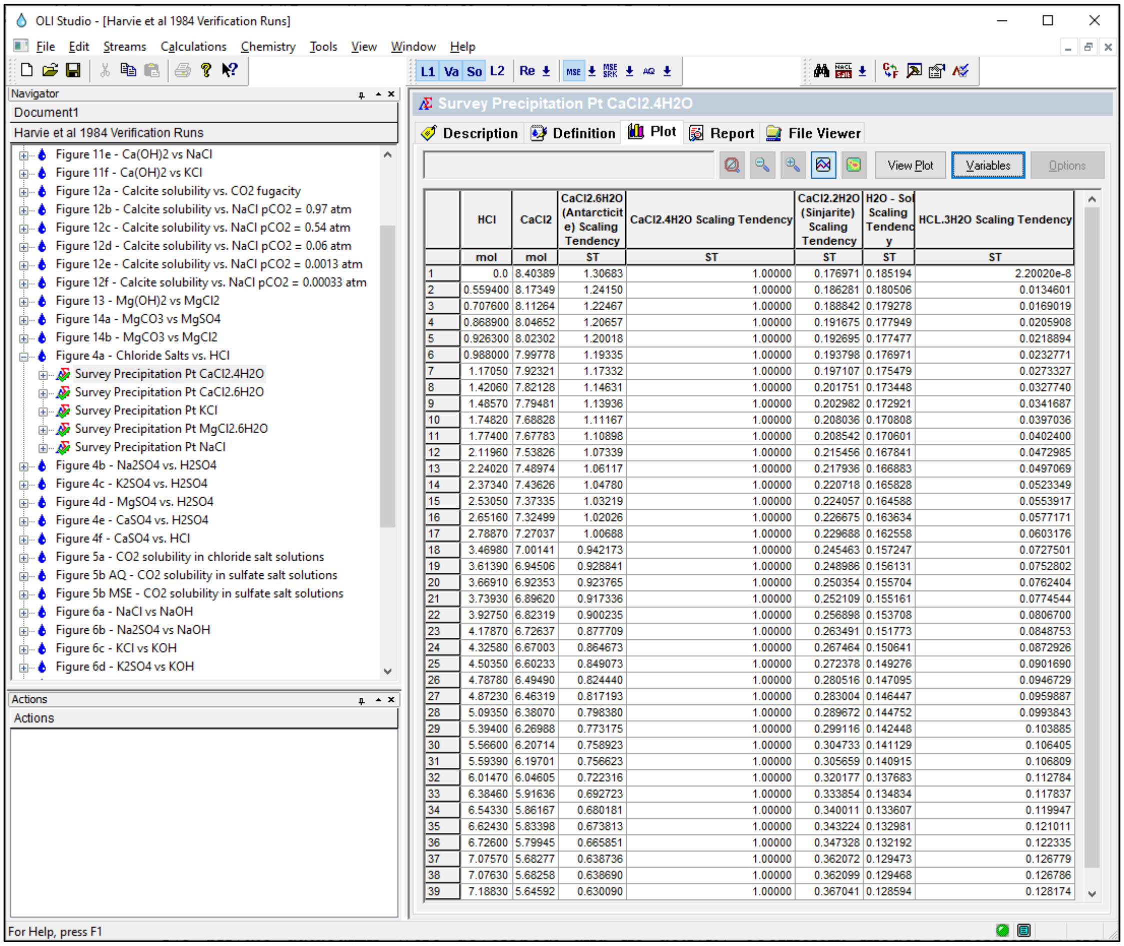
○ Temperature
○ Pressure

☑ Use Single Titrant
☑ Hide Related Inflows

Solid Precipitate:
- CaCl2.4H2O
- H2O - Sol
- HCL.1H2O
- HCL.2H2O
- HCL.3H2O
- KCl (sylvite) - Sol
- KCl.MgCl2.6H2O (Carnallite)
- KOH - Sol
- KOH.1H2O
- KOH.2H2O
- KOH.4H2O

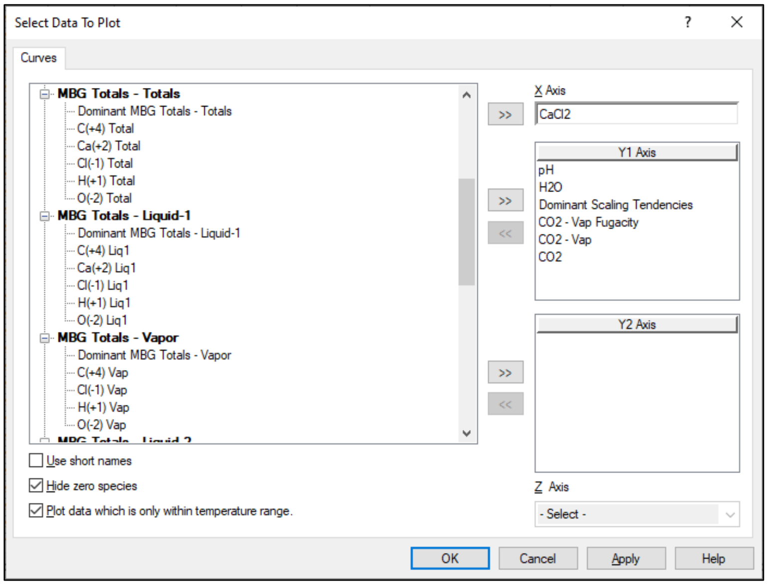
Adjusted Inflow:
- CaCl2
- CaCl2.4H2O
- H2O
- KCl
- MgCl2
- NaCl

Figure 3-3. Example Precipitation Point Calculation Type Specification for $CaCl_2.4H_2O$ Case.



	HCl	CaCl2	CaCl2.6H2O (Antarcticite) Scaling Tendency	CaCl2.4H2O Scaling Tendency	CaCl2.2H2O (Sinjarite) Scaling Tendency	H2O - Sol Scaling Tendency	HCL.3H2O Scaling Tendency
	mol	mol	ST	ST	ST	ST	ST
1	0.0	8.40389	1.30683	1.00000	0.176971	0.185194	2.20020e-8
2	0.559400	8.17349	1.24150	1.00000	0.186281	0.180506	0.0134601
3	0.707600	8.11264	1.22467	1.00000	0.188842	0.179278	0.0169019
4	0.868900	8.04652	1.20657	1.00000	0.191675	0.177949	0.0205908
5	0.926300	8.02302	1.20018	1.00000	0.192695	0.177477	0.0218894
6	0.988000	7.99778	1.19335	1.00000	0.193798	0.176971	0.0232771
7	1.17050	7.92321	1.17332	1.00000	0.197107	0.175479	0.0273327
8	1.42060	7.82128	1.14631	1.00000	0.201751	0.173448	0.0327740
9	1.48570	7.79481	1.13936	1.00000	0.202982	0.172921	0.0341687
10	1.74820	7.68828	1.11167	1.00000	0.208036	0.170808	0.0397036
11	1.77400	7.67783	1.10898	1.00000	0.208542	0.170601	0.0402400
12	2.11960	7.53826	1.07339	1.00000	0.215456	0.167841	0.0472985
13	2.24020	7.48974	1.06117	1.00000	0.217936	0.166883	0.0497069
14	2.37340	7.43626	1.04780	1.00000	0.220718	0.165828	0.0523349
15	2.53050	7.37335	1.03219	1.00000	0.224057	0.164588	0.0553917
16	2.65160	7.32499	1.02026	1.00000	0.226675	0.163634	0.0577171
17	2.78870	7.27037	1.00688	1.00000	0.229688	0.162558	0.0603176
18	3.46980	7.00141	0.942173	1.00000	0.245463	0.157247	0.0727501
19	3.61390	6.94506	0.928841	1.00000	0.248986	0.156131	0.0752802
20	3.66910	6.92353	0.923765	1.00000	0.250354	0.155704	0.0762404
21	3.73930	6.89620	0.917336	1.00000	0.252109	0.155161	0.0774544
22	3.92750	6.82319	0.900235	1.00000	0.256898	0.153708	0.0806700
23	4.17870	6.72637	0.877709	1.00000	0.263491	0.151773	0.0848753
24	4.32580	6.67003	0.864673	1.00000	0.267464	0.150641	0.0872926
25	4.50350	6.60233	0.849073	1.00000	0.272378	0.149276	0.0901690
26	4.78780	6.49490	0.824440	1.00000	0.280516	0.147095	0.0946729
27	4.87230	6.46319	0.817193	1.00000	0.283004	0.146447	0.0959887
28	5.09350	6.38070	0.798380	1.00000	0.289672	0.144752	0.0993843
29	5.39400	6.26988	0.773175	1.00000	0.299116	0.142448	0.103885
30	5.56600	6.20714	0.758923	1.00000	0.304733	0.141129	0.106405
31	5.59390	6.19701	0.756623	1.00000	0.305659	0.140915	0.106809
32	6.01470	6.04605	0.722316	1.00000	0.320177	0.137683	0.112784
33	6.38460	5.91636	0.692723	1.00000	0.333854	0.134834	0.117837
34	6.54330	5.86167	0.680181	1.00000	0.340011	0.133607	0.119947
35	6.62430	5.83398	0.673813	1.00000	0.343224	0.132981	0.121011
36	6.72600	5.79945	0.665851	1.00000	0.347328	0.132192	0.122335
37	7.07570	5.68277	0.638736	1.00000	0.362072	0.129473	0.126779
38	7.07630	5.68258	0.638690	1.00000	0.362099	0.129468	0.126786
39	7.18830	5.64592	0.630090	1.00000	0.367041	0.128594	0.128174

Figure 3-4. Example Output for $CaCl_2.4H_2O$ Solubility Case.



X Axis: CaCl2

Y1 Axis:
pH
H2O
Dominant Scaling Tendencies
CO2 - Vap Fugacity
CO2 - Vap
CO2

Z Axis: - Select -

☐ Use short names
☑ Hide zero species
☑ Plot data which is only within temperature range.

Figure 3-5. Material Balance Group Output Variables for CO_2 Solubility in Salt Solutions.

4.0 Results and Discussion

Appendix A summarizes the results of the OLI MSE model verification runs for the 41 model verification plots, which are sorted by the Harvie et al. (1984) figure number. Statistical measures are included on each worksheet for each verification plot to assess agreement between model and data. The measures include the mean, standard deviation, minimum, and maximum of the residuals in percent; the Pearson correlation coefficient (measure of precision); bias (location); scale differential; deviance (bias + scale differential + imprecision); accuracy (measure of combined impacts of bias and scale differential); and concordance (accuracy × precision). Appendix B provides the equations used to calculate these statistical measures.

In addition to visual comparison of the model-predicted curves to the data, agreement between model and data was assessed using two statistical measures: mean of the absolute value of the percent residuals and concordance. Appendix A, Page A-2, provides a color-coded summary of this statistical assessment for all 41 Harvie et al. (1984) figures. Color highlighting of each statistical measure is based on the key given in Table 4-1.

Table 4-1. Color Key for Assessing Agreement between Model and Data.

Highlight Color	Mean of Percent Residuals	Concordance
🟩	$\mu \leq 10\%$	$0.75 \leq C \leq 1.0$
🟨	$10\% < \mu \leq 25\%$	$0.50 \leq C < 0.75$
🟥	$25\% < \mu \leq 50\%$	$0.25 \leq C < 0.50$
🟧	$\mu > 50\%$	$C < 0.25$

Of the 41 model verification plots, 83% have a mean of the percent residuals less than or equal to 25%. Similarly, 75% display a concordance greater than or equal to 0.75. Only seven of the 41 verification plots fail to show good agreement between the model and data. Of these seven, three are relevant to the WIPP repository because they involve the Mg-OH-Cl-SO_4-CO_3 aqueous system (Harvie et al., 1984; Figures 13, 14a, and 14b). The remaining four (Harvie et al., 1984; Figures 4c, 5b, 6d, and 11a) address salt solubilities at the pH extremes (strong acid and strong base). It should be noted that in two of the three Mg-OH-Cl-SO_4-CO_3 system cases, the regressed Harvie et al. (1984) solubility curve also deviates from the data.

Lack of agreement between the OLI model-predicted solubility curves and the data is attributable to one or more of the following aspects:

1. **Missing Solid Species**: In five of the seven cases not showing good agreement, the OLI MSE thermodynamic database is missing one or more of the solid species included in the Harvie et al. (1984) regression of the data. For the three Mg-OH-Cl-SO_4-CO_3 system cases relevant to WIPP (Harvie et al., 1984; Figures 13, 14a, and 14b), missing solids included magnesium oxychloride [$Mg_2Cl(OH)_3 \cdot 4H_2O$] and nesquehonite [$MgCO_3 \cdot 3H_2O$]. Magnesium oxychloride is absent from both the MSE and AQ thermodynamic databases. Nesquehonite is included in OLI's AQ thermodynamic database; however, model predictions did not substantially improve relative to MSE model predictions, which are based on the combined solubility of magnesite [$MgCO_3$] plus brucite [$Mg(OH)_2$]. Missing solid species for the two cases not relevant to WIPP include $KHSO_4$ (Harvie et al., 1984; Figure 4c; MSE); $K_3H(SO_4)_2$ (Harvie et al., 1984; Figure 4c; MSE and AQ); $K_8H_6(SO_4)_7 \cdot H_2O$ (Harvie et al., 1984; Figure 4c; MSE and AQ); $CaCl_2.3Ca(OH)_2 \cdot 13H_2O$ (Harvie et al., 1984; Figure 11a; MSE and AQ); and $CaCl_2.Ca(OH)_2 \cdot H_2O$ (Harvie et al., 1984; Figure 11a; MSE).
2. **Variation in Different Solubility Datasets:** In some cases (Harvie et al., 1984; Figures 4b, 4c, and 13), multiple datasets from different sources depict fundamentally different solubility limits. This wide variation in measured solubility can be caused by differences in the (a) geomorphology of the solids due to aging; (b) experimental design (e.g., in situ precipitation from a supersaturated solution vs. dissolution of a crystalline solid); (c) experimental error (e.g., colloidal solids passing through a filter); (d) misidentification of the actual solid phase(s) present (e.g., magnesite vs. nesquehonite); and/or (e) presence of a second solid phase (e.g., brucite plus magnesite vs. magnesite alone). In Figure 13, Harvie et al. (1984) chose to fit their thermodynamic model to a blended dataset (brucite plus magnesium oxychloride) that was deemed most representative. The OLI-predicted solubility curve, however, is based on brucite only and splits the difference between the two solubility datasets.
3. **Thermodynamic Parameters Regressed Using Different Solubility Datasets:** OLI MSE thermodynamic parameters for a particular solid species may have been regressed against a different/more recent set(s) of solubility data than employed by Harvie et al. (1984) in their regressions.
4. **Activity Coefficient Parameters Not Regressed:** Mid-range and short-range interaction parameters were not regressed for the aqueous system of interest at high ionic strength such that deviations between model and data increase with increasing concentration (Harvie et al., 1984; potentially Figures 5b, 11e, 11f, 12e, and 12f).

5.0 Quality Assurance

The entire OLI software platform is classified as Level D per Software Classification Document X-SWCD-A-00007, Rev. 0 (Choi, 2019a) in accordance with SRS Manual 1Q, 20-1, Rev. 23, Software Quality Assurance (SRS, 2022). OLI software quality assurance is documented in the Software Quality Assurance Plan, X-SQP-A-00001 (Choi, 2019b).

Requirements for performing reviews of technical reports and the extent of review are established in Manual E7, Procedure 2.60 (SRS, 2021). SRNL documents the extent and type of review using the SRNL Technical Report Design Checklist (WSRC, 2004).

6.0 Conclusions

Verification testing of OLI Systems' MSE aqueous electrolyte thermodynamic model employed published solubility data for evaporite minerals compiled by Harvie et al. (1984) and displayed good agreement between the model and data. Of the 41 model verification plots, 83% have a mean of the percent residuals less than or equal to 25%. Similarly, 75% display a concordance greater than or equal to 0.75. Only seven of the 41 verification plots fail to show good agreement between the model and data. Of these seven, three are relevant to the WIPP repository because they involve the Mg-OH-Cl-SO_4-CO_3 aqueous system. Note that private databanks were not developed, and activity coefficient model regressions were not performed to improve model fits to the data. In other words, the verification runs are based on “out of the box” OLI model predictions.

7.0 Recommendations

Two recommendations to consider for future work are:

1. Conduct a literature review of solubility data for the Mg-OH-Cl-SO_4-CO_3 system at high ionic strength to evaluate whether additional datasets are available, particularly those containing hydromagnesite and magnesium oxychloride. If so, compare the additional solubility data to OLI MSE model predictions. Based on the results of this comparison, consider developing a private OLI MSE database that includes the missing species of interest and, where necessary, the regressed standard state properties and interaction parameters.
2. Perform similar verification testing of the OLI model for actinide solubility data.

8.0 References

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Appendix A. Results of Verification Testing and Summary Statistics

Verification Testing of OLI Systems Mixed Solvent Electrolyte Model for the Na-K-Mg-Ca-H-Cl-SO_4-OH-HCO_3-CO_3-CO_2-H_2O System to High Ionic Strength at 25°C

Data Source: **Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. *Geochimica et Cosmochimica Acta*, *48* (4), 723-751.**

		WIPP Relevant	Absolute Value of Residuals for MSE Model				Concordance	Concordance Titrant Precip. Pt. or Alt. Solid	Absolute Value of Residuals for AQ Model				Concordance
			Mean (%)	Std. Dev. (%)	Minimum (%)	Maximum (%)			Mean (%)	Std. Dev. (%)	Minimum (%)	Maximum (%)	
Figure 1	The mean activity coefficient of HCl in an HCl-H2O system	No	2.4	2.4	0.04	8.3	0.968	na	0.7	0.4	0.2	1.5	1.0
Figure 4a	The calculated and experimental solubilities of chloride salts in HCl solutions	No	3.1	5.3	0.1	24.7	0.768	na	na	na	na	na	na
Figure 4b	The calculated and experimental solubilities of Na sulfate salts in H2SO4 solutions	No	7.8	3.1	3.2	12.4	0.894	na	na	na	na	na	na
Figure 4c	The calculated and experimental solubilities of K sulfate salts in H2SO4 solutions	No	60.4	88.0	0.1	447.9	-0.064	na	55.2	18.8	2.1	69.6	0.071
Figure 4d	The calculated and experimental solubilities of Mg sulfate salts in H2SO4 solutions	No	11.7	11.6	0.1	35.3	0.229	na	na	na	na	na	na
Figure 4e	The calculated and experimental solubilities of Ca sulfate salts in H2SO4 solutions	No	4.0	5.4	0.4	18.0	0.950	na	na	na	na	na	na
Figure 4f	The calculated and experimental solubilities of Ca sulfate salts in HCl solutions	No	2.7	3.4	0.2	10.0	0.995	na	na	na	na	na	na
Figure 5a	The solubility of carbon dioxide in single electrolyte solutions: Chloride salts	No	5.0	3.9	0.2	19.9	0.784	na	na	na	na	na	na
Figure 5b	The solubility of carbon dioxide in single electrolyte solutions: Sulfate salts	No	26.4	43.4	0.8	167.5	0.479	na	21.0	24.8	0.4	96.4	0.405
Figure 6a	The solubilities of Na chloride salts in hydroxide solutions	No	2.0	1.9	0.05	6.3	0.995	na	na	na	na	na	na
Figure 6b	The solubilities of Na sulfate salts in hydroxide solutions	No	4.4	3.8	0.5	13.3	0.966	na	na	na	na	na	na
Figure 6c	The solubilities of K chloride salts in hydroxide solutions	No	2.0	1.1	0.7	3.3	0.999	na	na	na	na	na	na
Figure 6d	The solubilities of K sulfate salts in hydroxide solutions	No	28.7	38.3	0.5	91.2	0.964	na	na	na	na	na	na
Figure 7a	Salt solubilities in the Na-Cl-HCO3-H2O closed system	Yes	3.5	3.3	0.1	12.6	0.997	na	na	na	na	na	na
Figure 7b	Salt solubilities in the Na-SO4-HCO3-H2O closed system	Yes	9.5	13.6	3.0	33.8	0.924	na	na	na	na	na	na
Figure 7c	Salt solubilities in the Na-HCO3-CO3-H2O closed system	Yes	1.1	0.8	0.1	2.9	0.904	0.012	na	na	na	na	na
Figure 7d	Salt solubilities in the Na-Cl-CO3-H2O closed system	Yes	3.1	3.7	0.1	12.3	0.997	na	na	na	na	na	na
Figure 7e	Salt solubilities in the Na-SO4-CO3-H2O closed system	Yes	5.5	3.4	1.5	11.1	0.519	0.456	na	na	na	na	na
Figure 7f	Salt solubilities in the Na-OH-CO3-H2O closed system	Yes	7.3	5.5	0.9	17.7	0.911	na	na	na	na	na	na
Figure 9a	Salt solubilities in the K-Na-HCO3-H2O closed system	Yes	5.0	3.1	0.4	9.7	0.985	0.002	na	na	na	na	na
Figure 9b	Salt solubilities in the K-Cl-HCO3-H2O closed system	Yes	3.7	2.8	0.7	7.5	0.991	0.964	na	na	na	na	na
Figure 9c	Salt solubilities in the K-OH-CO3-H2O closed system	Yes	19.6	17.7	1.3	45.0	0.787	na	na	na	na	na	na
Figure 9d	Salt solubilities in the K-Cl-CO3-H2O closed system	Yes	1.6	0.9	0.2	2.3	na	0.114	na	na	na	na	na
Figure 9e	Salt solubilities in the Na-K-CO3-H2O closed system	Yes	13.5	10.2	1.8	31.3	0.919	na	na	na	na	na	na
Figure 9f	Salt solubilities in the K-CO3-SO4-H2O closed system	Yes	24.5	18.5	0.7	46.9	0.989	na	na	na	na	na	na
Figure 9g	Salt solubilities in the K-HCO3-CO3-H2O closed system	Yes	8.4	8.8	0.2	25.1	0.992	-0.157	na	na	na	na	na
Figure 11a	Ca(OH)2 solubility in CaCl2 solutions	No	52.5	54.5	0.2	151.4	-0.036	na	23.0	12.8	4.5	46.7	0.889
Figure 11b	Ca(OH)2 solubility in CaSO4 solutions	No	22.7	27.1	0.0	77.8	0.931	na	na	na	na	na	na
Figure 11c	Ca(OH)2 solubility in KOH solutions	No	13.4	9.9	0.2	31.3	0.992	na	na	na	na	na	na
Figure 11d	Ca(OH)2 solubility in NaOH solutions	No	13.0	9.9	0.2	28.0	0.993	na	na	na	na	na	na
Figure 11e	Ca(OH)2 solubility in NaCl solutions	No	11.8	8.7	1.4	23.6	0.682	na	na	na	na	na	na
Figure 11f	Ca(OH)2 solubility in KCl solutions	No	14.0	10.5	1.8	33.1	0.520	na	na	na	na	na	na
Figure 12a	Solubility of calcite in water as a function of pCO2	Yes	1.1	1.2	0.0	4.1	0.999	na	na	na	na	na	na
Figure 12b	Solubility of calcite in NaCl solutions at pCO2=0.97 atm	Yes	5.7	3.2	1.6	16.8	0.916	0.956	na	na	na	na	na
Figure 12c	Solubility of calcite in NaCl solutions at pCO2=0.54 atm	Yes	4.4	3.1	0.5	7.8	0.976	0.938	na	na	na	na	na
Figure 12d	Solubility of calcite in NaCl solutions at pCO2=0.06 atm	Yes	5.5	2.5	0.9	8.8	0.960	0.968	na	na	na	na	na
Figure 12e	Solubility of calcite in NaCl solutions at pCO2=0.0013 atm	Yes	12.7	10.0	1.0	31.2	0.787	0.833	na	na	na	na	na
Figure 12f	Solubility of calcite in NaCl solutions at pCO2=0.00033 atm	Yes	7.4	8.2	0.6	26.5	0.924	0.929	na	na	na	na	na
Figure 13	Predicted solubility of brucite and magnesium oxychloride in Mg-OH-Cl-H2O solutions	Yes	57.8	70.8	1.6	195.9	0.153	na	34.6	23.3	0.4	92.0	0.232
Figure 14a	Predicted solubility of MgCO3 in MgSO4 solutions	Yes	31.8	7.1	25.3	42.9	0.053	na	17.9	7.3	6.7	29.9	-0.013
Figure 14b	Predicted solubility of MgCO3 in MgCl2 solutions	Yes	54.3	62.2	1.9	214.5	0.284	na	106.0	127.8	9.9	438.7	-0.695

Mean (μ)	14.0
Std. Dev.	16.1
Minimum	1.1
Maximum	60.4

Mean (μ)	0.774
Std. Dev.	0.320
Minimum	-0.064
Maximum	0.999

Mean		Count (MSE)	% (MSE)
🟩	μ ≤ 10%	24	59%
🟨	10% < μ ≤ 25%	10	24%
🟥	25% < μ ≤ 50%	3	7%
🟧	μ > 50%	4	10%

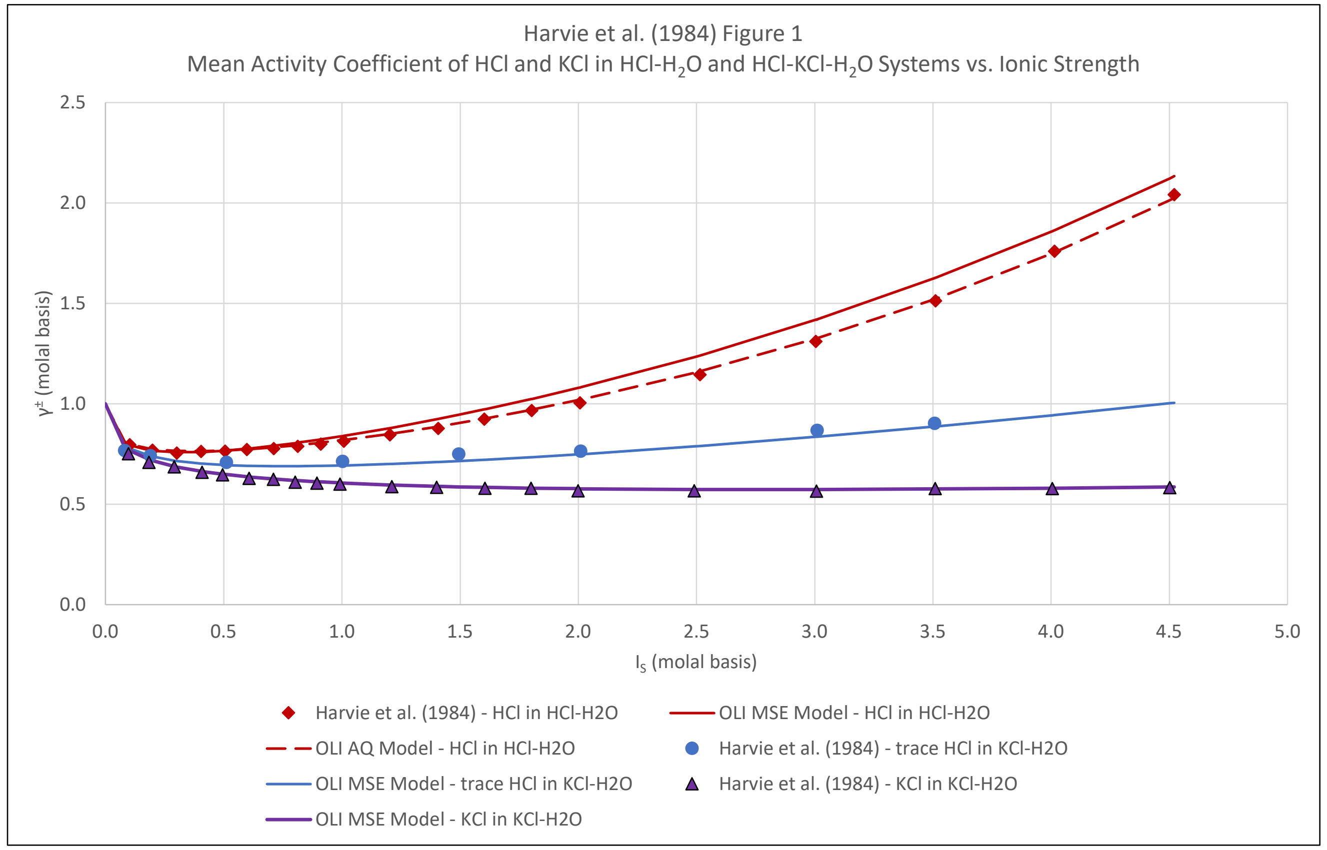
Concordance		Count (MSE)	% (MSE)
🟩	0.75 ≤ C ≤ 1.0	30	75%
🟨	0.50 ≤ C < 0.75	3	8%
🟥	0.25 ≤ C < 0.50	2	5%
🟧	C < 0.25	5	13%

Harvie et al (1984) Figure 1

Harvie et al (1984)				OLI Prediction - MSE Model														OLI Prediction - AQ Model				
I_S (molal)	$\gamma^{\pm 0}_{HCl}$	$\gamma^{\pm tr}_{HCl}$	$\gamma^{\pm 0}_{KCl}$	I_S (molal)	γ^{0}_{H+}	γ^{0}_{Cl-}	γ^{0}_{HCl}	$\gamma^{\pm 0}_{HCl}$ (molal)	Residual HCl (OLI - Harvie)/Harvie (%)	I_S (molal)	γ^{0}_{H+}	γ^{0}_{Cl-}	γ^{0}_{K+}	$\gamma^{\pm tr}_{HCl}$	$\gamma^{\pm 0}_{KCl}$	Residual HCl (OLI - Harvie)/Harvie (%)	Residual KCl (OLI - Harvie)/Harvie (%)	I_S (molal)	γ^{0}_{H+}	γ^{0}_{Cl-}	$\gamma^{\pm 0}_{HCl}$	Residual HCl (OLI - Harvie)/Harvie (%)
				1.01E-06	0.9988	0.9988	1.0000	0.9988	na	1.10E-06	0.9988	0.9988	0.9988	0.9988	0.9988	na	na	1.01E-06	0.999	0.999	0.9988	na
0.082		0.76721		0.082	0.8000	0.8000	0.9900	0.8041	na	0.082	0.8000	0.7820	0.7820	0.7909	0.7820	3.09	na	0.082	0.809	0.809	0.8086	na
0.097			0.75246	0.097	0.7909	0.7909	0.9881	0.7956	na	0.097	0.7909	0.7698	0.7698	0.7803	0.7698	na	2.30	0.097	0.801	0.801	0.8009	na
0.103	0.79672			0.103	0.7880	0.7880	0.9875	0.7930	-0.46	0.103	0.7881	0.7659	0.7659	0.7769	0.7659	na	na	0.103	0.799	0.799	0.7985	0.23
0.184			0.7082	0.184	0.7603	0.7603	0.9777	0.7689	na	0.184	0.7604	0.7225	0.7225	0.7412	0.7225	na	2.03	0.184	0.776	0.776	0.7763	na
0.189		0.74262		0.189	0.7591	0.7591	0.9771	0.7680	na	0.189	0.7593	0.7204	0.7204	0.7396	0.7204	-0.41	na	0.189	0.775	0.775	0.7755	na
0.200	0.76967			0.200	0.7570	0.7570	0.9758	0.7663	-0.43	0.200	0.7572	0.7163	0.7163	0.7365	0.7163	na	na	0.200	0.774	0.774	0.7739	0.55
0.291			0.68607	0.291	0.7454	0.7454	0.9649	0.7588	na	0.291	0.7457	0.6880	0.6880	0.7163	0.6880	na	0.28	0.291	0.766	0.766	0.7657	na
0.302	0.75492			0.302	0.7446	0.7446	0.9637	0.7585	0.47	0.302	0.7450	0.6853	0.6853	0.7145	0.6853	na	na	0.302	0.765	0.765	0.7653	1.37
0.404	0.7623			0.404	0.7415	0.7415	0.9516	0.7601	-0.29	0.404	0.7421	0.6639	0.6639	0.7019	0.6639	na	na	0.404	0.764	0.764	0.7644	0.27
0.409			0.65902	0.409	0.7415	0.7415	0.9511	0.7603	na	0.409	0.7421	0.6632	0.6632	0.7015	0.6632	na	0.63	0.409	0.764	0.764	0.7645	na
0.496			0.64672	0.496	0.7432	0.7432	0.9410	0.7662	na	0.496	0.7442	0.6496	0.6496	0.6953	0.6496	na	0.44	0.496	0.767	0.767	0.7674	na
0.507	0.76475			0.507	0.7436	0.7436	0.9397	0.7671	0.31	0.507	0.7446	0.6480	0.6480	0.6947	0.6480	na	na	0.507	0.768	0.768	0.7680	0.42
0.511		0.7082		0.511	0.7438	0.7438	0.9392	0.7675	na	0.511	0.7448	0.6474	0.6474	0.6944	0.6474	-1.95	na	0.511	0.768	0.768	0.7682	na
0.599	0.77213			0.599	0.7486	0.7486	0.9291	0.7766	0.58	0.599	0.7499	0.6367	0.6367	0.6910	0.6367	na	na	0.599	0.774	0.774	0.7739	0.22
0.608			0.62951	0.608	0.7492	0.7492	0.9280	0.7777	na	0.608	0.7506	0.6357	0.6357	0.6908	0.6357	na	0.99	0.608	0.775	0.775	0.7746	na
0.711			0.62459	0.711	0.7572	0.7572	0.9164	0.7910	na	0.711	0.7592	0.6257	0.6257	0.6892	0.6257	na	0.18	0.711	0.784	0.784	0.7836	na
0.712	0.77705			0.712	0.7573	0.7573	0.9162	0.7911	1.81	0.712	0.7593	0.6256	0.6256	0.6892	0.6256	na	na	0.712	0.784	0.784	0.7837	0.86
0.803			0.60984	0.803	0.7660	0.7660	0.9060	0.8048	na	0.803	0.7685	0.6182	0.6182	0.6893	0.6182	na	1.37	0.803	0.793	0.793	0.7934	na
0.814	0.78934			0.814	0.7672	0.7672	0.9047	0.8066	2.19	0.814	0.7698	0.6174	0.6174	0.6894	0.6174	na	na	0.814	0.795	0.795	0.7948	0.69
0.895			0.60492	0.895	0.7760	0.7760	0.8956	0.8200	na	0.895	0.7792	0.6118	0.6118	0.6905	0.6118	na	1.14	0.895	0.805	0.805	0.8046	na
0.911	0.79918			0.911	0.7780	0.7780	0.8938	0.8229	2.97	0.911	0.7812	0.6108	0.6108	0.6908	0.6108	na	na	0.911	0.807	0.807	0.8068	0.95
0.992			0.6	0.992	0.7878	0.7878	0.8848	0.8375	na	0.992	0.7916	0.6061	0.6061	0.6927	0.6061	na	1.01	0.992	0.818	0.818	0.8178	na
1.003		0.71311		1.003	0.7891	0.7891	0.8836	0.8395	na	1.003	0.7931	0.6055	0.6055	0.6930	0.6055	-2.82	na	1.003	0.819	0.819	0.8194	na
1.009	0.81393			1.009	0.7899	0.7899	0.8830	0.8406	3.28	1.009	0.7939	0.6052	0.6052	0.6931	0.6052	na	na	1.009	0.820	0.820	0.8202	0.77
1.203	0.8459			1.203	0.8164	0.8164	0.8617	0.8795	3.98	1.203	0.8222	0.5962	0.5962	0.7001	0.5962	na	na	1.203	0.851	0.851	0.8507	0.56
1.212			0.5877	1.212	0.8177	0.8177	0.8607	0.8813	na	1.212	0.8235	0.5958	0.5958	0.7005	0.5958	na	1.38	1.212	0.852	0.852	0.8521	na
1.401			0.58525	1.401	0.8465	0.8465	0.8404	0.9234	na	1.401	0.8546	0.5893	0.5893	0.7096	0.5893	na	0.69	1.401	0.886	0.886	0.8861	na
1.408	0.87787			1.408	0.8477	0.8477	0.8397	0.9251	5.38	1.408	0.8558	0.5891	0.5891	0.7100	0.5891	na	na	1.408	0.887	0.887	0.8875	1.09
1.494		0.75		1.494	0.8617	0.8617	0.8305	0.9455	na	1.494	0.8709	0.5866	0.5866	0.7148	0.5866	-4.70	na	1.494	0.904	0.904	0.9043	na
1.603	0.92459			1.603	0.8800	0.8800	0.8192	0.9723	5.16	1.603	0.8907	0.5840	0.5840	0.7212	0.5840	na	na	1.603	0.927	0.927	0.9266	0.22
1.606			0.58033	1.606	0.8805	0.8805	0.8189	0.9730	na	1.606	0.8912	0.5839	0.5839	0.7214	0.5839	na	0.62	1.606	0.927	0.927	0.9272	na
1.800			0.58033	1.800	0.9150	0.9150	0.7988	1.0238	na	1.800	0.9289	0.5801	0.5801	0.7341	0.5801	na	-0.04	1.800	0.970	0.970	0.9703	na
1.803	0.96639			1.803	0.9155	0.9155	0.7985	1.0245	6.01	1.803	0.9294	0.5801	0.5801	0.7343	0.5801	na	na	1.803	0.971	0.971	0.9709	0.47
2.000			0.56803	2.000	0.9527	0.9527	0.7786	1.0796	na	2.000	0.9702	0.5772	0.5772	0.7484	0.5772	na	1.62	2.000	1.018	1.018	1.0185	na
2.008	1.00574			2.008	0.9542	0.9542	0.7778	1.0820	7.58	2.008	0.9720	0.5771	0.5771	0.7490	0.5771	na	na	2.008	1.021	1.021	1.0205	1.47
2.010		0.7647		2.010	0.9546	0.9546	0.7776	1.0826	na	2.010	0.9724	0.5771	0.5771	0.7491	0.5771	-2.04	na	2.010	1.021	1.021	1.0210	na
2.491			0.56803	2.491	1.0540	1.0540	0.7308	1.2330	na	2.491	1.0831	0.5735	0.5735	0.7881	0.5735	na	0.96	2.491	1.154	1.154	1.1545	na
2.516	1.1459			2.516	1.0593	1.0593	0.7285	1.2412	8.31	2.516	1.0892	0.5734	0.5734	0.7903	0.5734	na	na	2.516	1.162	1.162	1.1619	1.40
3.005	1.31118			3.005	1.1725	1.1725	0.6834	1.4183	8.17	3.005	1.2181	0.5732	0.5732	0.8356	0.5732	na	na	3.005	1.325	1.325	1.3246	1.02
3.008			0.56557	3.008	1.1732	1.1732	0.6831	1.4195	na	3.008	1.2190	0.5733	0.5733	0.8359	0.5733	na	1.36	3.008	1.326	1.326	1.3257	na
3.010		0.86803		3.010	1.1737	1.1737	0.6829	1.4203	na	3.010	1.2196	0.5733	0.5733	0.8361	0.5733	-3.67	na	3.010	1.326	1.326	1.3265	na
3.507		0.90246		3.507	1.3002	1.3002	0.6396	1.6257	na	3.507	1.3671	0.5756	0.5756	0.8871	0.5756	-1.70	na	3.507	1.521	1.521	1.5210	na
3.510			0.57787	3.510	1.3010	1.3010	0.6394	1.6270	na	3.510	1.3680	0.5756	0.5756	0.8874	0.5756	na	-0.39	3.510	1.522	1.522	1.5222	na
3.511	1.5123			3.511	1.3013	1.3013	0.6393	1.6276	7.62	3.511	1.3684	0.5757	0.5757	0.8875	0.5757	na	na	3.511	1.523	1.523	1.5228	0.69
4.006			0.57787	4.006	1.4391	1.4391	0.5986	1.8601	na	4.006	1.5330	0.5799	0.5799	0.9429	0.5799	na	0.35	4.006	1.750	1.750	1.7498	na
4.015	1.76008			4.015	1.4418	1.4418	0.5978	1.8647	5.94	4.015	1.5363	0.5800	0.5800	0.9439	0.5800	na	na	4.015	1.754	1.754	1.7544	-0.32
4.502			0.58279	4.502	1.5888	1.5888	0.5601	2.1230	na	4.502	1.7164	0.5857	0.5857	1.0026	0.5857	na	0.49	4.502	2.015	2.015	2.0146	na
4.521	2.04112			4.521	1.5946	1.5946	0.5587	2.1333	4.52	4.521	1.7236	0.5859	0.5859	1.0049	0.5859	na	na	4.521	2.025	2.025	2.0252	-0.78
Mean	1.01	0.78	0.61					1.05						0.76	0.63						1.01	
Std. Dev.	0.37	0.07	0.05					0.40						0.07	0.06						0.36	
Mean of absolute values of residuals									3.8							2.5	0.9					0.7
Std. Dev. of absolute values of residuals									2.9							1.3	0.6					0.4
Minimum of absolute values of residuals									0.29							0.4	0.04					0.22
Maximum of absolute values of residuals									8.3							4.7	2.3					1.5
Pearson Correlation Coefficient (Precision)									0.998							0.966	0.997					1.000
Bias (Location)									0.00657							0.02239	0.02360					0.00010
Scale Differential									0.00415							0.00007	0.00452					0.00004
Imprecision (1 - r)									0.00169							0.03399	0.00264					0.00015
Deviance (Bias + Scale Diff. + Imprecision)									0.01241							0.05644	0.03076					0.00030
Accuracy = 1/(1 + Bias + Scale Diff.)									0.989							0.978	0.973					1.000
Concordance (Accuracy * Precision)									0.988							0.945	0.970					1.000

Mean of all residuals	2.4
Std. Dev. of all residuals	2.4
Minimum of all residuals	0.04
Maximum of all residuals	8.3
Mean Concordance	0.968

Harvie et al (1984) Figure 1



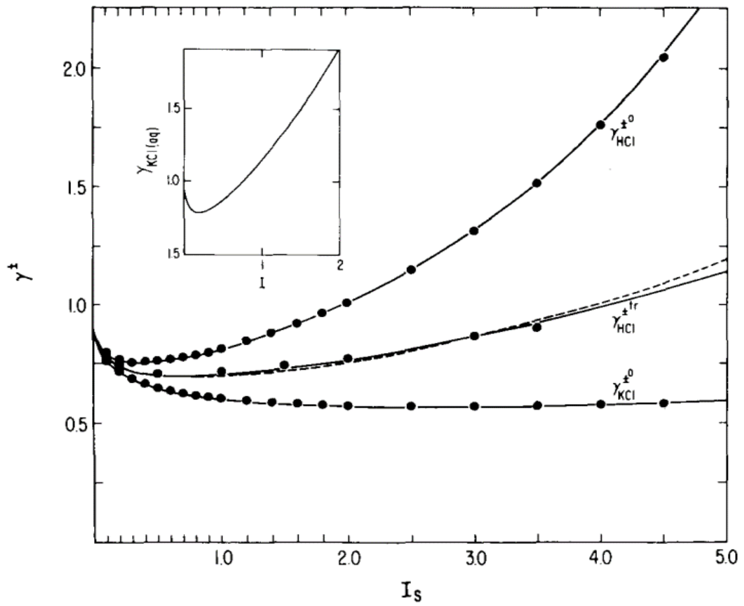


FIG. 1. The mean activity coefficient of HCL in an HCl-H_2O system, ($\gamma^{\pm 0}_{HCl}$), the mean activity coefficient of HCL in a KCl-H_2O system ($\gamma^{\pm tr}_{HCl}$), and the mean activity coefficient for KCl in a KCl-H_2O solution ($\gamma^{\pm 0}_{KCl}$) *versus* the stoichiometric ionic strength (I_s). The data points are from ROBINSON and STOKES (1968) and HARNED and OWEN (1958). The dashed curve is calculated from the literature data using Eqn. (2). The solid curves are calculated using Eqn. (A.3).

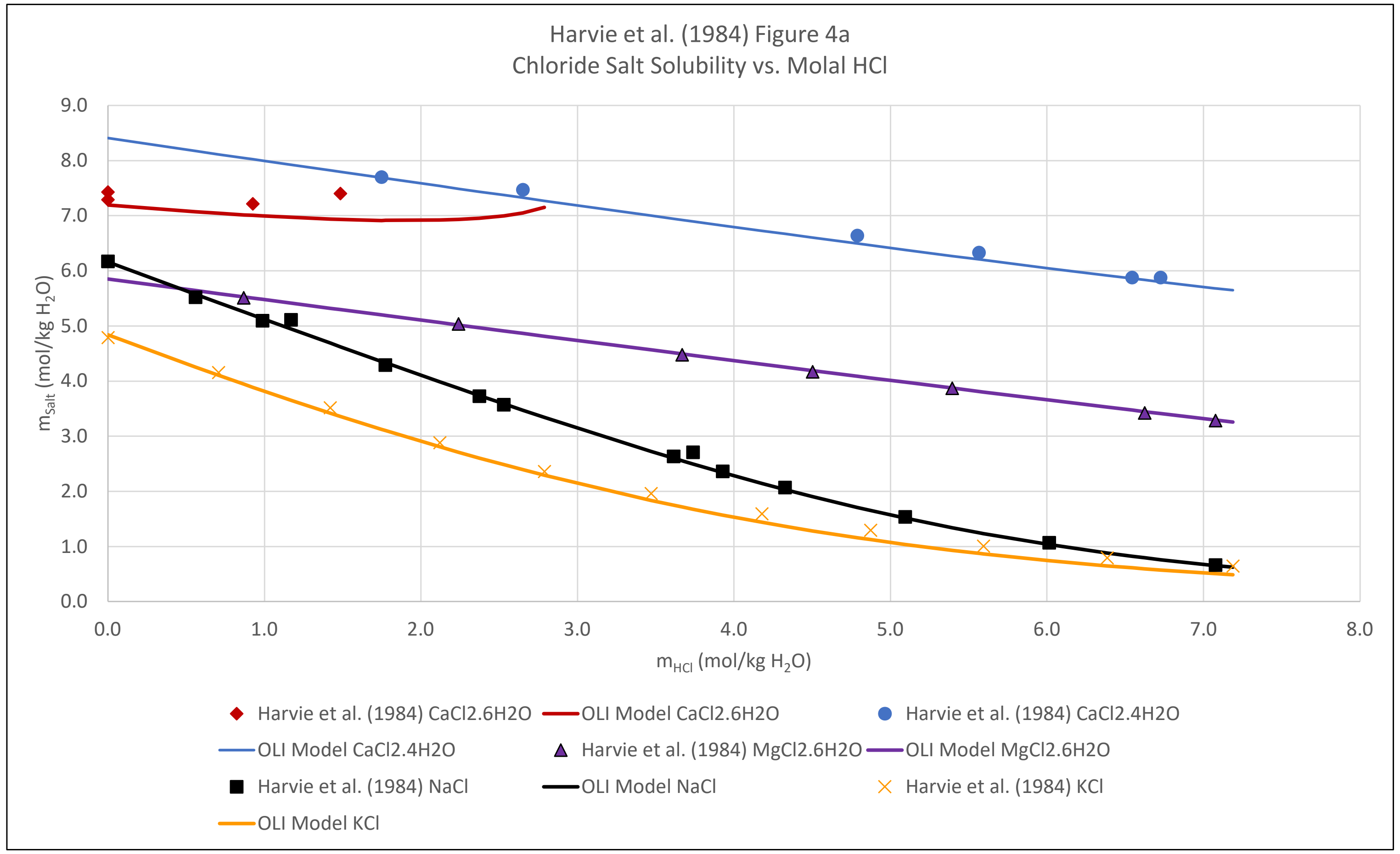
Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 4a

Harvie et al (1984)						OLI Prediction									
m_{HCl} (mol/kg H_2O)	$m_{CaCl2.4H2O}$ (mol/kg H_2O)	$m_{CaCl2.6H2O}$ (mol/kg H_2O) (Antarcticite)	$m_{MgCl2.6H2O}$ (mol/kg H_2O) (Bischofite)	m_{NaCl} (mol/kg H_2O) (Halite)	m_{KCl} (mol/kg H_2O) (Sylvite)	$CaCl_2.4H_2O$ (mol/kg H_2O)	Residual $CaCl_2.4H_2O$ (OLI - Harvie)/Harvie (%)	$CaCl_2.6H_2O$ (Antarcticite) (mol/kg H_2O)	Residual $CaCl_2.6H_2O$ (OLI - Harvie)/Harvie (%)	$MgCl_2.6H_2O$ (Bischofite) (mol/kg H_2O)	Residual $MgCl_2.6H_2O$ (OLI - Harvie)/Harvie (%)	NaCl (Halite) (mol/kg H_2O)	Residual NaCl (OLI - Harvie)/Harvie (%)	KCl (Sylvite) (mol/kg H_2O)	Residual KCl (OLI - Harvie)/Harvie (%)
0.00		7.43					na		na		na		na		na
0.00		7.29		6.17	4.79	8.40	na	7.19	-1.3	5.85	na	6.16	-0.2	4.84	1.1
0.56				5.52		8.17	na	7.07	na	5.64	na	5.58	1.0	4.25	na
0.71					4.15	8.11	na	7.04	na	5.59	na	5.42	na	4.10	-1.2
0.87			5.51			8.05	na	7.02	na	5.53	0.3	5.26	na	3.94	na
0.93		7.21				8.02	na	7.01	-2.9	5.51	na	5.20	na	3.89	na
0.99				5.09		8.00	na	7.00	na	5.48	na	5.13	0.8	3.83	na
1.17				5.11		7.92	na		na	5.41	na	4.94	-3.2	3.65	na
1.42					3.52	7.82	na	6.94	na	5.32	na	4.69	na	3.42	-2.9
1.49		7.40				7.79	na	6.93	-6.3	5.30	na	4.62	na	3.36	na
1.75	7.70					7.69	-0.1	6.91	na	5.20	na	4.36	na	3.12	na
1.77				4.29		7.68	na	6.91	na	5.19	na	4.33	0.9	3.10	na
2.12					2.88	7.54	na	6.92	na	5.06	na	3.99	na	2.81	-2.6
2.24			5.04			7.49	na	6.93	na	5.02	-0.4	3.87	na	2.71	na
2.37				3.72		7.44	na	6.95	na	4.97	na	3.74	0.4	2.61	na
2.53				3.57		7.37	na	7.00	na	4.91	na	3.59	0.4	2.48	na
2.65	7.47					7.32	-1.9	7.05	na	4.87	na	3.47	na	2.39	na
2.79					2.36	7.27	na	7.15	na	4.82	na	3.34	na	2.29	-2.9
3.47					1.96	7.00	na		na	4.57	na	2.73	na	1.84	-6.5
3.61				2.63		6.95	na		na	4.51	na	2.60	-1.2	1.75	na
3.67			4.48			6.92	na		na	4.49	0.3	2.56	na	1.72	na
3.74				2.71		6.90	na		na	4.47	na	2.50	-7.7	1.68	na
3.93				2.36		6.82	na		na	4.40	na	2.34	-0.7	1.57	na
4.18					1.59	6.73	na		na	4.31	na	2.15	na	1.44	-9.7
4.33				2.07		6.67	na		na	4.25	na	2.03	-1.7	1.37	na
4.50			4.17			6.60	na		na	4.19	0.6	1.91	na	1.28	na
4.79	6.64					6.49	-2.2		na	4.09	na	1.71	na	1.16	na
4.87					1.29	6.46	na		na	4.06	na	1.65	na	1.12	-13.1
5.09				1.53		6.38	na		na	3.98	na	1.52	-1.1	1.04	na
5.39			3.87			6.27	na		na	3.87	0.1	1.34	na	0.93	na
5.57	6.33					6.21	-1.9		na	3.81	na	1.25	na	0.87	na
5.59					1.01	6.20	na		na	3.80	na	1.24	na	0.87	-14.1
6.01				1.07		6.05	na		na	3.66	na	1.03	-3.2	0.74	na
6.38					0.79	5.92	na		na	3.53	na	0.88	na	0.65	-18.0
6.54	5.88					5.86	-0.3		na	3.47	na	0.82	na	0.61	na
6.62			3.42			5.83	na		na	3.45	0.8	0.80	na	0.60	na
6.73	5.88					5.80	-1.3		na	3.41	na	0.76	na	0.57	na
7.08				0.66		5.68	na		na	3.29	na	0.65	-1.0	0.51	na
7.08			3.29			5.68	na		na	3.29	0.3	0.65	na	0.51	na
7.19					0.65	5.65	na		na	3.26	na	0.62	na	0.49	-24.7
Mean	6.65	7.30	4.25	3.32	2.27	6.54	na	7.04	na	4.05	na	3.30	na	2.17	na
Std. Dev.	0.78	0.09	0.82	1.74	1.41	0.81	na	0.13	na	0.65	na	1.75	na	1.46	na
Mean of absolute values of residuals							1.3		3.5		0.4		1.7		8.8
Std. Dev. of absolute values of residuals							0.9		2.6		0.2		2.0		7.8
Minimum of absolute values of residuals							0.1		1.3		0.1		0.2		1.1
Maximum of absolute values of residuals							2.2		6.3		0.8		7.7		24.7
Pearson Correlation Coefficient (Precision)							0.997		-0.386		1.000		0.999		1.000
Bias (Location)							0.01045		3.90517		0.04347		0.00012		0.00286
Scale Differential							0.00039		0.06437		0.02654		0.00003		0.00083
Imprecision (1 - r)							0.00312		1.38592		0.00015		0.00089		0.00020
Deviance (Bias + Scale Diff. + Imprecision)							0.01396		5.35546		0.07016		0.00103		0.00389
Accuracy = 1/(1 + Bias + Scale Diff.)							0.989		0.201		0.935		1.000		0.996
Concordance (Accuracy * Precision)							0.986		-0.078		0.934		0.999		0.996

Mean of all residuals	3.1
Std. Dev. of all residuals	5.3
Minimum of all residuals	0.1
Maximum of all residuals	24.7
Mean Concordance	0.768

Harvie et al (1984) Figure 4a



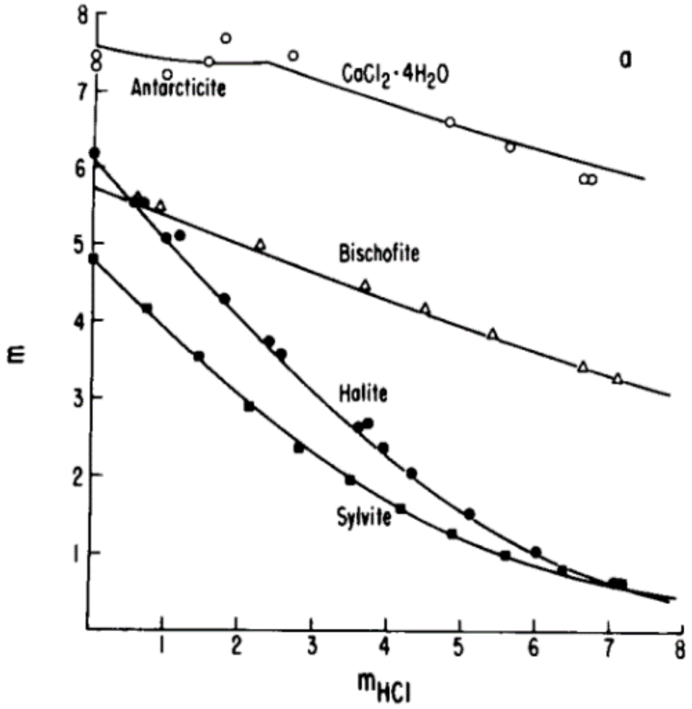
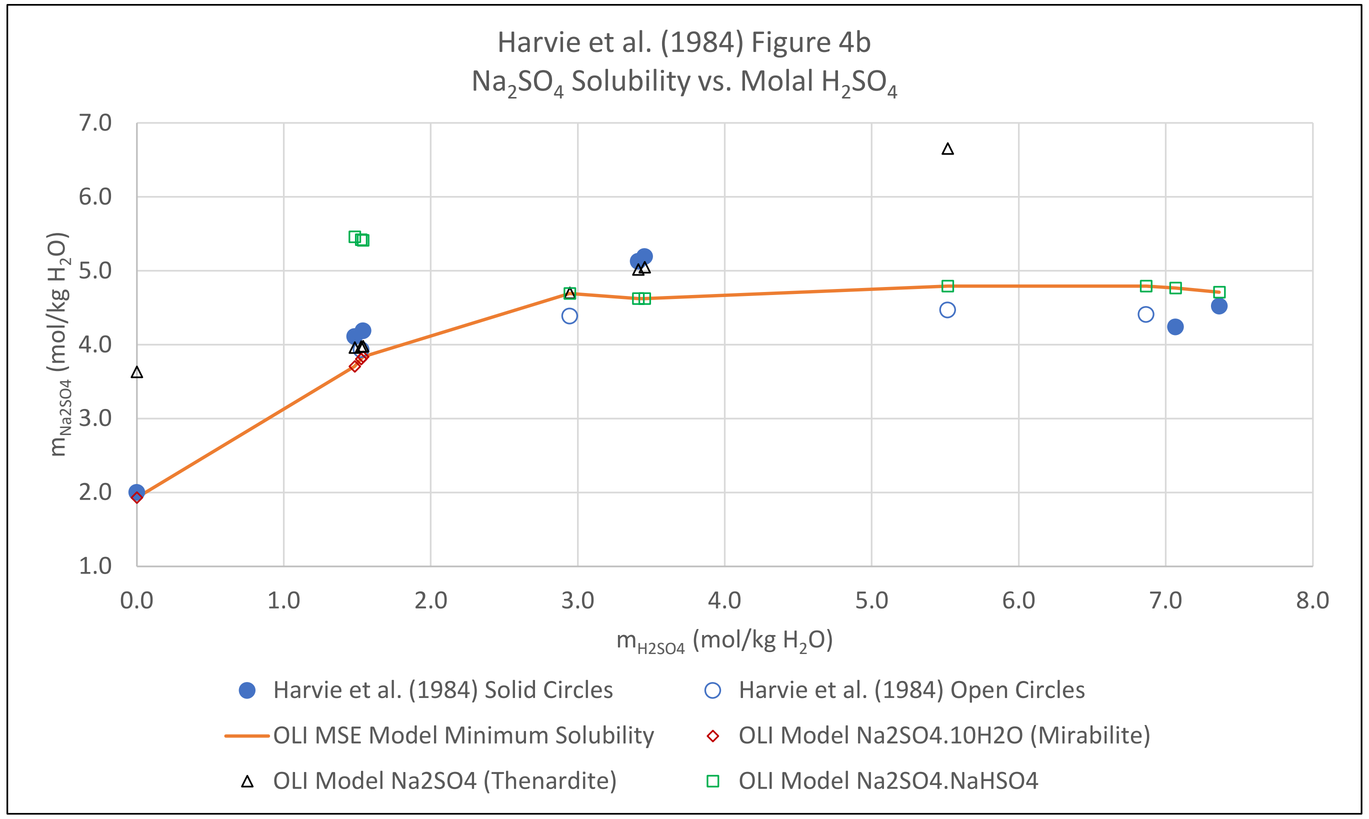


FIG. 4. The calculated and experimental solubilities of salts in acidic solutions. The model is also in agreement with various emf and isopiestic measurements (see text). Curves a–e were used in parameterization. Curve f was predicted using fully parameterized model for acidic solutions.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 4b

Harvie et al (1984)			OLI Prediction				Residual
m_{H2SO4} (mol/kg H_2O)	m_{Na2SO4} (mol/kg H_2O) Solid Circles	m_{Na2SO4} (mol/kg H_2O) Open Circles	$Na_2SO_4.10H_2O$ (Mirabilite) (mol/kg H_2O)	Na_2SO_4 (Thenardite) (mol/kg H_2O)	$Na_2SO_4.NaHSO_4$ (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	2.00		1.93	3.63		1.93	-3.5
1.48	4.11		3.71	3.96	5.46	3.71	-9.8
1.53		3.93	3.80	3.98	5.42	3.80	-3.2
1.54	4.19		3.84	3.98	5.41	3.84	-8.4
2.95		4.39		4.70	4.69	4.69	7.1
3.41	5.13			5.02	4.63	4.63	-9.8
3.45	5.19			5.05	4.62	4.62	-11.0
5.52		4.47		6.65	4.79	4.79	7.3
6.87		4.41			4.79	4.79	8.8
7.07	4.24				4.77	4.77	12.4
7.36	4.52				4.71	4.71	4.2
Mean	4.23		na	na	na	4.21	na
Std. Dev.	0.84		na	na	na	0.87	na
Mean of absolute values of residuals							7.8
Std. Dev. of absolute values of residuals							3.1
Minimum of absolute values of residuals							3.2
Maximum of absolute values of residuals							12.4
Pearson Correlation Coefficient (Precision)							0.895
Bias (Location)							0.00050
Scale Differential							0.00076
Imprecision (1 - r)							0.10473
Deviance (Bias + Scale Diff. + Imprecision)							0.10599
Accuracy = 1/(1 + Bias + Scale Diff.)							0.999
Concordance (Accuracy * Precision)							0.894



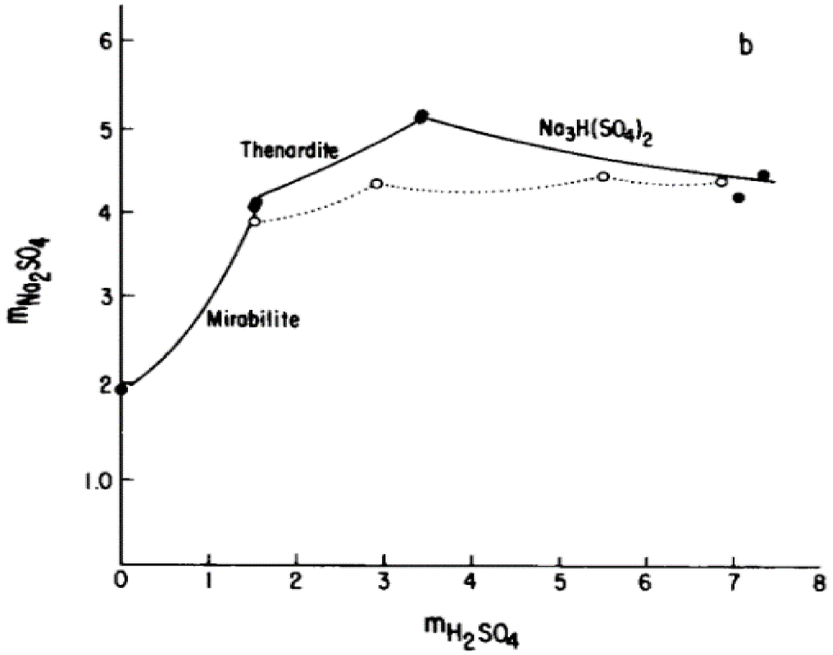


FIG. 4. The calculated and experimental solubilities of salts in acidic solutions. The model is also in agreement with various emf and isopiestic measurements (see text). Curves a–e were used in parameterization. Curve f was predicted using fully parameterized model for acidic solutions.

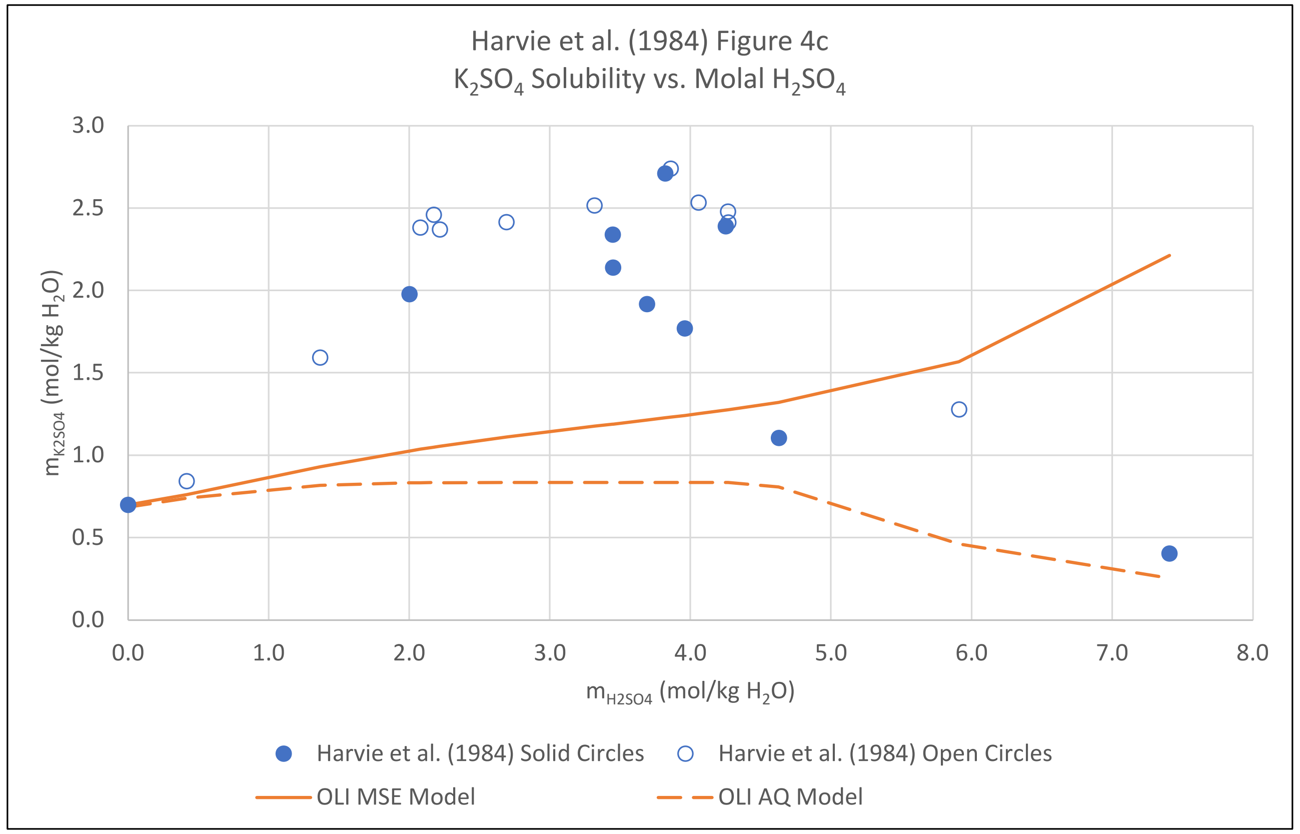
Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 4c

Harvie et al (1984)			OLI Prediction - MSE Model		OLI Prediction - AQ Model	
m_{H2SO4} (mol/kg H_2O)	m_{K2SO4} (mol/kg H_2O) Solid Circles	m_{K2SO4} (mol/kg H_2O) Open Circles	K_2SO_4 (Arcanite)* (mol/kg H_2O)	Residual (OLI - Harvie)/Harvie (%)	K_2SO_4 (Arcanite)** (mol/kg H_2O)	Residual (OLI - Harvie)/Harvie (%)
0.00	0.70		0.70	-0.06	0.68	-2.11
0.42		0.84	0.76	-9.95	0.74	-12.49
1.37		1.59	0.93	-41.62	0.82	-48.74
2.00	1.98		1.02	-48.16	0.83	-57.89
2.08		2.38	1.04	-56.52	0.83	-65.02
2.17		2.46	1.05	-57.42	0.83	-66.11
2.22		2.37	1.05	-55.56	0.83	-64.84
2.69		2.42	1.11	-54.08	0.83	-65.49
3.32		2.52	1.18	-53.29	0.83	-66.87
3.45	2.34		1.19	-49.19	0.83	-64.36
3.45	2.14		1.19	-44.45	0.83	-61.04
3.69	1.92		1.21	-36.77	0.83	-56.54
3.82	2.71		1.23	-54.75	0.83	-69.24
3.86		2.74	1.23	-55.09	0.83	-69.57
3.96	1.77		1.24	-29.85	0.83	-52.87
4.06		2.53	1.25	-50.62	0.83	-67.11
4.25	2.39		1.27	-46.75	0.83	-65.12
4.27		2.48	1.28	-48.57	0.83	-66.37
4.27		2.41	1.28	-47.15	0.83	-65.45
4.63	1.10		1.32	19.50	0.81	-26.96
5.91		1.28	1.57	22.52	0.46	-63.93
7.41	0.40		2.21	447.92	0.25	-37.20
Mean	1.98		1.20	na	0.78	na
Std. Dev.	0.69		0.30	na	0.14	na
Mean of absolute values of residuals				60.4	na	55.2
Std. Dev. of absolute values of residuals				88.0	na	18.8
Minimum of absolute values of residuals				0.1	na	2.1
Maximum of absolute values of residuals				447.9	na	69.6
Pearson Correlation Coefficient (Precision)				-0.188	na	0.715
Bias (Location)				1.56354	na	7.53450
Scale Differential				0.38677	na	1.50347
Imprecision (1 - r)				1.18767	na	0.28504
Deviance (Bias + Scale Diff. + Imprecision)				3.13798	na	9.32301
Accuracy = 1/(1 + Bias + Scale Diff.)				0.339	na	0.100
Concordance (Accuracy * Precision)				-0.064	na	0.071

* Only K_2SO_4 solid included in MSE databank

** Only K_2SO_4 and $KHSO_4$ solids included in AQ databank



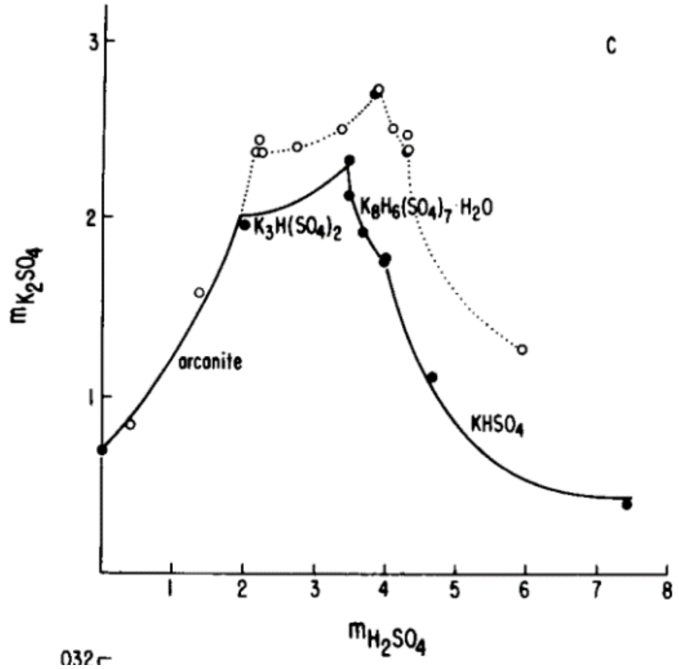


FIG. 4. The calculated and experimental solubilities of salts in acidic solutions. The model is also in agreement with various emf and isopiestic measurements (see text). Curves a–e were used in parameterization. Curve f was predicted using fully parameterized model for acidic solutions.

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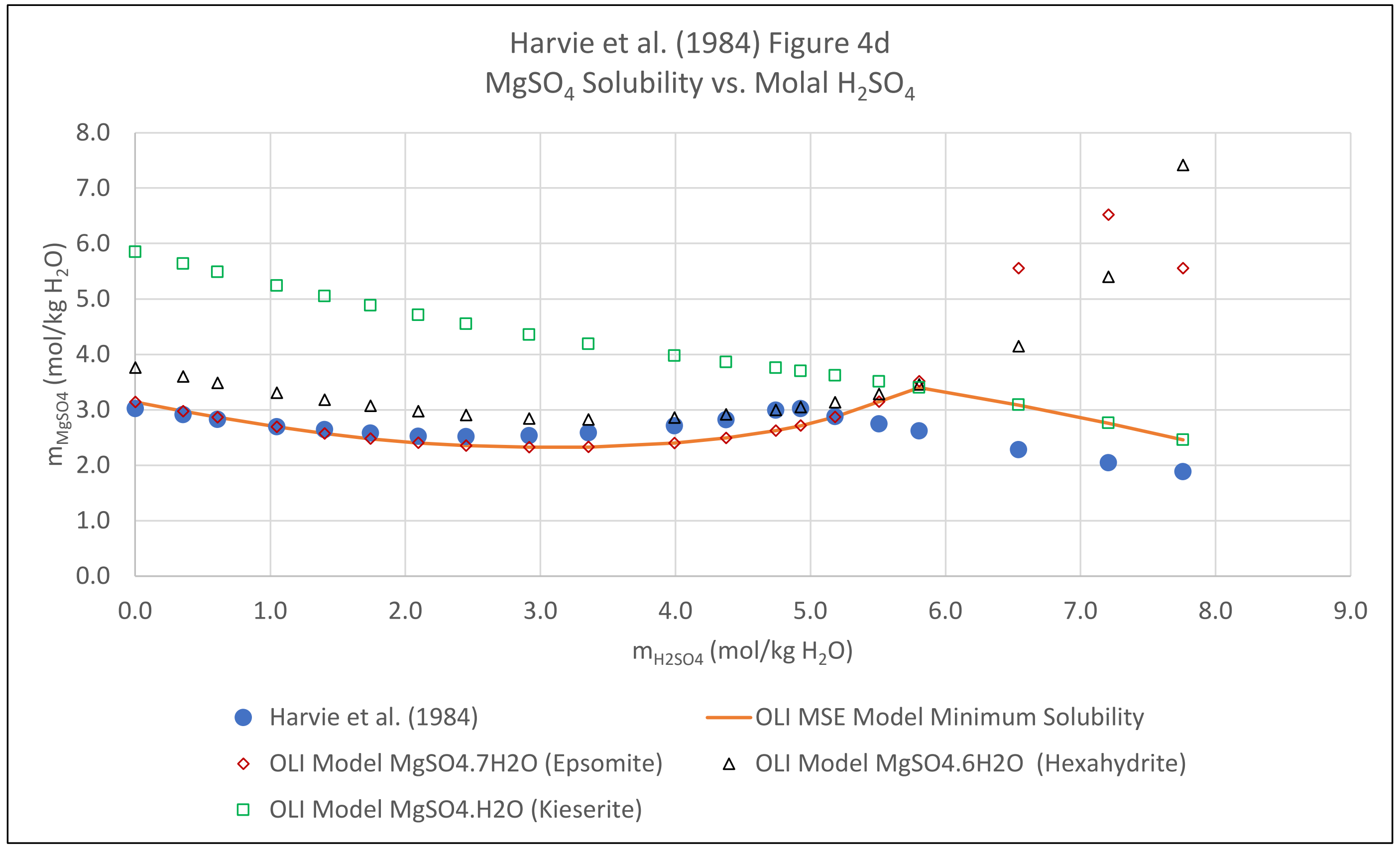
Harvie et al (1984) Figure 4d

Harvie et al (1984)		OLI Prediction				Residual
m_{H2SO4} (mol/kg H_2O)	m_{MgSO4} (mol/kg H_2O)	Epsomite (mol/kg H_2O)	Hexahydrite (mol/kg H_2O)	Kieserite (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	3.02	3.14	3.76	5.85	3.14	4.0
0.35	2.91	2.98	3.60	5.63	2.98	2.3
0.61	2.83	2.87	3.49	5.48	2.87	1.4
1.05	2.70	2.69	3.31	5.24	2.69	-0.1
1.40	2.64	2.57	3.18	5.05	2.57	-2.5
1.74	2.58	2.48	3.07	4.88	2.48	-3.8
2.10	2.52	2.40	2.98	4.71	2.40	-4.7
2.45	2.52	2.35	2.90	4.55	2.35	-6.4
2.92	2.53	2.32	2.85	4.35	2.32	-8.2
3.36	2.59	2.33	2.83	4.19	2.33	-9.9
3.99	2.71	2.40	2.86	3.98	2.40	-11.3
4.38	2.82	2.49	2.91	3.86	2.49	-11.6
4.74	2.99	2.63	3.00	3.75	2.63	-12.3
4.93	3.02	2.71	3.05	3.70	2.71	-10.1
5.18	2.88	2.87	3.14	3.62	2.87	-0.2
5.51	2.74	3.15	3.28	3.51	3.15	14.7
5.81	2.62	3.52	3.46	3.40	3.40	29.7
6.54	2.28	5.55	4.15	3.09	3.09	35.3
7.21	2.05	6.52	5.40	2.76	2.76	34.9
7.76	1.88	5.55	7.42	2.46	2.46	30.8
Mean	2.64	na	na	na	2.71	na
Std. Dev.	0.30	na	na	na	0.32	na
Mean of absolute values of residuals						11.7
Std. Dev. of absolute values of residuals						11.6
Minimum of absolute values of residuals						0.1
Maximum of absolute values of residuals						35.3
Pearson Correlation Coefficient (Precision)						0.235
Bias (Location)						0.02261
Scale Differential						0.00119
Imprecision (1 - r)						0.76523
Deviance (Bias + Scale Diff. + Imprecision)						0.78903
Accuracy = 1/(1 + Bias + Scale Diff.)						0.977
Concordance (Accuracy * Precision)						0.229



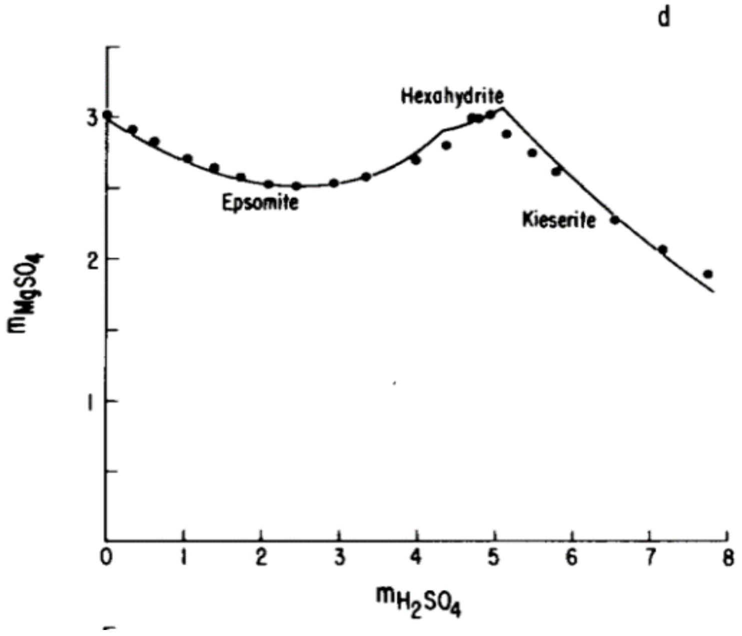


FIG. 4. The calculated and experimental solubilities of salts in acidic solutions. The model is also in agreement with various emf and isopiestic measurements (see text). Curves a–e were used in parameterization. Curve f was predicted using fully parameterized model for acidic solutions.

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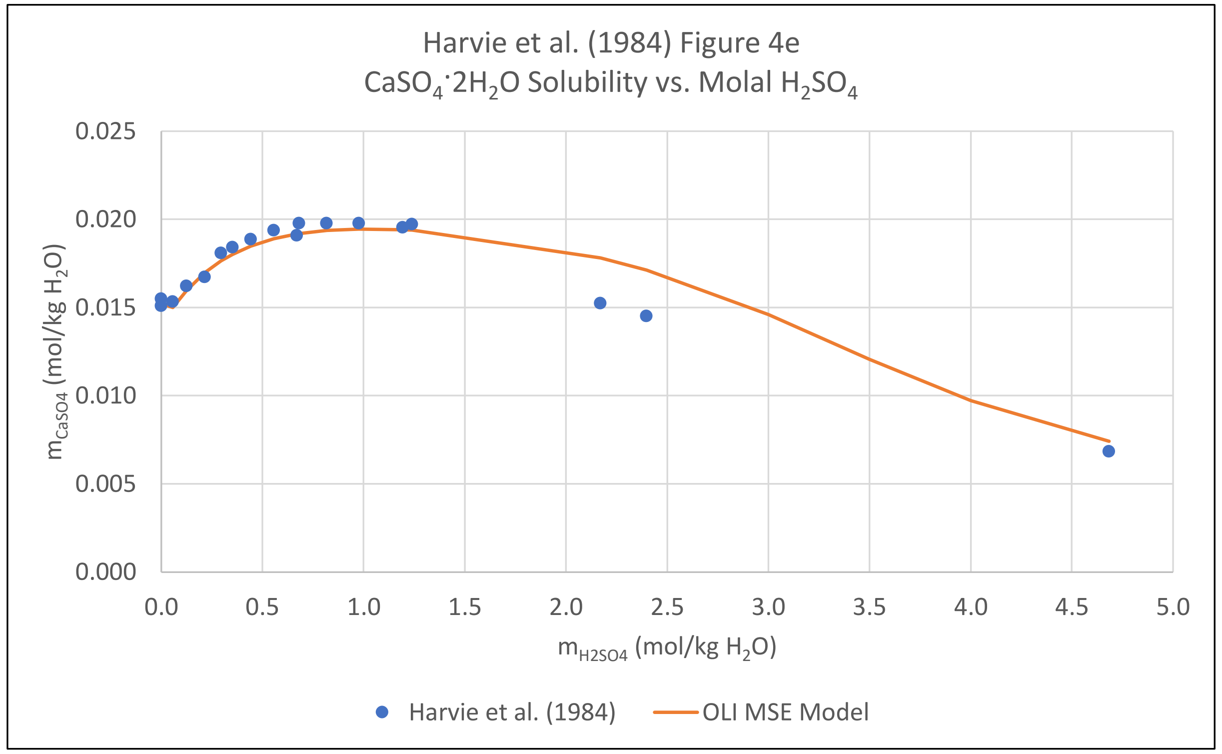
Harvie et al (1984) Figure 4e

Harvie et al (1984)		OLI Prediction (mol/kg H_2O)	Residual (OLI - Harvie)/Harvie (%)
m_{H2SO4} (mol/kg H_2O)	m_{CaSO4} (mol/kg H_2O) $CaSO_4.2H_2O$ (Gypsum)		
0.000	0.015		na
0.000	0.015	0.015	0.8
0.057	0.015	0.015	-2.2
0.125	0.016	0.016	-1.7
0.216	0.017	0.017	1.5
0.296	0.018	0.018	-2.4
0.352	0.018	0.018	-2.2
0.443	0.019	0.018	-2.0
0.557	0.019	0.019	-2.5
0.671	0.019	0.019	0.4
0.682	0.020	0.019	-2.9
0.819	0.020	0.019	-2.0
0.978	0.020	0.019	-1.6
1.194	0.020	0.019	-0.7
1.239	0.020	0.019	-1.7
2.171	0.015	0.018	16.9
2.399	0.015	0.017	18.0
3.000		0.015	na
3.500		0.012	na
4.000		0.010	na
4.684	0.007	0.007	8.5
Mean	0.02	0.02	na
Std. Dev.	0.003	0.003	na
Mean of absolute values of residuals			4.0
Std. Dev. of absolute values of residuals			5.4
Minimum of absolute values of residuals			0.4
Maximum of absolute values of residuals			18.0
Pearson Correlation Coefficient (Precision)			0.957
Bias (Location)			0.00087
Scale Differential			0.00593
Imprecision (1 - r)			0.04326
Deviance (Bias + Scale Diff. + Imprecision)			0.05007
Accuracy = 1/(1 + Bias + Scale Diff.)			0.993
Concordance (Accuracy * Precision)			0.950



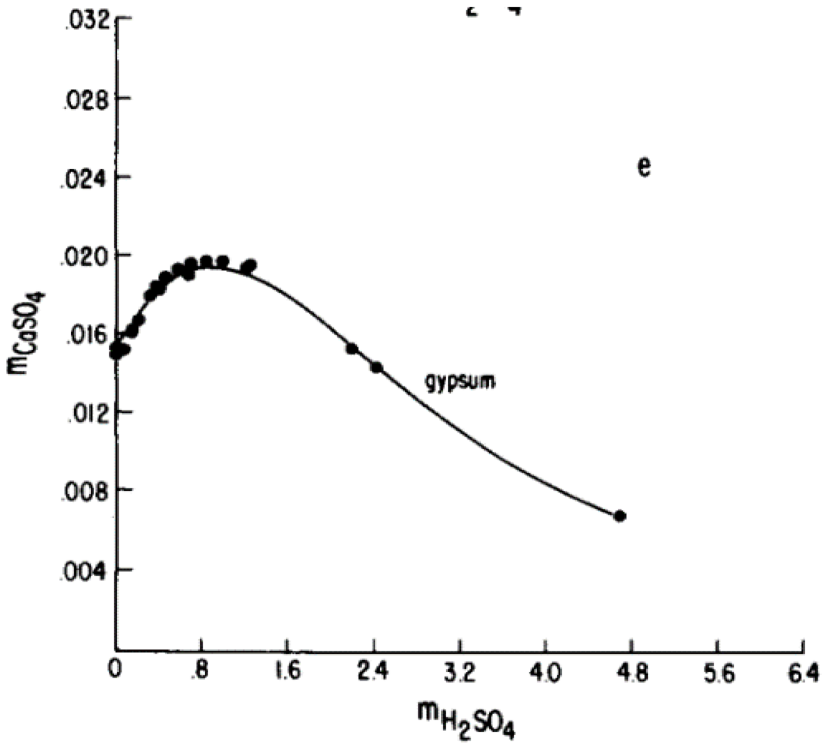


FIG. 4. The calculated and experimental solubilities of salts in acidic solutions. The model is also in agreement with various emf and isopiestic measurements (see text). Curves a–e were used in parameterization. Curve f was predicted using fully parameterized model for acidic solutions.

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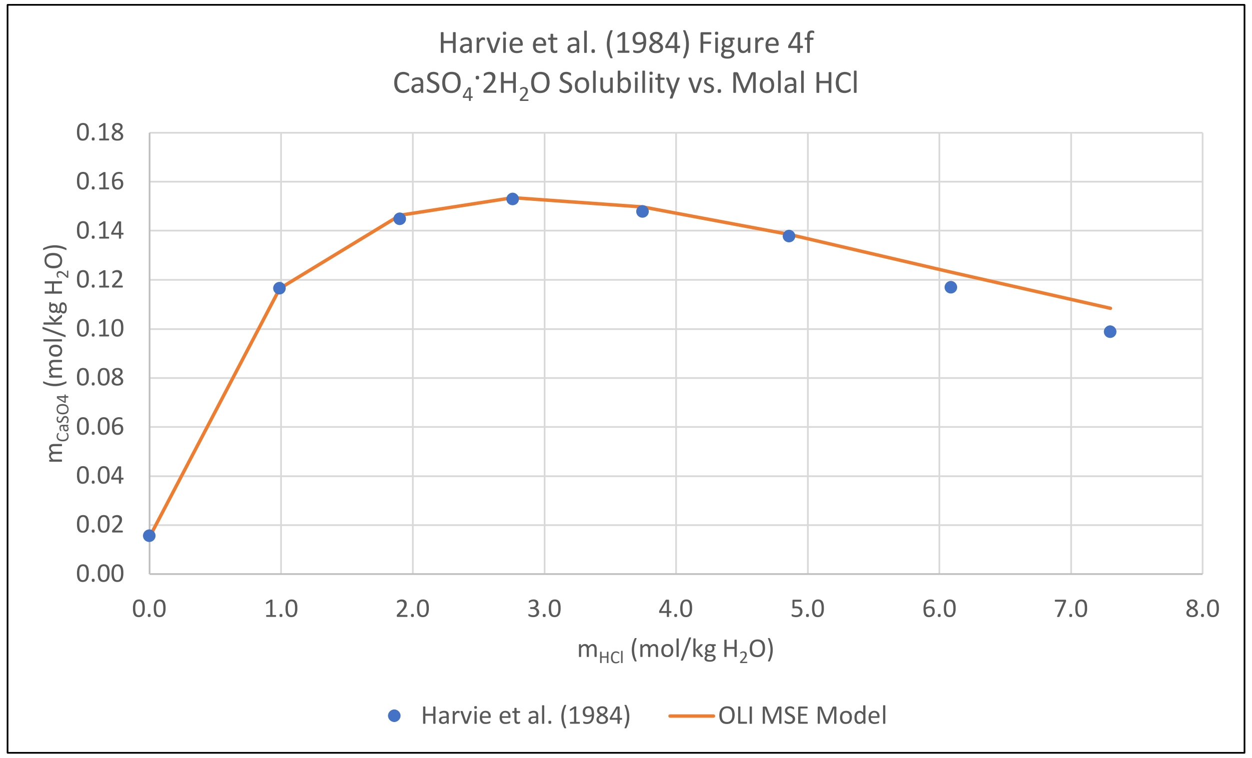
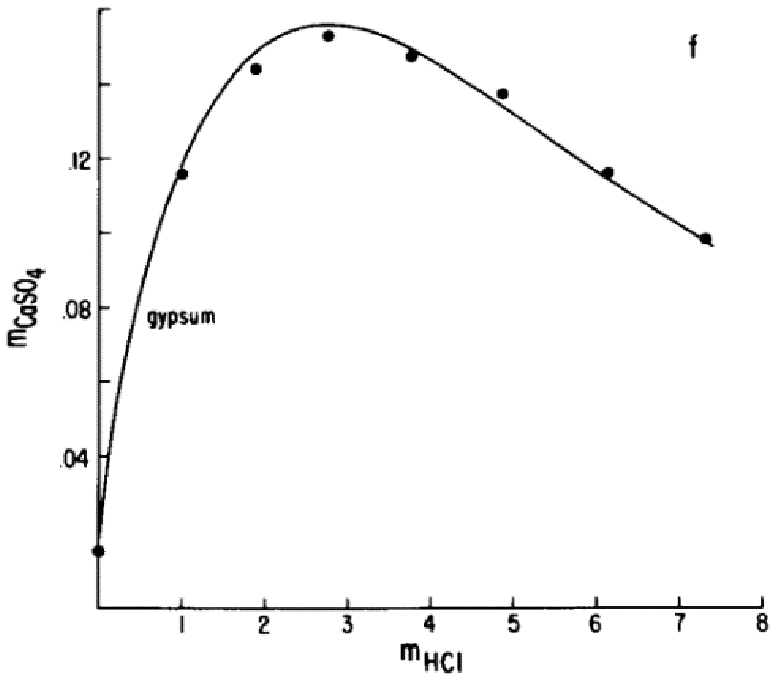
Harvie et al (1984) Figure 4f

Harvie et al (1984)		OLI Prediction (mol/kg H_2O)	Residual (OLI - Harvie)/Harvie (%)
m_{HCl} (mol/kg H_2O)	m_{CaSO4} (mol/kg H_2O) $CaSO_4.2H_2O$ (Gypsum)		
0.00	0.02	0.02	-1.8
0.99	0.12	0.12	0.2
1.90	0.14	0.15	1.2
2.76	0.15	0.15	0.5
3.75	0.15	0.15	1.4
4.86	0.14	0.14	0.6
6.09	0.12	0.12	5.6
7.30	0.10	0.11	10.0
Mean	0.12	0.12	na
Std. Dev.	0.04	0.05	na
Mean of absolute values of residuals			2.7
Std. Dev. of absolute values of residuals			3.4
Minimum of absolute values of residuals			0.2
Maximum of absolute values of residuals			10.0
Pearson Correlation Coefficient (Precision)			0.997
Bias (Location)			0.00208
Scale Differential			0.00001
Imprecision (1 - r)			0.00315
Deviance (Bias + Scale Diff. + Imprecision)			0.00524
Accuracy = 1/(1 + Bias + Scale Diff.)			0.998
Concordance (Accuracy * Precision)			0.995





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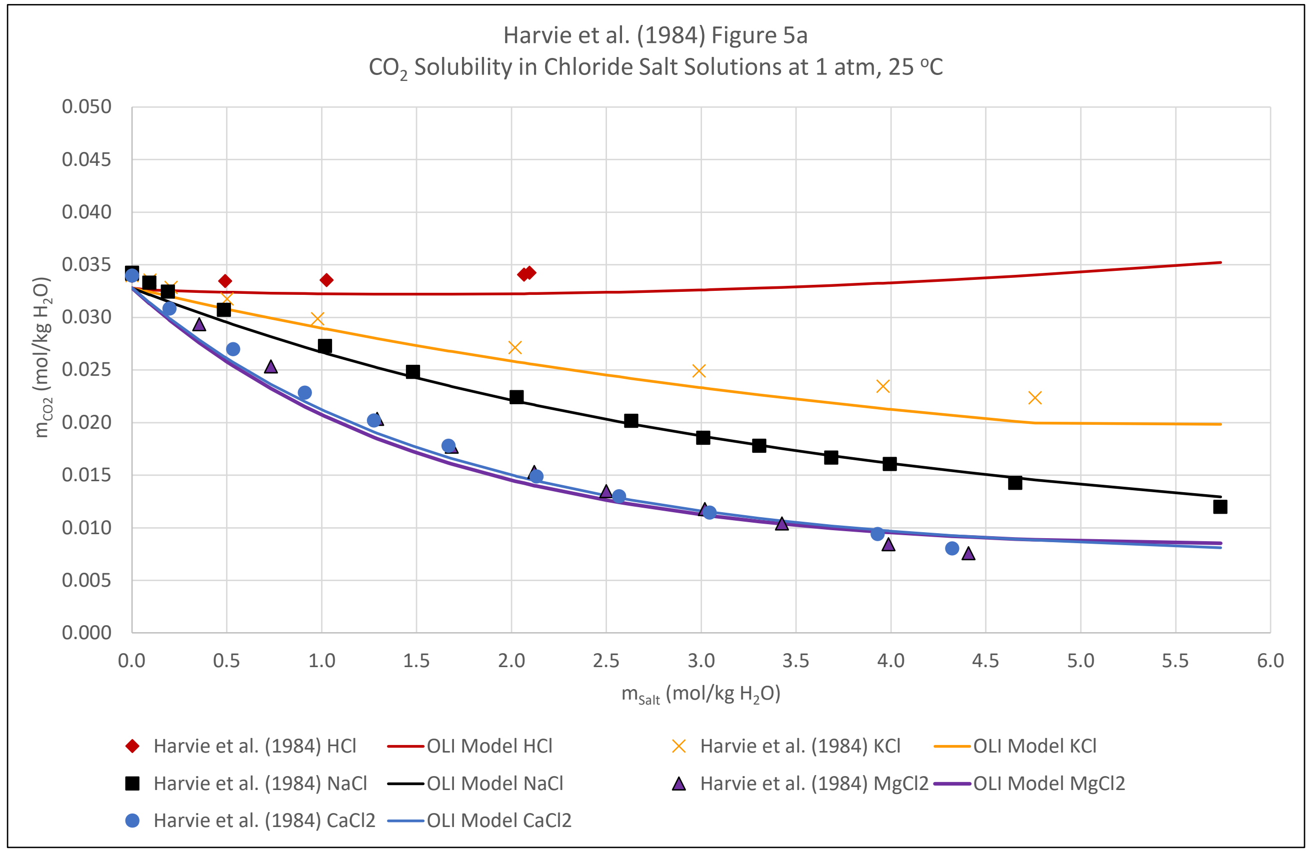
Harvie et al (1984) Figure 5a

m_{salt} (mol/kg H_2O)	m_{CO2} (mol/kg H_2O) - Harvie et al (1984)									OLI Prediction									
	HCl	HCl Translated	KCl	KCl Translated	NaCl	NaCl Translated	$MgCl_2$	$MgCl_2$ Translated	$CaCl_2$	HCl (mol/kg H_2O)	Residual HCl (OLI - Harvie)/Harvie (%)	KCl (mol/kg H_2O)	Residual KCl (OLI - Harvie)/Harvie (%)	NaCl (mol/kg H_2O)	Residual NaCl (OLI - Harvie)/Harvie (%)	$MgCl_2$ (mol/kg H_2O)	Residual $MgCl_2$ (OLI - Harvie)/Harvie (%)	$CaCl_2$ (mol/kg H_2O)	Residual $CaCl_2$ (OLI - Harvie)/Harvie (%)
0.0	0.054	0.034	0.049	0.034	0.044	0.034	0.039	0.034	0.034	0.0328	-3.5	0.0328	-3.5	0.0328	-4.3	0.0328	-4.1	0.0328	-3.6
0.093					0.043	0.033				0.0326	na	0.0324	na	0.0322	-3.5	0.0313	na	0.0314	na
0.095			0.049	0.034						0.0326	na	0.0324	-3.4	0.0321	na	0.0313	na	0.0314	na
0.191					0.042	0.032				0.0325	na	0.0320	na	0.0315	-2.9	0.0299	na	0.0300	na
0.199									0.031	0.0325	na	0.0320	na	0.0315	na	0.0298	na	0.0299	-3.0
0.207			0.048	0.033						0.0325	na	0.0320	-2.8	0.0314	na	0.0296	na	0.0298	na
0.355							0.034	0.029		0.0325	na	0.0314	na	0.0304	na	0.0276	-6.0	0.0279	na
0.485					0.041	0.031				0.0324	na	0.0309	na	0.0296	-3.6	0.0260	na	0.0263	na
0.492	0.053	0.033								0.0324	-3.2	0.0308	na	0.0296	na	0.0259	na	0.0262	na
0.502			0.047	0.032						0.0324	na	0.0308	-3.0	0.0295	na	0.0258	na	0.0261	na
0.534									0.027	0.0324	na	0.0307	na	0.0293	na	0.0254	na	0.0257	-4.6
0.733							0.030	0.025		0.0323	na	0.0299	na	0.0282	na	0.0232	-8.3	0.0237	na
0.912									0.023	0.0323	na	0.0293	na	0.0272	na	0.0215	na	0.0220	-3.9
0.979			0.045	0.030						0.0323	na	0.0290	-2.8	0.0268	na	0.0209	na	0.0214	na
1.018					0.037	0.027				0.0322	na	0.0289	na	0.0266	-2.6	0.0206	na	0.0211	na
1.026	0.054	0.034								0.0322	-3.9	0.0289	na	0.0266	na	0.0205	na	0.0210	na
1.276									0.020	0.0322	na	0.0280	na	0.0253	na	0.0186	na	0.0191	-5.4
1.293							0.025	0.020		0.0322	na	0.0280	na	0.0252	na	0.0185	-9.3	0.0190	na
1.481					0.035	0.025				0.0322	na	0.0274	na	0.0243	-1.9	0.0172	na	0.0178	na
1.669									0.018	0.0322	na	0.0268	na	0.0235	na	0.0162	na	0.0167	-6.4
1.686							0.023	0.018		0.0322	na	0.0268	na	0.0234	na	0.0161	-9.3	0.0166	na
2.019			0.042	0.027						0.0322	na	0.0258	-4.9	0.0221	na	0.0144	na	0.0149	na
2.028					0.032	0.022				0.0322	na	0.0258	na	0.0220	-1.7	0.0144	na	0.0149	na
2.067	0.054	0.034								0.0323	-5.4	0.0257	na	0.0219	na	0.0142	na	0.0147	na
2.095	0.054	0.034								0.0323	-5.8	0.0256	na	0.0218	na	0.0141	na	0.0146	na
2.120							0.020	0.015		0.0323	na	0.0255	na	0.0217	na	0.0140	-8.5	0.0145	na
2.132									0.015	0.0323	na	0.0255	na	0.0216	na	0.0140	na	0.0144	-3.0
2.499							0.019	0.014		0.0324	na	0.0245	na	0.0203	na	0.0126	-6.5	0.0131	na
2.567									0.013	0.0324	na	0.0244	na	0.0201	na	0.0124	na	0.0128	-1.3
2.632					0.030	0.020				0.0324	na	0.0242	na	0.0199	-1.6	0.0122	na	0.0126	na
2.988			0.040	0.025						0.0326	na	0.0233	-6.3	0.0188	na	0.0113	na	0.0116	na
3.011					0.029	0.019				0.0326	na	0.0233	na	0.0187	0.6	0.0112	na	0.0116	na
3.019							0.017	0.012		0.0326	na	0.0233	na	0.0187	na	0.0112	-5.0	0.0116	na
3.044									0.011	0.0326	na	0.0232	na	0.0186	na	0.0112	na	0.0115	0.2
3.306					0.028	0.018				0.0328	na	0.0226	na	0.0179	0.3	0.0106	na	0.0109	na
3.426							0.015	0.010		0.0329	na	0.0224	na	0.0175	na	0.0104	-0.4	0.0107	na
3.685					0.027	0.017				0.0330	na	0.0219	na	0.0169	1.1	0.0100	na	0.0102	na
3.929									0.009	0.0332	na	0.0214	na	0.0163	na	0.0096	na	0.0098	3.9
3.958			0.038	0.023						0.0333	na	0.0213	-9.1	0.0162	na	0.0096	na	0.0097	na
3.988							0.013	0.008		0.0333	na	0.0213	na	0.0161	na	0.0096	12.9	0.0097	na
3.994					0.026	0.016				0.0333	na	0.0213	na	0.0161	0.3	0.0095	na	0.0097	na
4.322									0.008	0.0336	na	0.0207	na	0.0154	na	0.0092	na	0.0093	15.2
4.409							0.013	0.008		0.0337	na	0.0205	na	0.0152	na	0.0091	19.9	0.0092	na
4.654					0.024	0.014				0.0339	na	0.0201	na	0.0148	3.2	0.0089	na	0.0089	na
4.759			0.037	0.022						0.0340	na	0.0199	-10.8	0.0146	na	0.0089	na	0.0088	na
5.736					0.022	0.012				0.0352	na	0.0198	na	0.0129	7.8	0.0085	na	0.0081	na
Mean	na	0.034	na	0.029	na	0.023	na	0.018	0.019	0.032	na	0.027	na	0.023	na	0.017	na	0.019	na
Std. Dev.	na	0.0003	na	0.005	na	0.008	na	0.009	0.009	0.0002	na	0.005	na	0.007	na	0.008	na	0.008	na
Mean of absolute values of residuals											4.3		5.2		2.5		8.2		4.6
Std. Dev. of absolute values of residuals											1.2		3.0		2.0		5.1		3.9
Minimum of absolute values of residuals											3.2		2.8		0.3		0.4		0.2
Maximum of absolute values of residuals											5.8		10.8		7.8		19.9		15.2
Pearson Correlation Coefficient (Precision)											0.009		0.998		1.000		0.995		0.998
Bias (Location)											17.39634		0.04796		0.00122		0.00533		0.00194
Scale Differential											0.08532		0.00509		0.00427		0.00552		0.00284
Imprecision (1 - r)											0.99111		0.00168		0.00025		0.00511		0.00158
Deviance (Bias + Scale Diff. + Imprecision)											18.47278		0.05473		0.00574		0.01596		0.00637
Accuracy = 1/(1 + Bias + Scale Diff.)											0.054		0.950		0.995		0.989		0.995
Concordance (Accuracy * Precision)											0.0005		0.948		0.994		0.984		0.994

Mean of all residuals	5.0
Std. Dev. of all residuals	3.9
Minimum of all residuals	0.2
Maximum of all residuals	19.9
Mean Concordance	0.784

Harvie et al (1984) Figure 5a



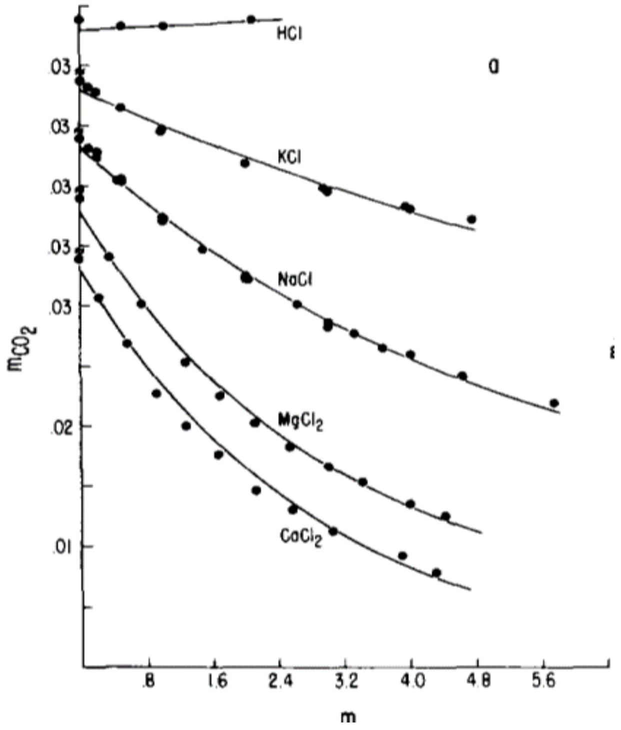


FIG. 5. The solubility of carbon dioxide in single electrolyte solutions. The curves in $MgSO_4$ and K_2SO_4 solutions were predicted using the model fully parameterized from the other data.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

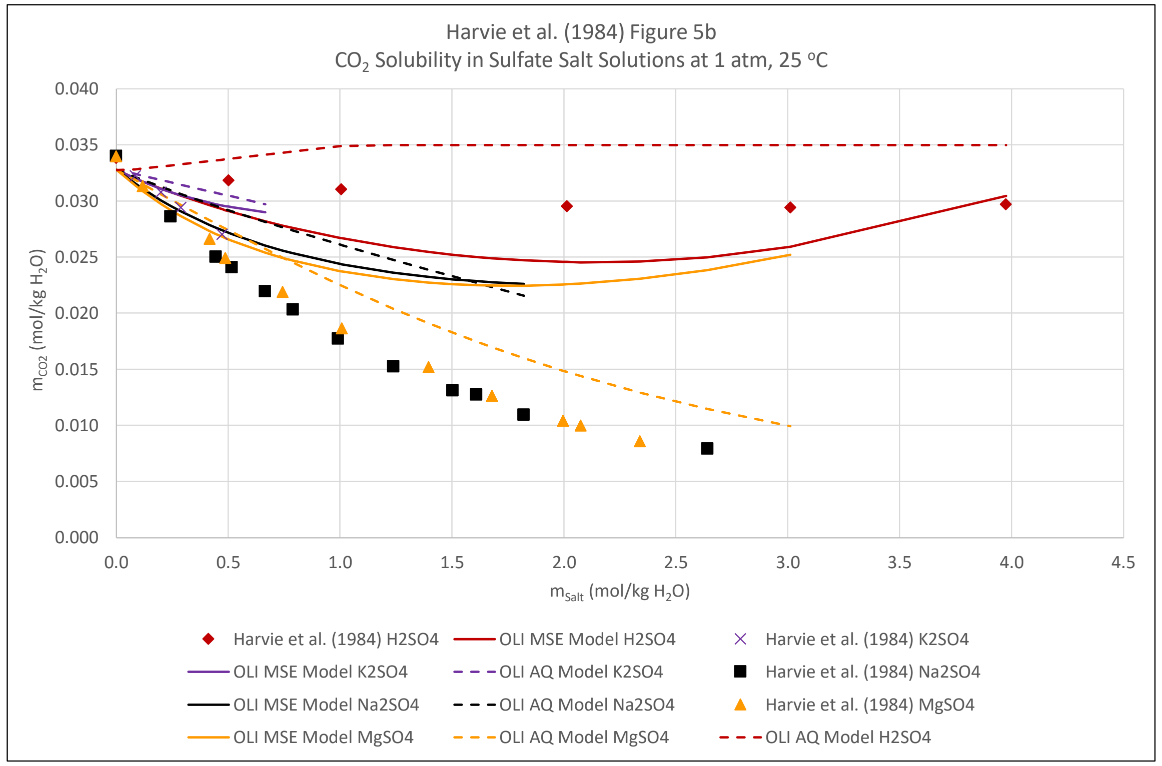
Harvie et al (1984) Figure 5b

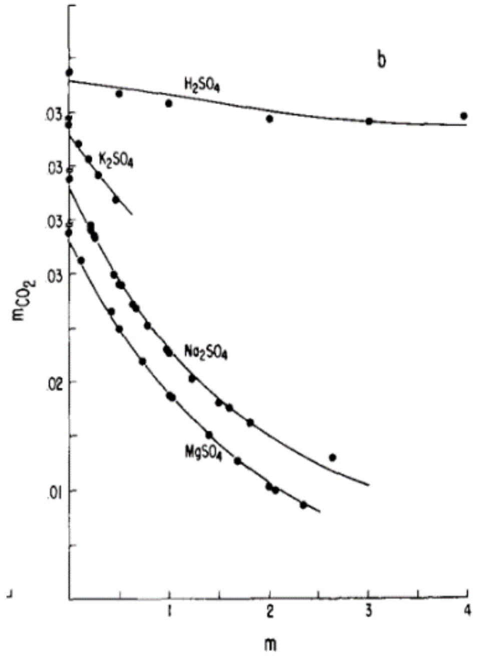
m_{salt} (mol/kg H_2O)	m_{CO2} (mol/kg H_2O) - Harvie et al (1984)							OLI Prediction - MSE Model								OLI Prediction - AQ Model							
	H_2SO_4	H_2SO_4 Translated	K_2SO_4	K_2SO_4 Translated	Na_2SO_4	Na_2SO_4 Translated	$MgSO_4$	H_2SO_4 (mol/kg H_2O)	Residual H_2SO_4 (OLI - Harvie)/Harvie (%)	K_2SO_4 (mol/kg H_2O)	Residual K_2SO_4 (OLI - Harvie)/Harvie (%)	Na_2SO_4 (mol/kg H_2O)	Residual Na_2SO_4 (OLI - Harvie)/Harvie (%)	$MgSO_4$ (mol/kg H_2O)	Residual $MgSO_4$ (OLI - Harvie)/Harvie (%)	H_2SO_4 (mol/kg H_2O)	Residual H_2SO_4 (OLI - Harvie)/Harvie (%)	K_2SO_4 (mol/kg H_2O)	Residual K_2SO_4 (OLI - Harvie)/Harvie (%)	Na_2SO_4 (mol/kg H_2O)	Residual Na_2SO_4 (OLI - Harvie)/Harvie (%)	$MgSO_4$ (mol/kg H_2O)	Residual $MgSO_4$ (OLI - Harvie)/Harvie (%)
0.0	0.0489	0.0339	0.0441	0.0341	0.0390	0.0340	0.0340	0.0328	-3.18	0.0328	-3.80	0.0328	-3.70	0.0328	-3.60	0.0328	-3.20	0.0328	-3.83	0.0328	-3.73	0.0328	-3.63
0.0854			0.0423	0.0323				0.0320	na	0.0320	-0.84	0.0315	na	0.0314	na	0.0328	na	0.0324	0.38	0.0321	na	0.0319	na
0.1182							0.0314	0.0317	na	0.0317	na	0.0311	na	0.0309	-1.54	0.0329	na	0.0322	na	0.0319	na	0.0315	0.48
0.1999			0.0408	0.0308				0.0311	na	0.0311	0.84	0.0301	na	0.0297	na	0.0331	na	0.0319	3.36	0.0313	na	0.0306	na
0.2424					0.0336	0.0286		0.0308	na	0.0308	na	0.0296	3.20	0.0292	na	0.0332	na	0.0317	na	0.0309	8.02	0.0301	na
0.2880			0.0395	0.0295				0.0305	na	0.0305	3.57	0.0291	na	0.0286	na	0.0333	na	0.0314	6.77	0.0306	na	0.0296	na
0.4176							0.0266	0.0296	na	0.0298	na	0.0278	na	0.0273	2.50	0.0335	na	0.0308	na	0.0297	na	0.0283	6.11
0.4449					0.0301	0.0251		0.0294	na	0.0297	na	0.0276	10.21	0.0271	na	0.0336	na	0.0307	na	0.0295	17.94	0.0280	na
0.4731			0.0371	0.0271				0.0293	na	0.0296	9.42	0.0274	na	0.0268	na	0.0337	na	0.0306	13.10	0.0294	na	0.0277	na
0.4879							0.0249	0.0292	na	0.0295	na	0.0273	na	0.0267	7.05	0.0337	na	0.0305	na	0.0293	na	0.0275	10.45
0.5019	0.0469	0.0319						0.0291	-8.71	0.0295	na	0.0272	na	0.0266	na	0.0337	5.87	0.0305	na	0.0292	na	0.0274	na
0.5154					0.0291	0.0241		0.0290	na	0.0294	na	0.0271	12.21	0.0265	na	0.0338	na	0.0304	na	0.0291	20.62	0.0273	na
0.6651					0.0270	0.0220		0.0282	na	0.0290	na	0.0260	18.51	0.0254	na	0.0341	na	0.0297	na	0.0281	28.03	0.0257	na
0.7435							0.0219	0.0278	na		na	0.0256	na	0.0249	13.65	0.0343	na		na	0.0276	na	0.0250	13.77
0.7885					0.0253	0.0203		0.0276	na		na	0.0253	24.57	0.0247	na	0.0344	na		na	0.0274	34.54	0.0245	na
0.9912					0.0228	0.0178		0.0267	na		na	0.0244	37.41	0.0238	na	0.0349	na		na	0.0262	47.22	0.0226	na
1.0056	0.0461	0.0311						0.0267	-14.15		na	0.0244	na	0.0237	na	0.0349	12.28		na	0.0261	na	0.0225	na
1.0079							0.0187	0.0267	na		na	0.0244	na	0.0237	26.97	0.0349	na		na	0.0261	na	0.0224	20.13
1.2381					0.0203	0.0153		0.0259	na		na	0.0236	54.44	0.0230	na	0.0350	na		na	0.0247	61.93	0.0204	na
1.3960							0.0152	0.0255	na		na	0.0232	na	0.0227	49.12	0.0350	na		na	0.0239	na	0.0191	25.32
1.5028					0.0181	0.0131		0.0252	na		na	0.0230	75.21	0.0226	na	0.0350	na		na	0.0233	77.26	0.0183	na
1.6088					0.0178	0.0128		0.0250	na		na	0.0229	78.67	0.0225	na	0.0350	na		na	0.0227	77.57	0.0175	na
1.6783							0.0127	0.0249	na		na	0.0228	na	0.0225	77.40	0.0350	na		na	0.0223	na	0.0170	34.00
1.8205					0.0160	0.0110		0.0247	na		na	0.0226	105.93	0.0225	na	0.0350	na		na	0.0216	96.37	0.0160	na
1.9960							0.0104	0.0246	na		na		na	0.0226	116.28	0.0350	na		na		na	0.0149	42.58
2.0129	0.0446	0.0296						0.0246	-16.95		na		na	0.0226	na	0.0350	18.36		na		na	0.0148	na
2.0754							0.0100	0.0245	na		na		na	0.0226	126.40	0.0350	na		na		na	0.0144	43.93
2.3403							0.0086	0.0246	na		na		na	0.0231	167.54	0.0350	na		na		na	0.0129	49.86
2.6418					0.0130	0.0080		0.0250	na		na		na	0.0238	na	0.0350	na		na		na	0.0115	na
3.0117	0.0444	0.0294						0.0259	-11.94		na		na	0.0252	na	0.0350	18.91		na		na	0.0099	na
3.9752	0.0447	0.0297						0.0304	2.43		na		na		na	0.0350	17.73		na		na		na
Mean	na	0.031	na	0.031	na	0.019	0.019	0.0282	na	0.0312	na	0.0252	na	0.0254	na	0.0344	na	0.0318	na	0.0264	na	0.0223	na
Std. Dev.	na	0.0017	na	0.0027	na	0.0078	0.0089	0.0031	na	0.0012	na	0.0023	na	0.0036	na	0.0009	na	0.0008	na	0.0032	na	0.0071	na
Mean of absolute values of residuals									9.6		3.7		38.6		53.8		12.7		5.5		43.0		22.8
Std. Dev. of absolute values of residuals									5.9		3.5		35.1		59.2		6.8		4.8		31.3		17.6
Minimum of absolute values of residuals									2.4		0.8		3.2		1.5		3.2		0.4		3.7		0.5
Maximum of absolute values of residuals									17.0		9.4		105.9		167.5		18.9		13.1		96.4		49.9
Pearson Correlation Coefficient (Precision)									0.737		0.995		0.986		0.940		-0.954		0.996		0.990		0.996
Bias (Location)									0.8043		0.0393		1.0346		0.6030		4.4636		0.3192		1.0845		0.0697
Scale Differential									0.1719		0.3087		0.8151		0.4390		0.1923		0.7387		0.4271		0.0248
Imprecision (1 - r)									0.2634		0.0046		0.0136		0.0598		1.9536		0.0042		0.0098		0.0039
Deviance (Bias + Scale Diff. + Imprecision)									1.2396		0.3526		1.8632		1.1018		6.6095		1.0621		1.5215		0.0985
Accuracy = 1/(1 + Bias + Scale Diff.)									0.506		0.742		0.351		0.490		0.177		0.486		0.398		0.914
Concordance (Accuracy * Precision)									0.373		0.738		0.346		0.460		-0.169		0.484		0.394		0.910

Mean of all residuals	26.4
Std. Dev. of all residuals	43.4
Minimum of all residuals	0.8
Maximum of all residuals	167.5
Mean Concordance	0.479

Mean of all residuals	21.0
Std. Dev. of all residuals	24.8
Minimum of all residuals	0.4
Maximum of all residuals	96.4
Mean Concordance	0.405

Harvie et al (1984) Figure 5b





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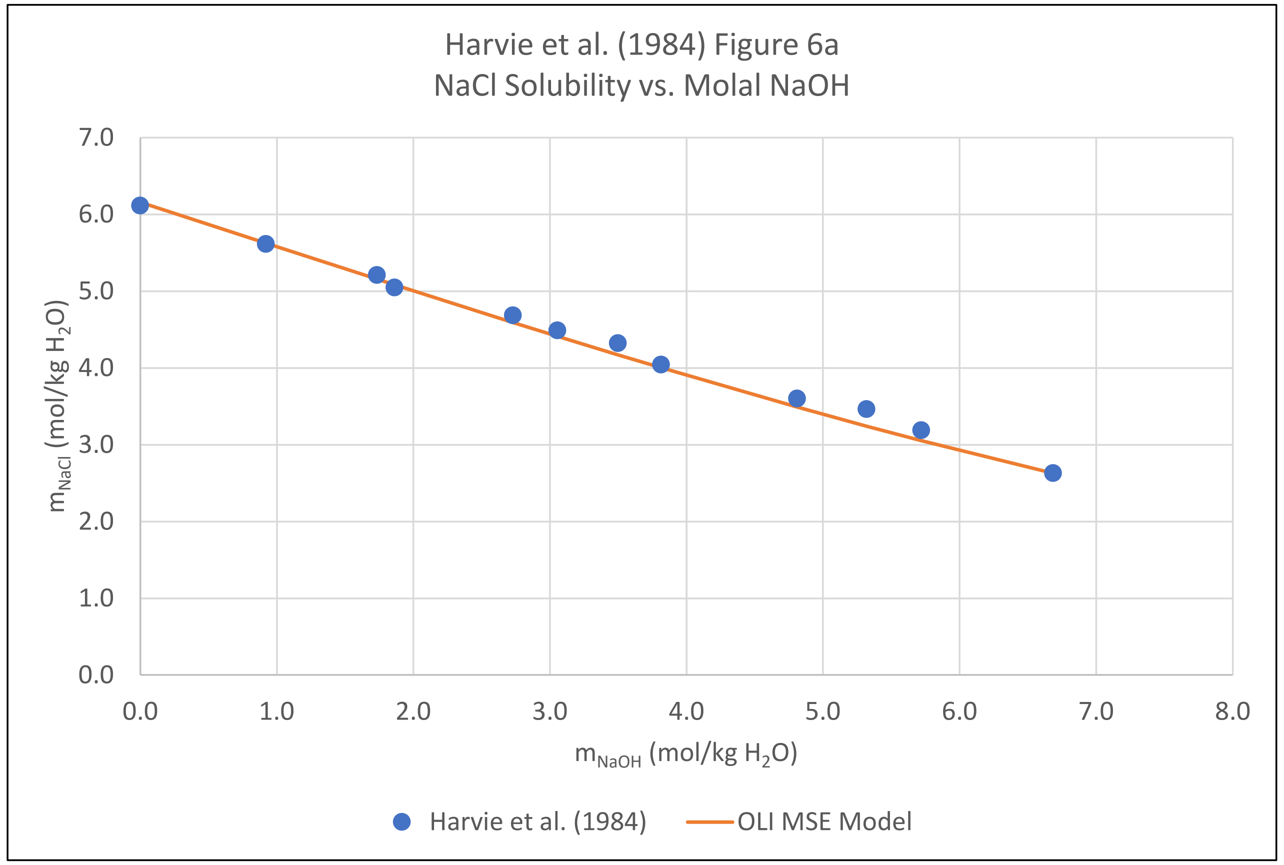
Harvie et al (1984) Figure 6a

Harvie et al (1984)		OLI Prediction	Residual
m_{NaOH} (mol/kg H_2O)	m_{NaCl} (mol/kg H_2O) Halite	Halite (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	6.11	6.16	0.8
0.92	5.61	5.62	0.2
1.73	5.21	5.16	-1.0
1.86	5.04	5.08	0.7
2.73	4.68	4.59	-1.9
3.06	4.48	4.41	-1.6
3.50	4.32	4.17	-3.5
3.81	4.04	4.00	-0.9
4.81	3.60	3.49	-3.0
5.32	3.46	3.24	-6.3
5.72	3.19	3.05	-4.2
6.69	2.63	2.63	0.05
Mean	4.52	4.45	na
Std. Dev.	1.04	1.08	na
Mean of absolute values of residuals			2.0
Std. Dev. of absolute values of residuals			1.9
Minimum of absolute values of residuals			0.05
Maximum of absolute values of residuals			6.3
Pearson Correlation Coefficient (Precision)			0.998
Bias (Location)			0.00233
Scale Differential			0.00096
Imprecision (1 - r)			0.00203
Deviance (Bias + Scale Diff. + Imprecision)			0.00531
Accuracy = 1/(1 + Bias + Scale Diff.)			0.997
Concordance (Accuracy * Precision)			0.995



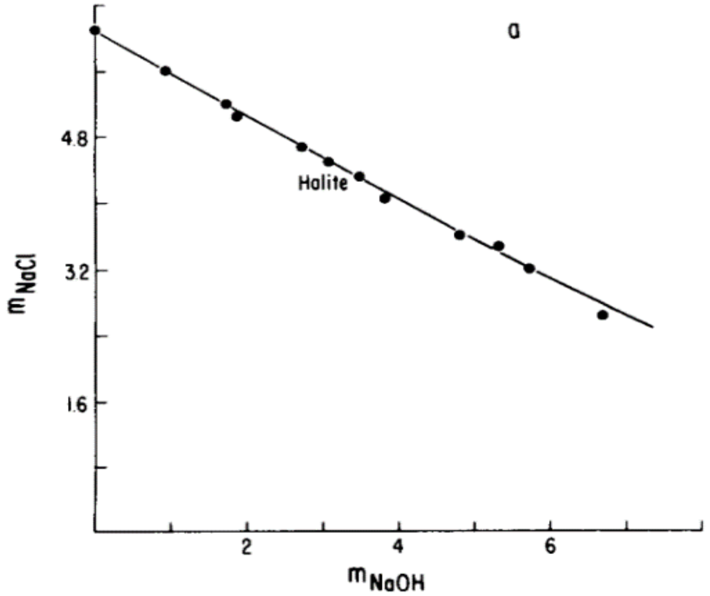


FIG. 6. The solubilities of sodium and potassium salts in hydroxide solutions. The model is also in agreement with emf data at lower concentrations.

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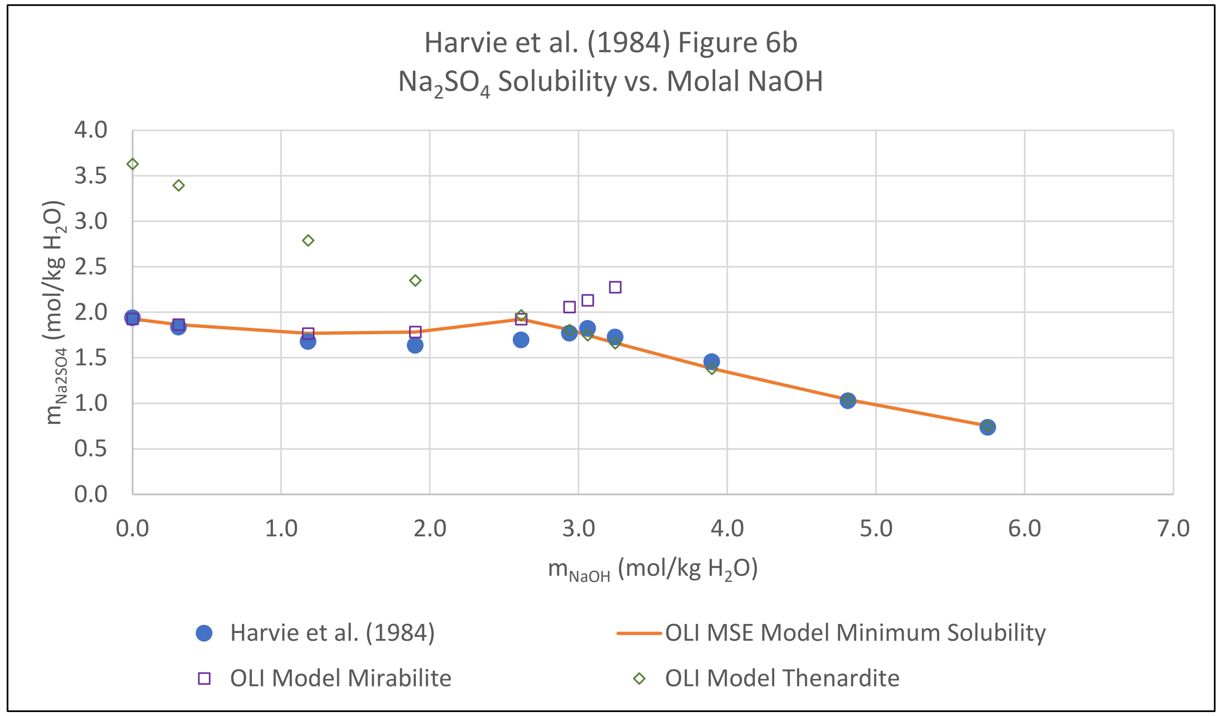
Harvie et al (1984) Figure 6b

Harvie et al (1984)		OLI Prediction			Residual
m_{NaOH} (mol/kg H_2O)	$m_{Na2SO4.10H2O}$ (mol/kg H_2O)	$Na_2SO_4.10H_2O$ (Mirabilite) (mol/kg H_2O)	Na_2SO_4 (Thenardite) (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	1.94	1.93	3.63	1.93	-0.5
0.31	1.84	1.86	3.39	1.86	1.6
1.18	1.68	1.77	2.79	1.77	5.3
1.90	1.64	1.78	2.35	1.78	9.0
2.61	1.70	1.92	1.97	1.92	13.3
2.94	1.77	2.06	1.81	1.81	2.0
3.06	1.82	2.13	1.75	1.75	-4.1
3.25	1.73	2.28	1.66	1.66	-3.9
3.90	1.46		1.38	1.38	-5.1
4.81	1.03		1.04	1.04	1.0
5.75	0.74		0.75	0.75	2.2
Mean	1.58	na	na	1.61	na
Std. Dev.	0.37	na	na	0.39	na
Mean of absolute values of residuals					4.4
Std. Dev. of absolute values of residuals					3.8
Minimum of absolute values of residuals					0.5
Maximum of absolute values of residuals					13.3
Pearson Correlation Coefficient (Precision)					0.970
Bias (Location)					0.00340
Scale Differential					0.00095
Imprecision (1 - r)					0.03026
Deviance (Bias + Scale Diff. + Imprecision)					0.03461
Accuracy = 1/(1 + Bias + Scale Diff.)					0.996
Concordance (Accuracy * Precision)					0.966



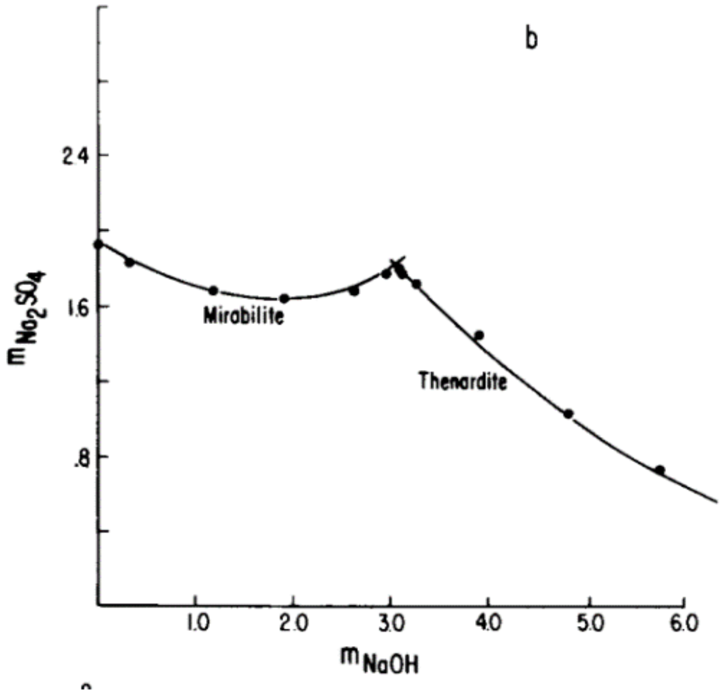


FIG. 6. The solubilities of sodium and potassium salts in hydroxide solutions. The model is also in agreement with emf data at lower concentrations.

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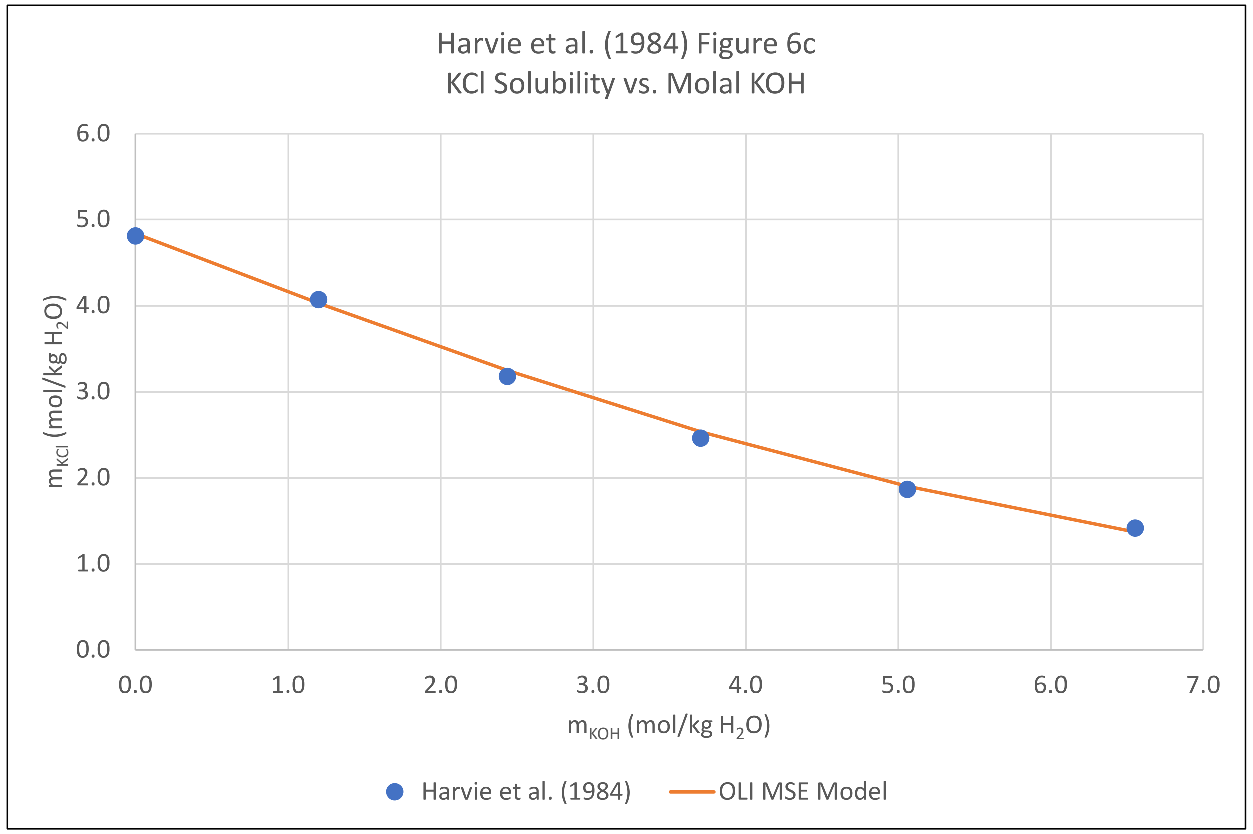
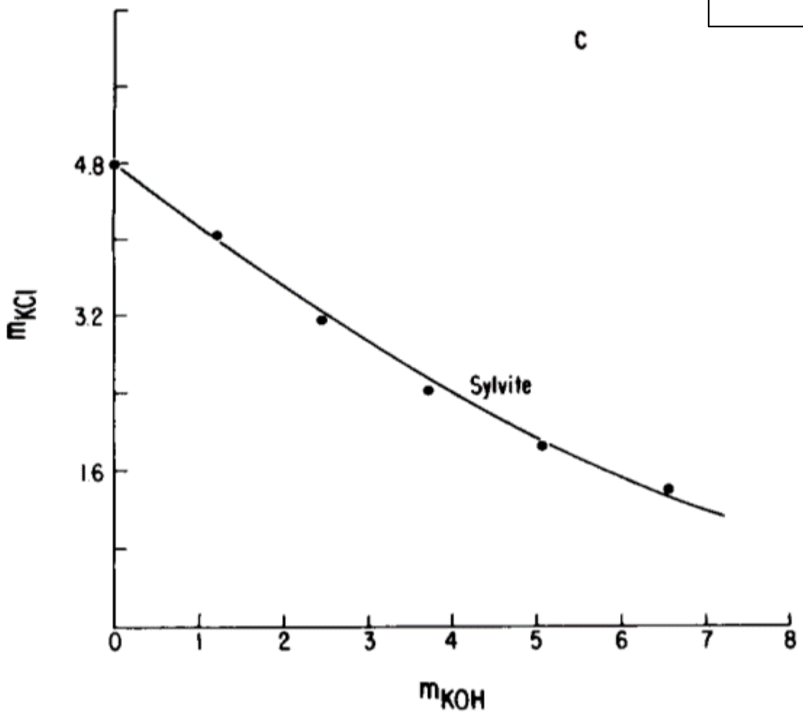
Harvie et al (1984) Figure 6c

Harvie et al (1984)		OLI Prediction	Residual
m_{KOH} (mol/kg H_2O)	m_{KCl} (mol/kg H_2O) Sylvite	KCl (Sylvite) (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	4.81	4.84	0.7
1.20	4.07	4.03	-0.9
2.44	3.17	3.25	2.3
3.71	2.46	2.53	3.0
5.06	1.86	1.90	1.9
6.56	1.41	1.37	-3.3
Mean	2.96	2.99	na
Std. Dev.	1.31	1.31	na
Mean of absolute values of residuals			2.0
Std. Dev. of absolute values of residuals			1.1
Minimum of absolute values of residuals			0.7
Maximum of absolute values of residuals			3.3
Pearson Correlation Coefficient (Precision)			0.999
Bias (Location)			0.00017
Scale Differential			0.00001
Imprecision (1 - r)			0.00080
Deviance (Bias + Scale Diff. + Imprecision)			0.00098
Accuracy = 1/(1 + Bias + Scale Diff.)			0.9998
Concordance (Accuracy * Precision)			0.999





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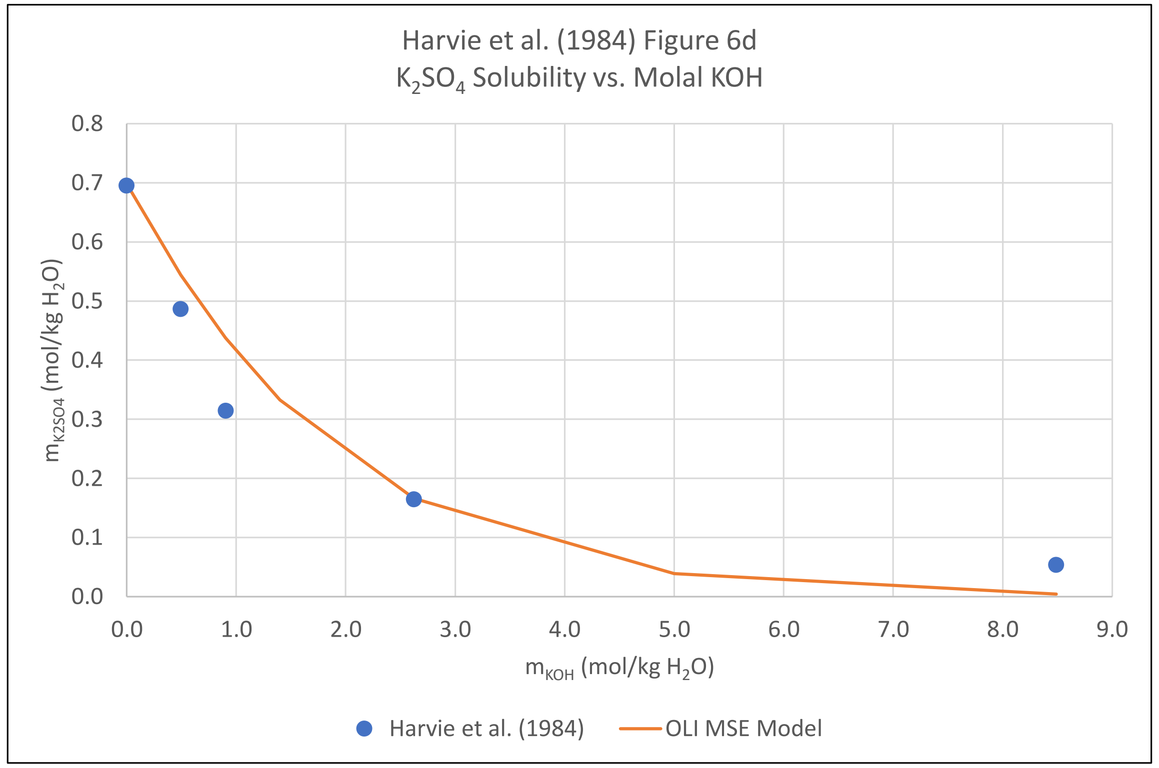
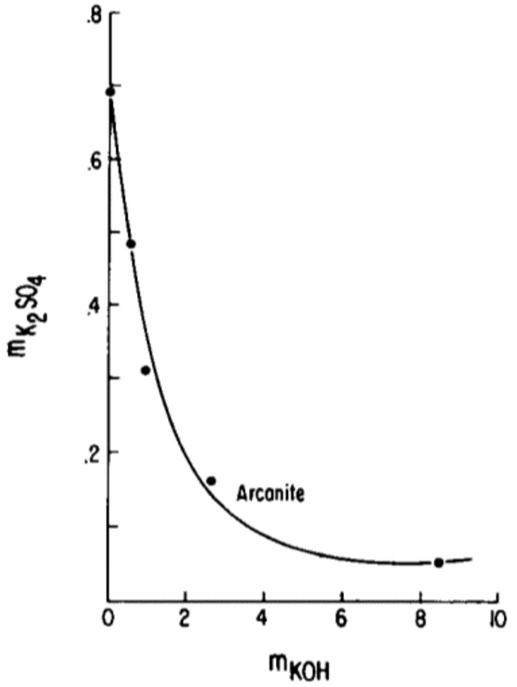
Harvie et al (1984) Figure 6d

Harvie et al (1984)		OLI Prediction	Residual
m_{KOH} (mol/kg H_2O)	m_{K2SO4} (mol/kg H_2O) Arcanite	K_2SO_4 (Arcanite) (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	0.70	0.70	0.5
0.49	0.49	0.54	11.9
0.90	0.31	0.44	39.2
1.40		0.33	na
2.62	0.16	0.17	0.9
5.00		0.04	na
8.49	0.05	0.005	-91.2
Mean	0.34	0.37	na
Std. Dev.	0.26	0.28	na
Mean of absolute values of residuals			28.7
Std. Dev. of absolute values of residuals			38.3
Minimum of absolute values of residuals			0.5
Maximum of absolute values of residuals			91.2
Pearson Correlation Coefficient (Precision)			0.975
Bias (Location)			0.00647
Scale Differential			0.00484
Imprecision (1 - r)			0.02497
Deviance (Bias + Scale Diff. + Imprecision)			0.03628
Accuracy = 1/(1 + Bias + Scale Diff.)			0.989
Concordance (Accuracy * Precision)			0.964





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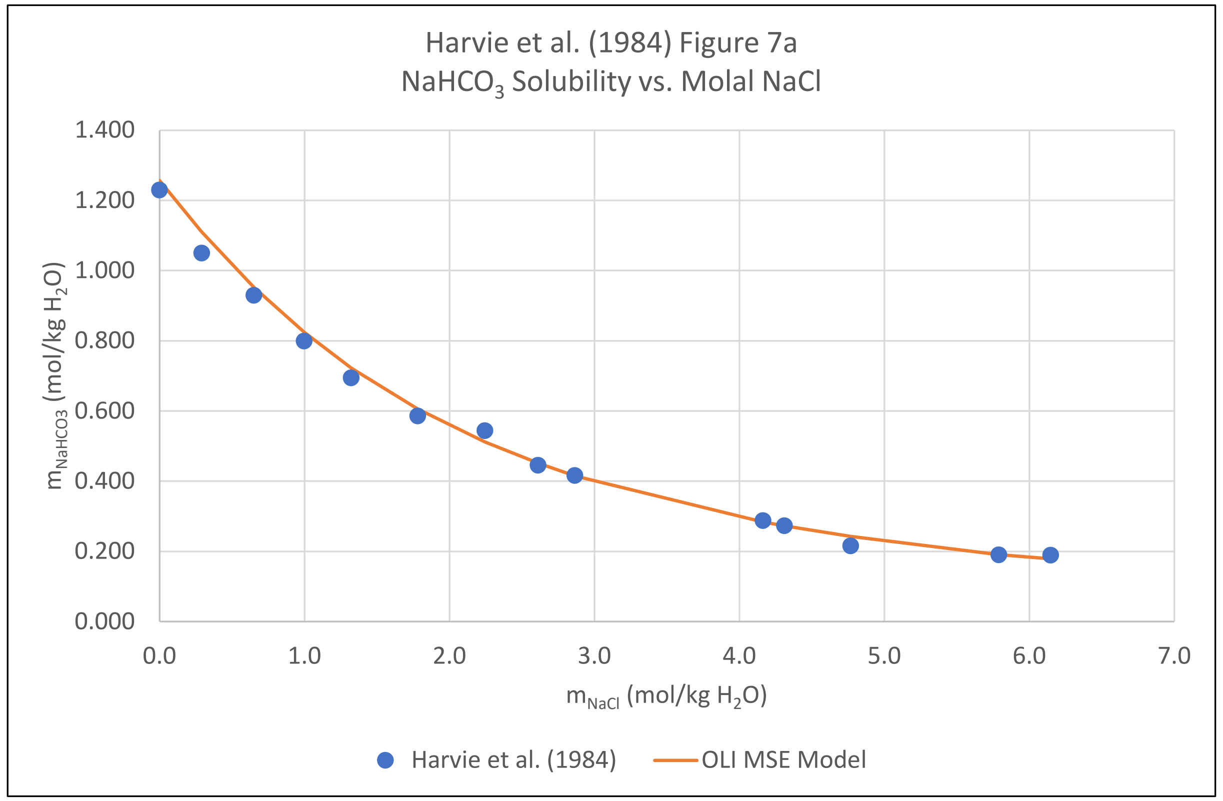
Harvie et al (1984) Figure 7a

Harvie et al (1984)		OLI Prediction		Residual
m_{NaCl} (mol/kg H_2O)	m_{NaHCO3} (mol/kg H_2O) Nahcolite	$NaHCO_3$ (Nahcolite) (mol/kg H_2O)	Comment	(OLI - Harvie)/Harvie (%)
0.00	1.23	1.26		2.2
0.29	1.05	1.11		5.7
0.65	0.93	0.95		2.4
1.00	0.80	0.82		3.1
1.32	0.69	0.72		4.1
1.78	0.59	0.61		3.3
2.24	0.54	0.51		-5.9
2.61	0.45	0.45		1.2
2.86	0.42	0.42		-0.1
4.16	0.29	0.28		-1.3
4.31	0.27	0.27		-0.3
4.77	0.22	0.24		12.6
5.79	0.19	0.19		0.5
6.15	0.19	0.18	NaCl precipitates	-5.5
Mean	0.56	0.57	na	na
Std. Dev.	0.34	0.35	na	na
Mean of absolute values of residuals				3.5
Std. Dev. of absolute values of residuals				3.3
Minimum of absolute values of residuals				0.1
Maximum of absolute values of residuals				12.6
Pearson Correlation Coefficient (Precision)				0.999
Bias (Location)				0.00065
Scale Differential				0.00088
Imprecision (1 - r)				0.00124
Deviance (Bias + Scale Diff. + Imprecision)				0.00277
Accuracy = 1/(1 + Bias + Scale Diff.)				0.998
Concordance (Accuracy * Precision)				0.997



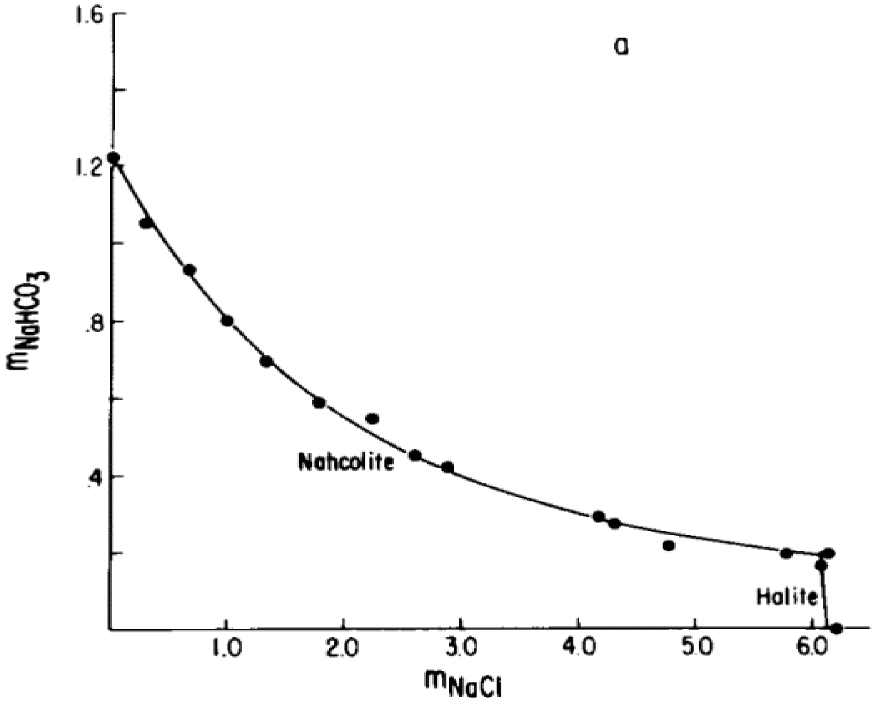


FIG. 7. Salt solubilities in the Na-Cl-SO_4-HCO_3-CO_3-OH-H_2O system. Closed systems.

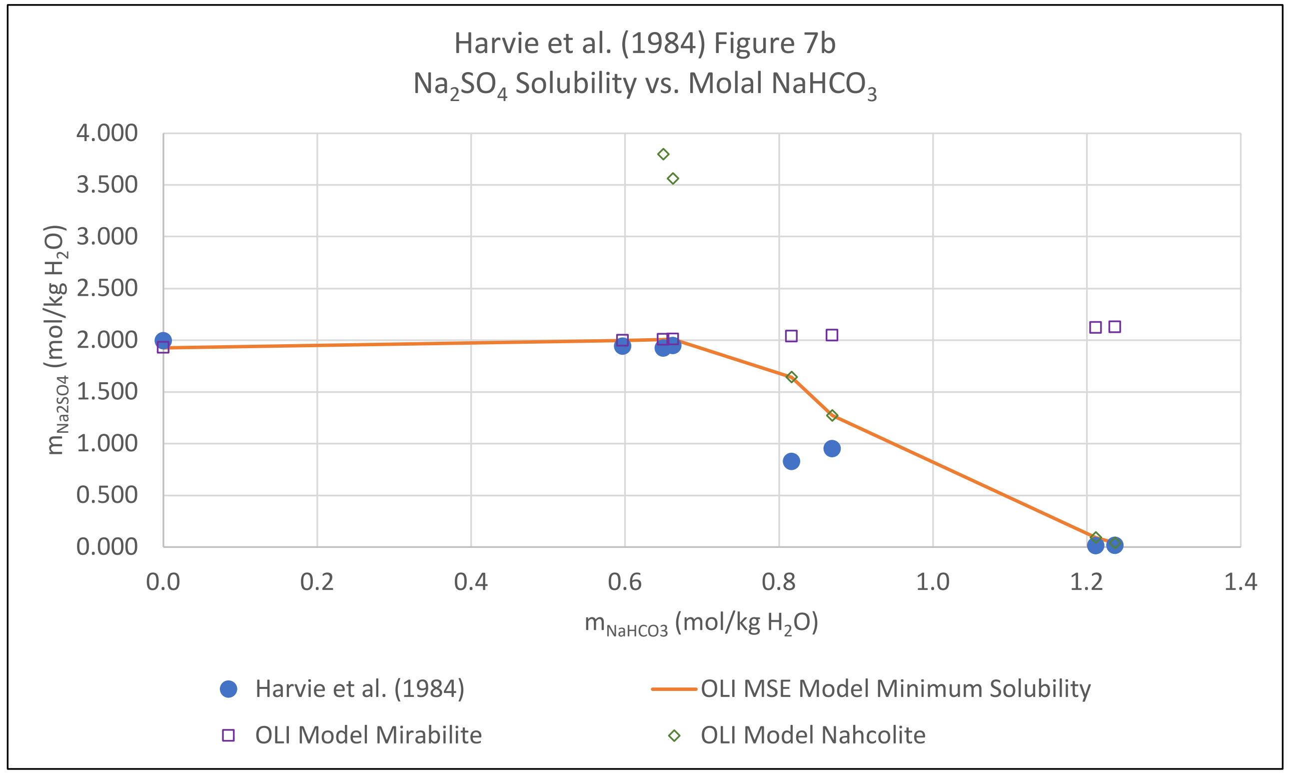
Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 7b

Harvie et al (1984)		OLI Prediction			Residual
m_{NaHCO3} (mol/kg H_2O)	m_{Na2SO4} (mol/kg H_2O)	$Na_2SO_4.10H_2O$ (Mirabilite) (mol/kg H_2O)	$NaHCO_3$ (Nahcolite) (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	1.99	1.93		1.93	-3.3
0.60	1.94	2.00		2.00	3.0
0.65	1.92	2.01	3.80	2.01	4.3
0.66	1.95	2.01	3.56	2.01	3.1
0.82	0.83	2.04	1.64	1.64	**
0.87	0.95	2.05	1.27	1.27	33.8
1.21	0.01	2.12	0.09	0.09	***
1.24	0.02	2.13	0.04	0.04	***
Mean	1.20	na	na	1.37	na
Std. Dev.	0.87	na	na	0.85	na
Mean of absolute values of residuals					9.5
Std. Dev. of absolute values of residuals					13.6
Minimum of absolute values of residuals					3.0
Maximum of absolute values of residuals					33.8
Pearson Correlation Coefficient (Precision)					0.946
Bias (Location)					0.02315
Scale Differential					0.00034
Imprecision (1 - r)					0.05396
Deviance (Bias + Scale Diff. + Imprecision)					0.07745
Accuracy = 1/(1 + Bias + Scale Diff.)					0.977
Concordance (Accuracy * Precision)					0.924

** Not calculated because data were excluded from Harvie et al. (1984) regression in Fig. 7

*** Not included in residual calculations because of large uncertainty in digitized values located at x axis



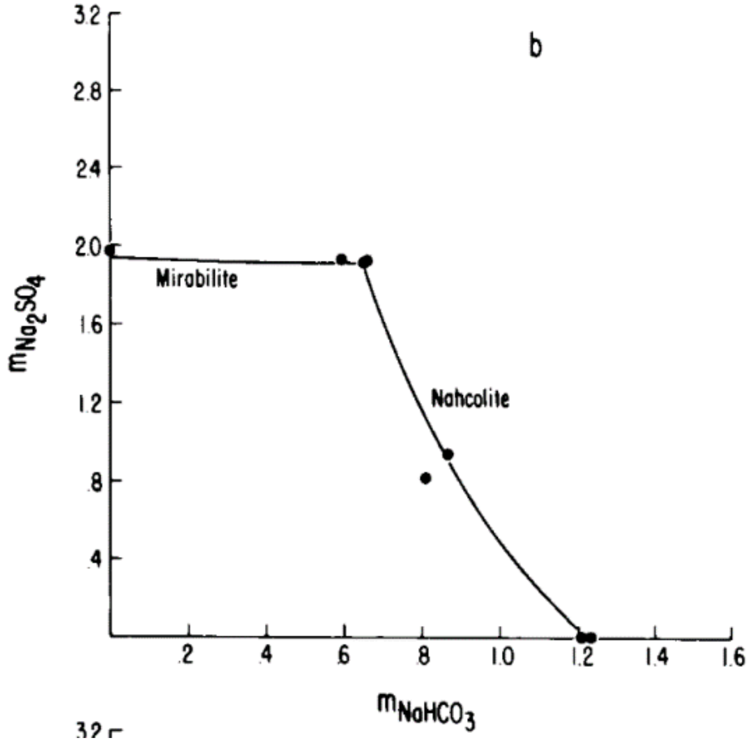


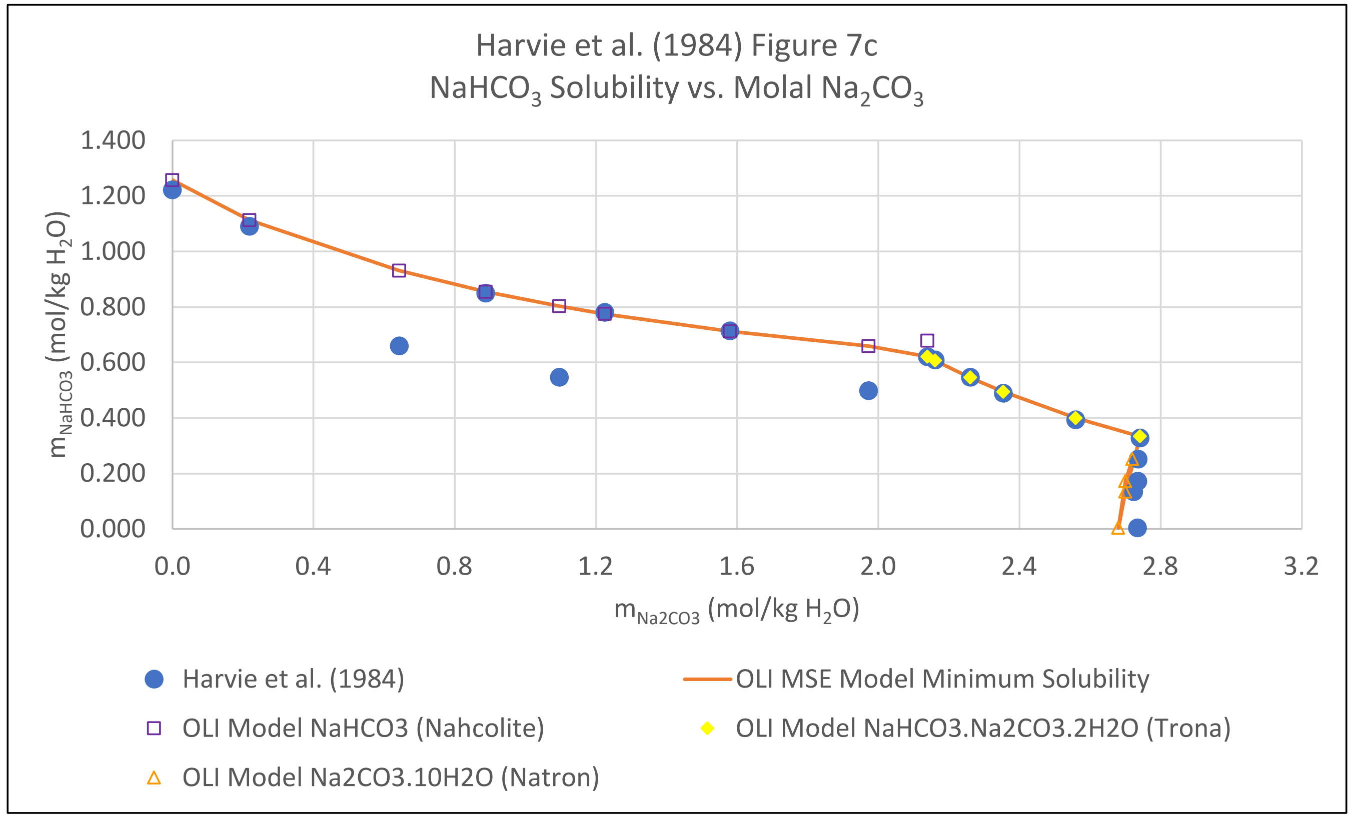
FIG. 7. Salt solubilities in the Na-Cl-SO_4-HCO_3-CO_3-OH-H_2O system. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 7c

Harvie et al (1984)		OLI Prediction				Residual
m_{Na2CO3} (mol/kg H_2O)	m_{NaHCO3} (mol/kg H_2O)	$NaHCO_3$ (Nahcolite) (mol/kg H_2O)	$NaHCO_3.Na_2CO_3.2H_2O$ (Trona) (mol/kg H_2O)	$Na_2CO_3.10H_2O$ (Natron) (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	1.22	1.26			1.26	2.9
0.22	1.09	1.11			1.11	2.0
0.64	0.66	0.93			0.93	**
0.89	0.85	0.85			0.85	0.6
1.10	0.55	0.80			0.80	**
1.23	0.78	0.77			0.77	-0.7
1.58	0.71	0.71			0.71	-0.4
1.97	0.50	0.66			0.66	**
2.14	0.62	0.68	0.62		0.62	0.1
2.16	0.61		0.61		0.61	-0.5
2.26	0.55		0.55		0.55	-0.2
2.35	0.49		0.49		0.49	0.9
2.56	0.39		0.40		0.40	1.6
2.74	0.33		0.33		0.33	1.7
2.72	0.13			2.70		-0.9
2.73	0.00			2.68		-2.0
2.74	0.17			2.70		-1.3
2.74	0.25			2.72		-0.6
Mean	0.67	na	na	2.70	0.72	na
Std. Dev.	0.25	na	na	0.01	0.26	na
					Mean of absolute values of residuals	1.1
					Std. Dev. of absolute values of residuals	0.8
					Minimum of absolute values of residuals	0.1
					Maximum of absolute values of residuals	2.9
Hahcolite and Trona					Pearson Correlation Coefficient Nahcolite + Trona (Precision)	0.926
					Bias (Location)	0.02398
					Scale Differential	0.00052
					Imprecision (1 - r)	0.07382
					Deviance (Bias + Scale Diff. + Imprecision)	0.09831
					Accuracy = 1/(1 + Bias + Scale Diff.)	0.976
					Concordance (Accuracy * Precision)	0.904
Natron					Pearson Correlation Coefficient Natron (Precision)	0.125
					Bias (Location)	8.77144
					Scale Differential	0.45640
					Imprecision (1 - r)	0.87511
					Deviance (Bias + Scale Diff. + Imprecision)	10.10296
					Accuracy = 1/(1 + Bias + Scale Diff.)	0.098
					Concordance (Accuracy * Precision)	0.012

** Not calculated because data were excluded from Harvie et al. (1984) regression in Fig. 7



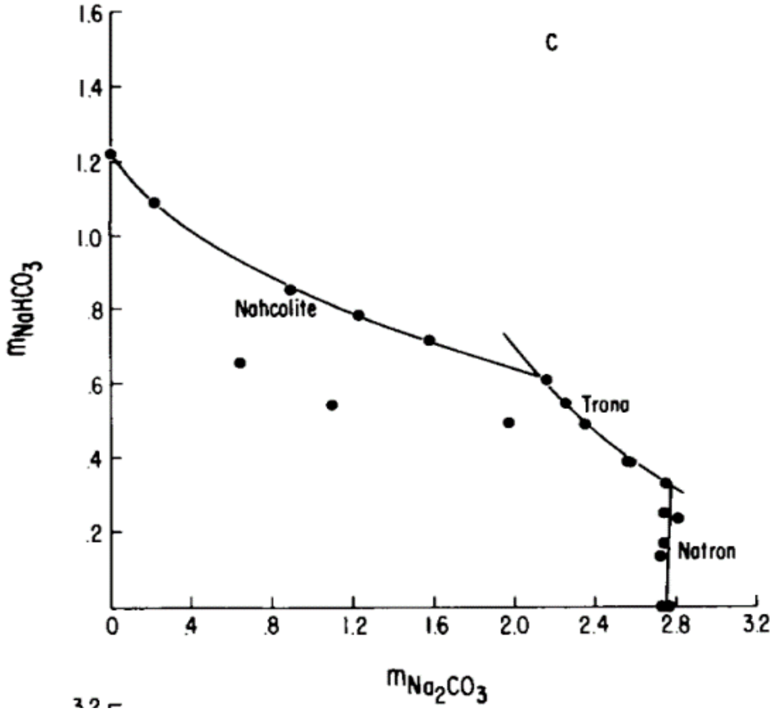


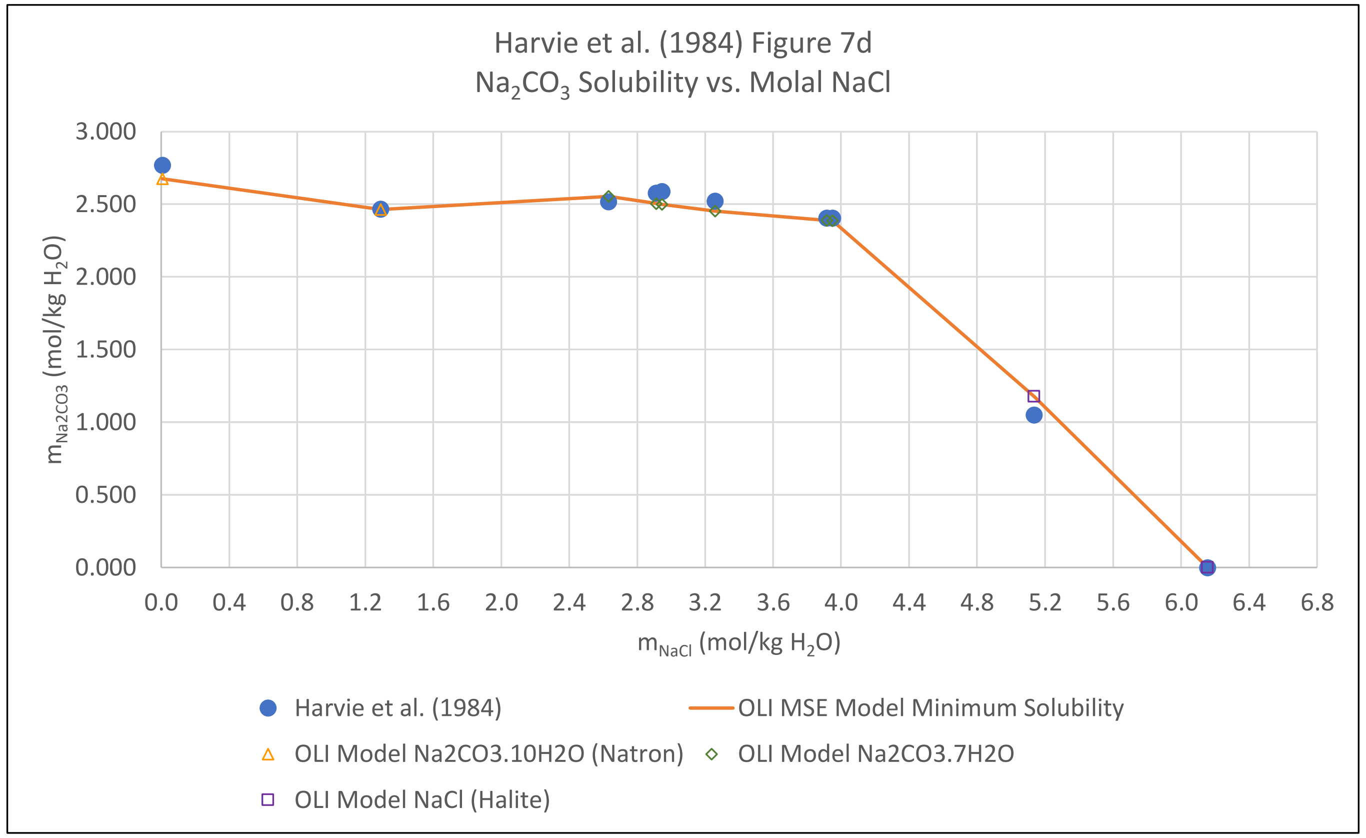
FIG. 7. Salt solubilities in the Na-Cl-SO_4-HCO_3-CO_3-OH-H_2O system. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 7d

Harvie et al (1984)		OLI Prediction				Residual
m_{NaCl} (mol/kg H_2O)	m_{Na2CO3} (mol/kg H_2O)	$Na_2CO_3.10H_2O$ (Natron) (mol/kg H_2O)	$Na_2CO_3.7H_2O$ (mol/kg H_2O)	NaCl (Halite) (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.01	2.77	2.68			2.68	-3.4
1.29	2.47	2.46			2.46	-0.1
2.63	2.52		2.55		2.55	1.5
2.91	2.58		2.50		2.50	-2.8
2.95	2.59		2.50		2.50	-3.4
3.26	2.52		2.45		2.45	-2.7
3.92	2.40		2.39		2.39	-0.7
3.95	2.40		2.39		2.39	-0.7
5.14	1.05			1.18	1.18	12.3
6.16	0.00			0.002	0.002	**
Mean	2.13	na	na	na	2.11	na
Std. Dev.	0.89	na	na	na	0.85	na
Mean of absolute values of residuals						3.1
Std. Dev. of absolute values of residuals						3.7
Minimum of absolute values of residuals						0.1
Maximum of absolute values of residuals						12.3
Pearson Correlation Coefficient (Precision)						0.998
Bias (Location)						0.00026
Scale Differential						0.00083
Imprecision (1 - r)						0.00220
Deviance (Bias + Scale Diff. + Imprecision)						0.00329
Accuracy = 1/(1 + Bias + Scale Diff.)						0.999
Concordance (Accuracy * Precision)						0.997

** Not calculated because of large uncertainty in digitized values extracted from Fig. 7 by Harvie et al. (1984)



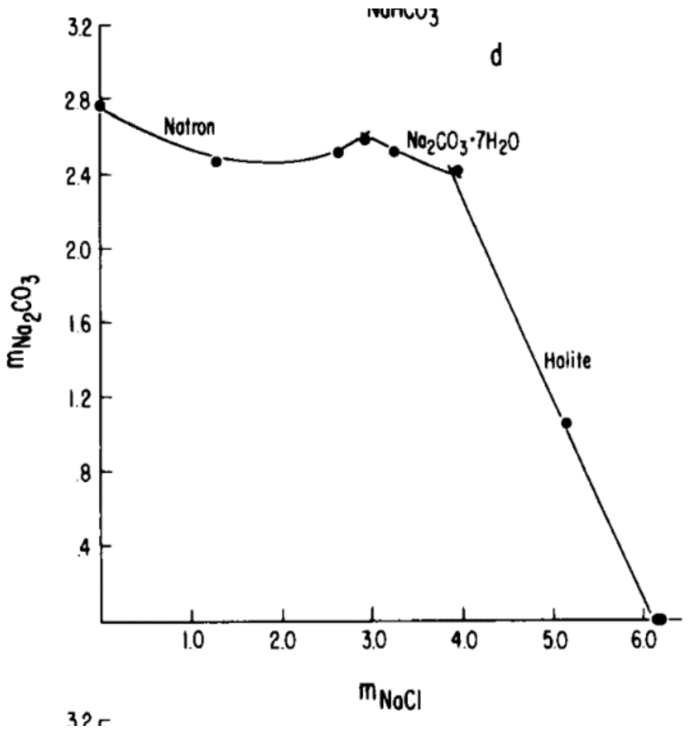
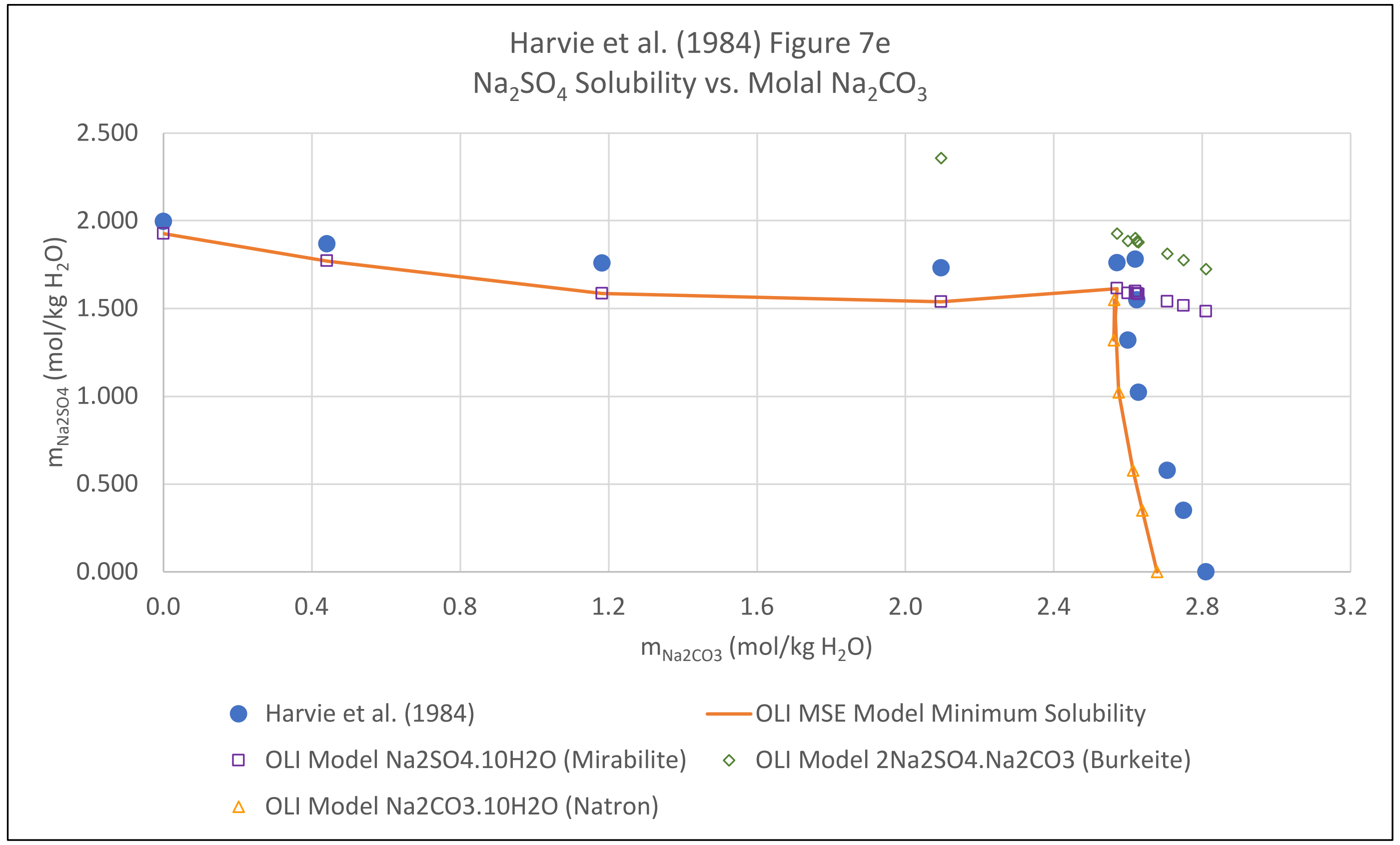


FIG. 7. Salt solubilities in the Na-Cl-SO$_4$-HCO$_3$-CO$_3$-OH-H$_2$O system. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 7e

Harvie et al (1984)		OLI Prediction				Residual
m_{Na2CO3} (mol/kg H_2O)	m_{Na2SO4} (mol/kg H_2O)	$Na_2SO_4.10H_2O$ (Mirabilite) (mol/kg H_2O)	$2Na_2SO_4.Na_2CO_3$ (Burkeite) (mol/kg H_2O)	$Na_2CO_3.10H_2O$ (Natron) (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	2.00	1.93			1.93	-3.4
0.44	1.87	1.77			1.77	-5.2
1.18	1.76	1.59			1.59	-9.8
2.10	1.73	1.54	2.36		1.54	-11.1
2.57	1.76	1.61	1.93		1.61	-8.3
2.62	1.78	1.60	1.90		1.60	-10.3
2.60	1.32	1.59	1.88	2.56		-1.5
2.62	1.55	1.59	1.88	2.56		-2.3
2.63	1.02	1.58	1.88	2.58		-2.0
2.71	0.58	1.54	1.81	2.61		-3.4
2.75	0.35	1.52	1.77	2.64		-4.0
2.81	0.00	1.48	1.72	2.68		-4.7
Mean	1.82	na	na	2.61	1.67	na
Std. Dev.	0.10	na	na	0.05	0.15	na
Mean of absolute values of residuals						5.5
Std. Dev. of absolute values of residuals						3.4
Minimum of absolute values of residuals						1.5
Maximum of absolute values of residuals						11.1
Mirabilite	Pearson Correlation Coefficient Mirabilite (Precision)					0.992
	Bias (Location)					0.83455
	Scale Differential					0.07761
	Imprecision (1 - r)					0.00776
	Deviance (Bias + Scale Diff. + Imprecision)					0.91993
	Accuracy = 1/(1 + Bias + Scale Diff.)					0.523
	Concordance (Accuracy * Precision)					0.519
Natron	Pearson Correlation Coefficient Natron (Precision)					0.995
	Bias (Location)					1.01494
	Scale Differential					0.16675
	Imprecision (1 - r)					0.00462
	Deviance (Bias + Scale Diff. + Imprecision)					1.18632
	Accuracy = 1/(1 + Bias + Scale Diff.)					0.458
	Concordance (Accuracy * Precision)					0.456



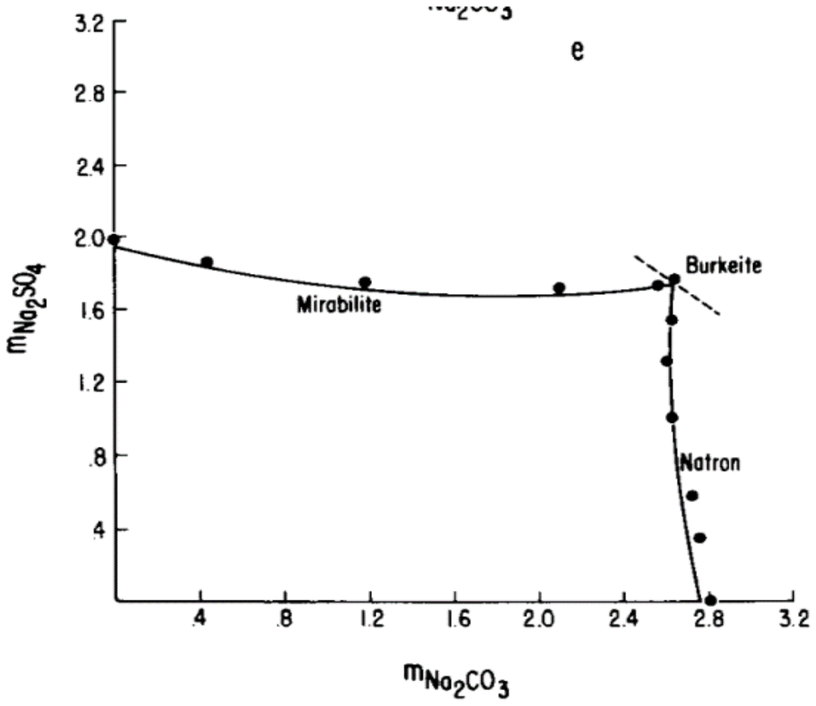
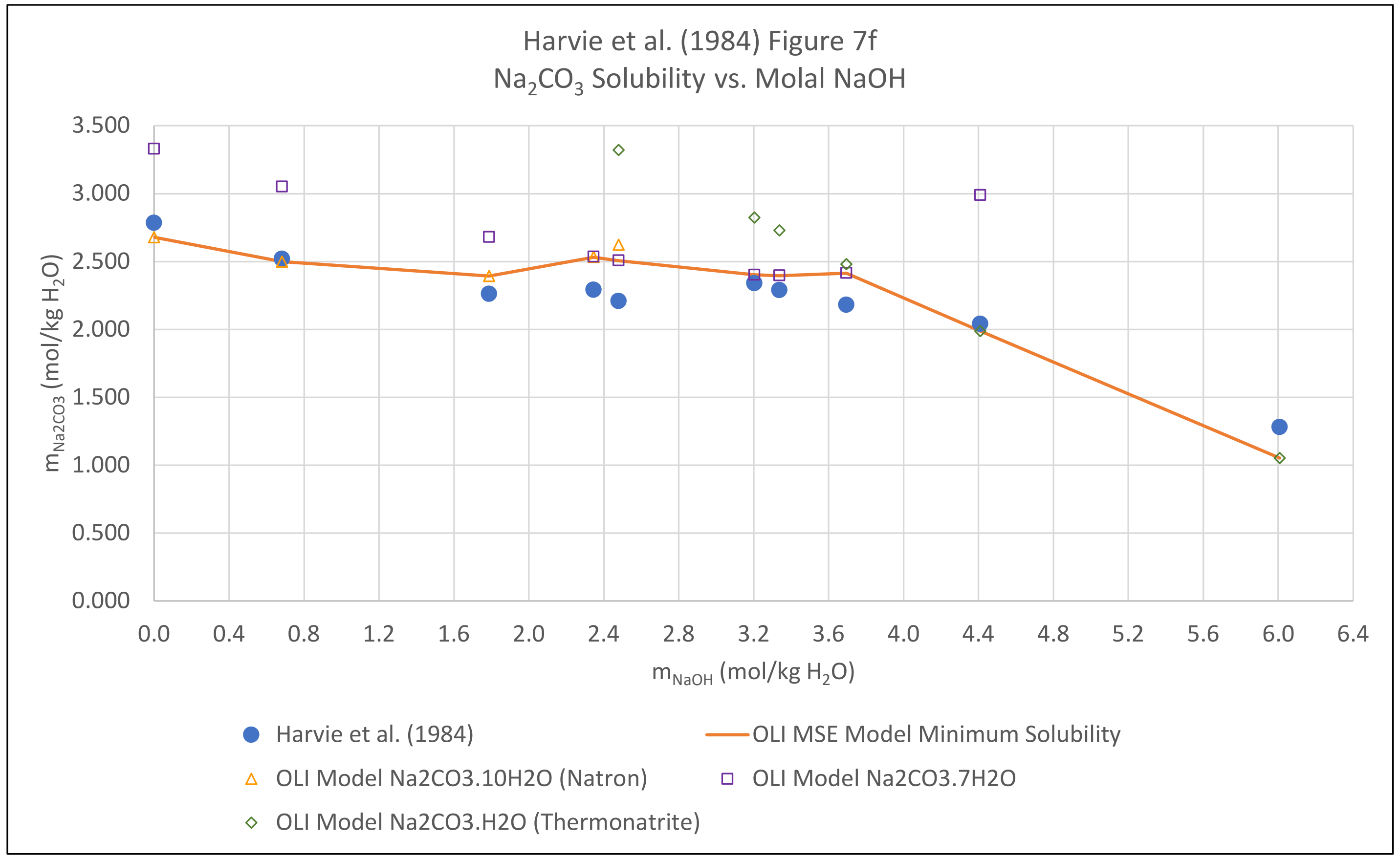


FIG. 7. Salt solubilities in the Na-Cl-SO$_4$-HCO$_3$-CO$_3$-OH-H$_2$O system. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 7f

Harvie et al (1984)		OLI Prediction				Residual
m_{NaOH} (mol/kg H_2O)	m_{Na2CO3} (mol/kg H_2O)	$Na_2CO_3.10H_2O$ (Natron) (mol/kg H_2O)	$Na_2CO_3.7H_2O$ (mol/kg H_2O)	$Na_2CO_3.H_2O$ (Thermonatrite) (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	2.78	2.68	3.33		2.68	-3.8
0.68	2.52	2.50	3.05		2.50	-0.9
1.79	2.26	2.39	2.68		2.39	5.8
2.35	2.29	2.53	2.54		2.53	10.5
2.48	2.21	2.62	2.51	3.32	2.51	13.5
3.20	2.34		2.40	2.82	2.40	2.7
3.34	2.29		2.40	2.73	2.40	4.7
3.70	2.18		2.42	2.48	2.42	10.7
4.41	2.04		2.99	1.99	1.99	-2.6
6.01	1.28			1.05	1.05	-17.7
Mean	2.22	na	na	na	2.29	na
Std. Dev.	0.39	na	na	na	0.47	na
Mean of absolute values of residuals						7.3
Std. Dev. of absolute values of residuals						5.5
Minimum of absolute values of residuals						0.9
Maximum of absolute values of residuals						17.7
Pearson Correlation Coefficient (Precision)						0.940
Bias (Location)						0.01360
Scale Differential						0.01797
Imprecision (1 - r)						0.06050
Deviance (Bias + Scale Diff. + Imprecision)						0.09207
Accuracy = 1/(1 + Bias + Scale Diff.)						0.969
Concordance (Accuracy * Precision)						0.911



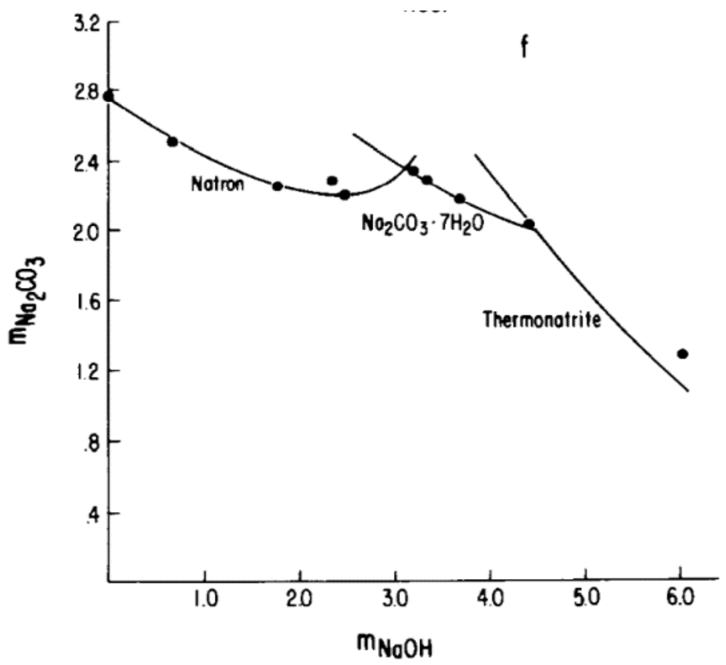
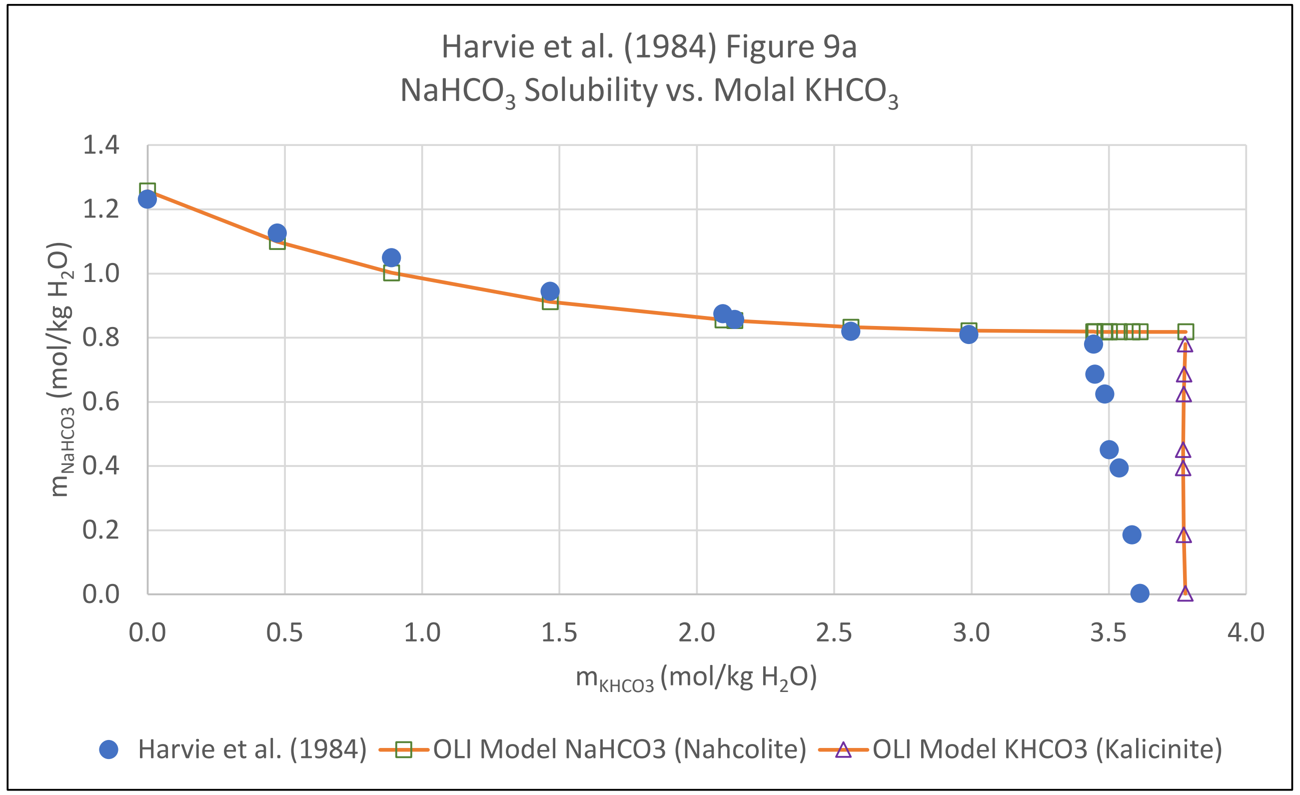


FIG. 7. Salt solubilities in the Na-Cl-SO_4-HCO_3-CO_3-OH-H_2O system. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 9a

Harvie et al (1984)		OLI Prediction		Residual
m_{KHCO3} (mol/kg H_2O)	m_{NaHCO3} (mol/kg H_2O)	$NaHCO_3$ (Nahcolite) Solubility Limit (mol/kg H_2O)	$KHCO_3$ (Kalicinite) Solubility Limit (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	1.23	1.26		2.0
0.47	1.13	1.10		-2.3
0.89	1.05	1.00		-4.4
1.47	0.94	0.91		-3.4
2.09	0.87	0.86		-2.1
2.14	0.86	0.85		-0.4
2.56	0.82	0.83		1.6
2.99	0.81	0.82		1.5
3.45	0.78	0.82	3.78	9.7
3.45	0.69	0.82	3.77	9.4
3.49	0.62	0.82	3.77	8.2
3.50	0.45	0.82	3.77	7.7
3.54	0.39	0.82	3.77	6.6
3.59	0.19	0.82	3.77	5.2
3.61	0.002	0.82	3.78	4.6
3.78		0.82	3.78	na
Mean	0.96	0.95	3.77	na
Std. Dev.	0.16	0.16	0.004	na
Mean of absolute values of residuals				5.0
Std. Dev. of absolute values of residuals				3.1
Minimum of absolute values of residuals				0.4
Maximum of absolute values of residuals				9.7
Nahcolite	Pearson Correlation Coefficient NaHCO3 (Precision)			0.987
	Bias (Location)			0.00207
	Scale Differential			0.00000
	Imprecision (1 - r)			0.01312
	Deviance (Bias + Scale Diff. + Imprecision)			0.01520
	Accuracy = 1/(1 + Bias + Scale Diff.)			0.998
	Concordance (Accuracy * Precision)			0.985
Kalicinite	Pearson Correlation Coefficient KHCO3 (Precision)			0.429
	Bias (Location)			169.47474
	Scale Differential			8.27403
	Imprecision (1 - r)			0.57131
	Deviance (Bias + Scale Diff. + Imprecision)			178.32008
	Accuracy = 1/(1 + Bias + Scale Diff.)			0.006
	Concordance (Accuracy * Precision)			0.002



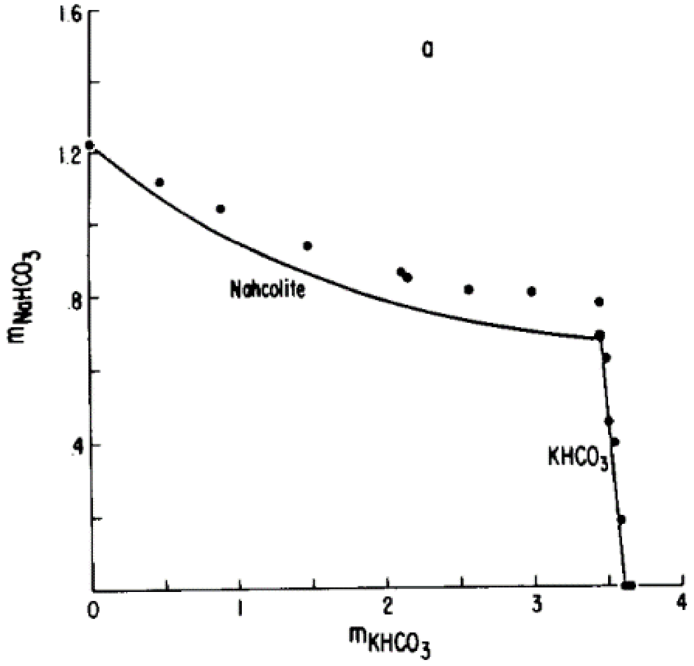
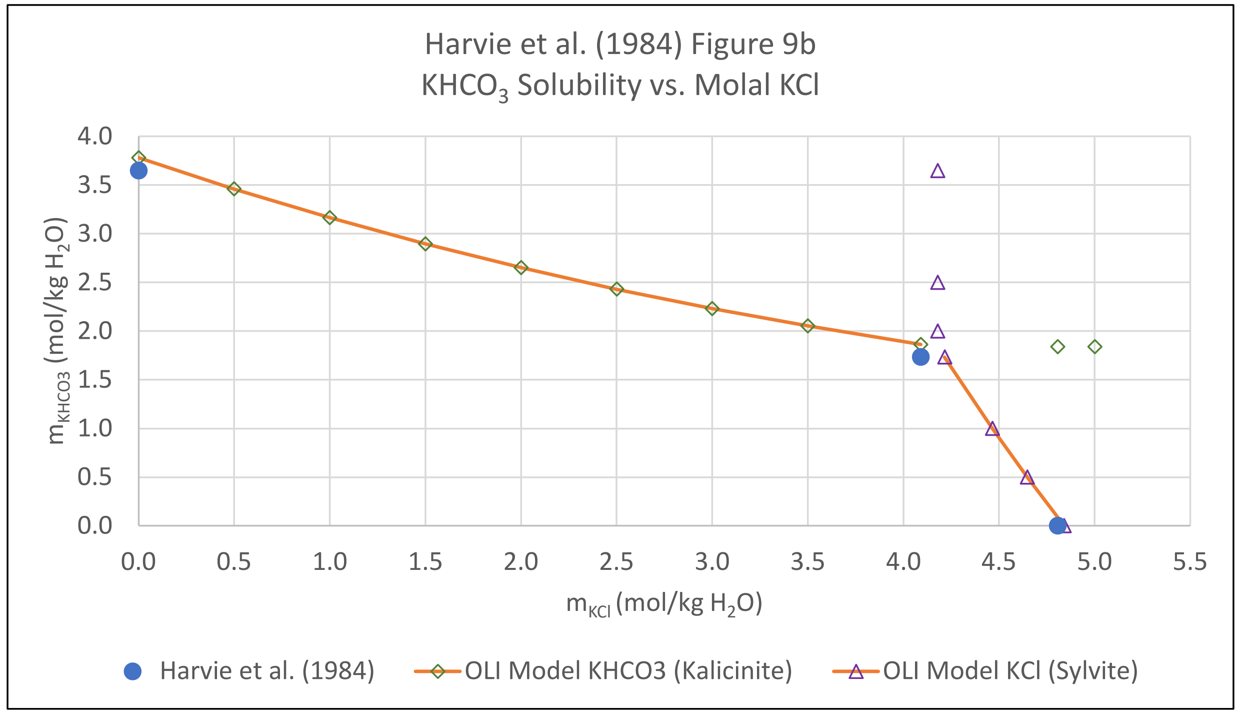


FIG. 9. Salt solubilities in potassium carbonate systems. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 9b

Harvie et al (1984)		OLI Prediction	Residual
m_{KCl} (mol/kg H_2O)	m_{KHCO3} (mol/kg H_2O)	$KHCO_3$ (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.0	3.6	3.8	3.6
0.5		3.5	na
1.0		3.2	na
1.5		2.9	na
2.0		2.7	na
2.5		2.4	na
3.0		2.2	na
3.5		2.1	na
4.1	1.7	1.9	7.5
4.8	0.0	1.8	na
5.0		1.8	na
Mean	2.69	2.82	na
Std. Dev.	1.35	1.35	na
Pearson Correlation Coefficient (Precision)			1.000
Bias (Location)			0.00934
Scale Differential			0.00000
Imprecision (1 - r)			0.00000
Deviance (Bias + Scale Diff. + Imprecision)			0.00934
Accuracy = 1/(1 + Bias + Scale Diff.)			0.991
Concordance (Accuracy * Precision)			0.991



Harvie et al (1984)		OLI Prediction	Residual
m_{KHCO3} (mol/kg H_2O)	m_{KCl} (mol/kg H_2O)	KCl (Sylvite) (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
3.6		4.2	na
2.5		4.2	na
2.0		4.2	na
1.7	4.1	4.2	3.0
1.0		4.5	na
0.5		4.6	na
0.0	4.8	4.8	0.7
Mean	4.45	4.53	na
Std. Dev.	0.51	0.44	na
Mean of absolute values of residuals			3.7
Std. Dev. of absolute values of residuals			2.8
Minimum of absolute values of residuals			0.71
Maximum of absolute values of residuals			7.5
Pearson Correlation Coefficient (Precision)			1.000
Bias (Location)			0.02802
Scale Differential			0.00912
Imprecision (1 - r)			0.00000
Deviance (Bias + Scale Diff. + Imprecision)			0.03714
Accuracy = 1/(1 + Bias + Scale Diff.)			0.964
Concordance (Accuracy * Precision)			0.964

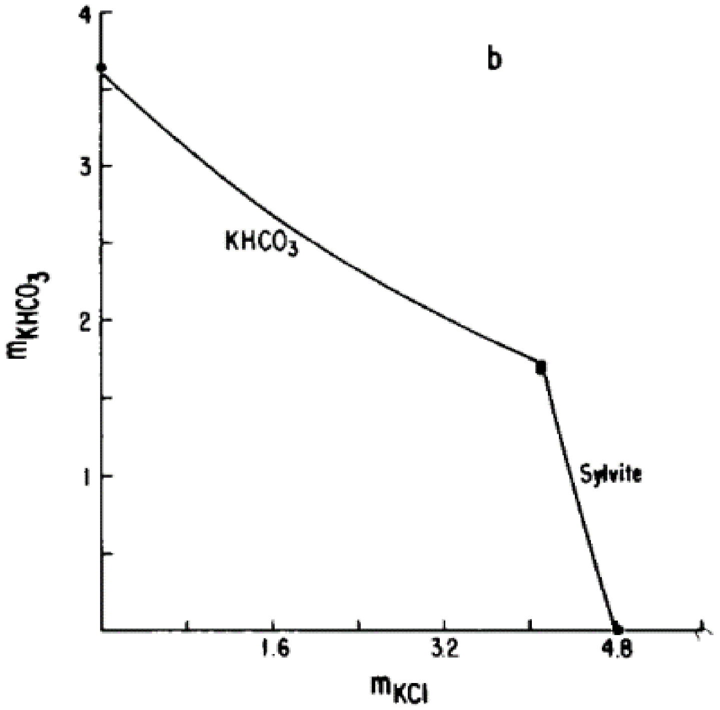
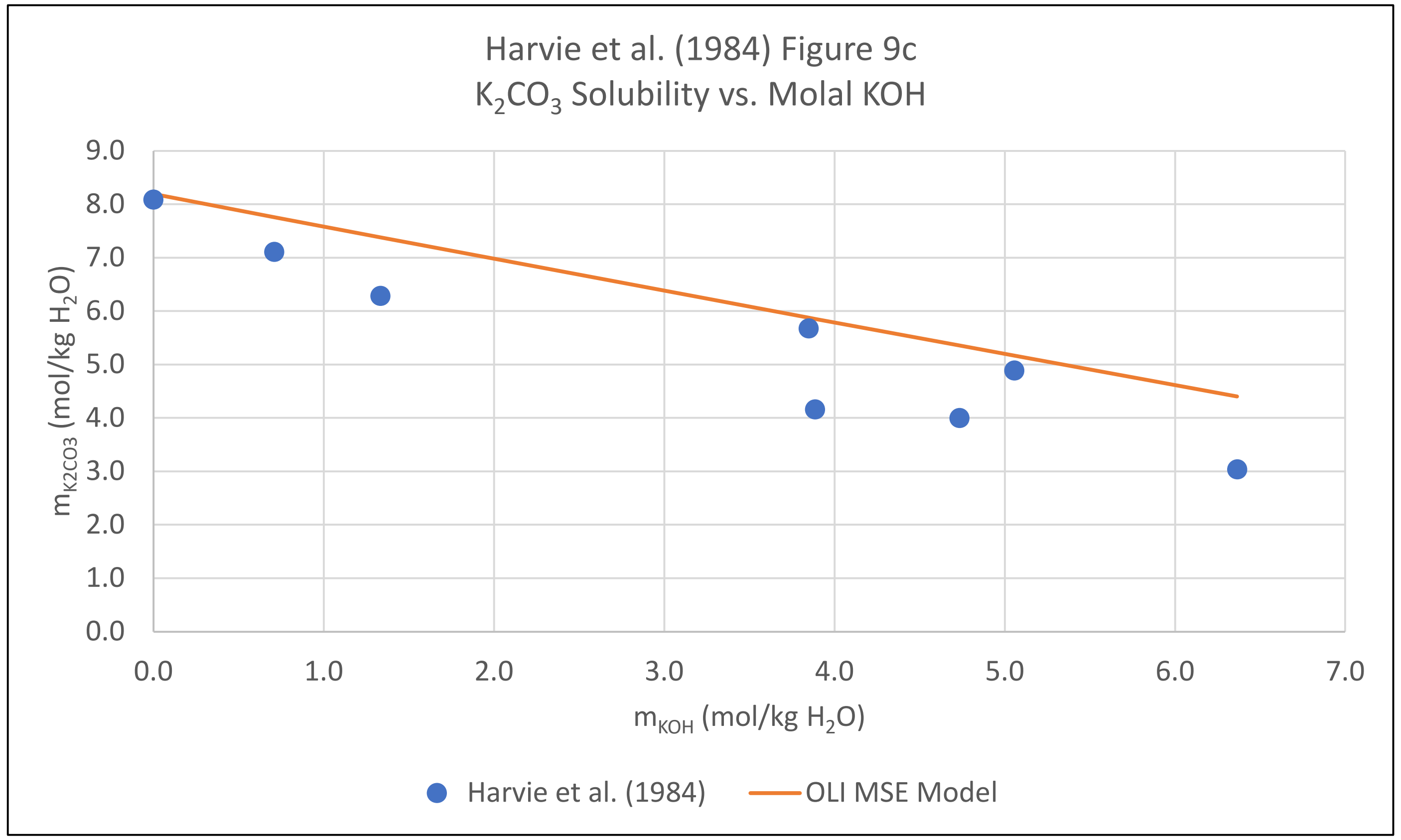


FIG. 9. Salt solubilities in potassium carbonate systems. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 9c

Harvie et al (1984)		OLI Prediction	Residual
m_{KOH} (mol/kg H_2O)	m_{K2CO3} (mol/kg H_2O)	$K_2CO_3.1.5H_2O$ (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	8.09	8.20	1.3
0.71	7.11	7.76	9.1
1.33	6.28	7.38	17.5
3.85	5.68	5.88	3.5
3.89	4.16	5.85	40.6
4.73	4.00	5.36	33.9
5.06	4.89	5.16	5.6
6.36	3.04	4.40	45.0
Mean	5.41	6.25	na
Std. Dev.	1.70	1.36	na
Mean of absolute values of residuals			19.6
Std. Dev. of absolute values of residuals			17.7
Minimum of absolute values of residuals			1.33
Maximum of absolute values of residuals			45.0
Pearson Correlation Coefficient (Precision)			0.944
Bias (Location)			0.17411
Scale Differential			0.02490
Imprecision (1 - r)			0.05609
Deviance (Bias + Scale Diff. + Imprecision)			0.25510
Accuracy = 1/(1 + Bias + Scale Diff.)			0.834
Concordance (Accuracy * Precision)			0.787



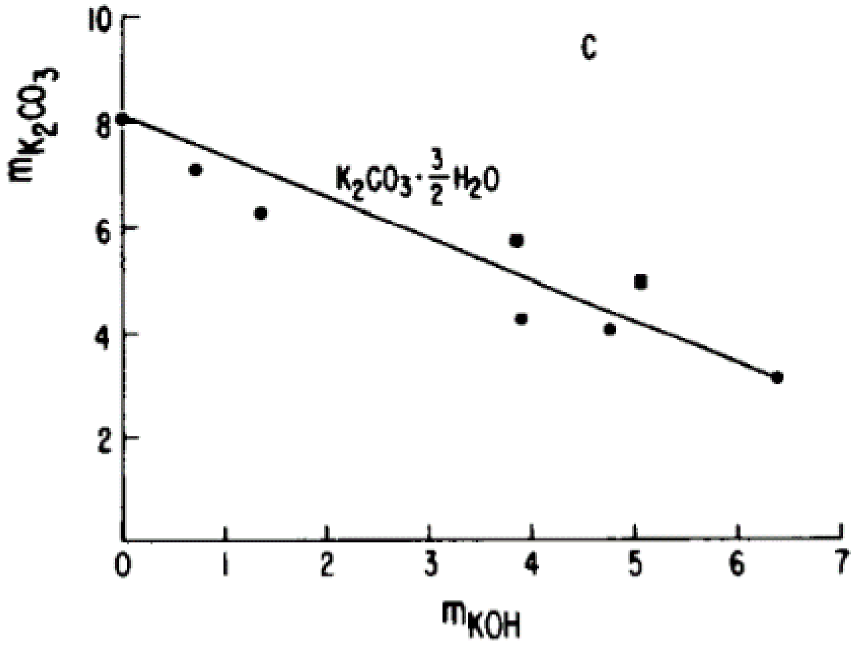
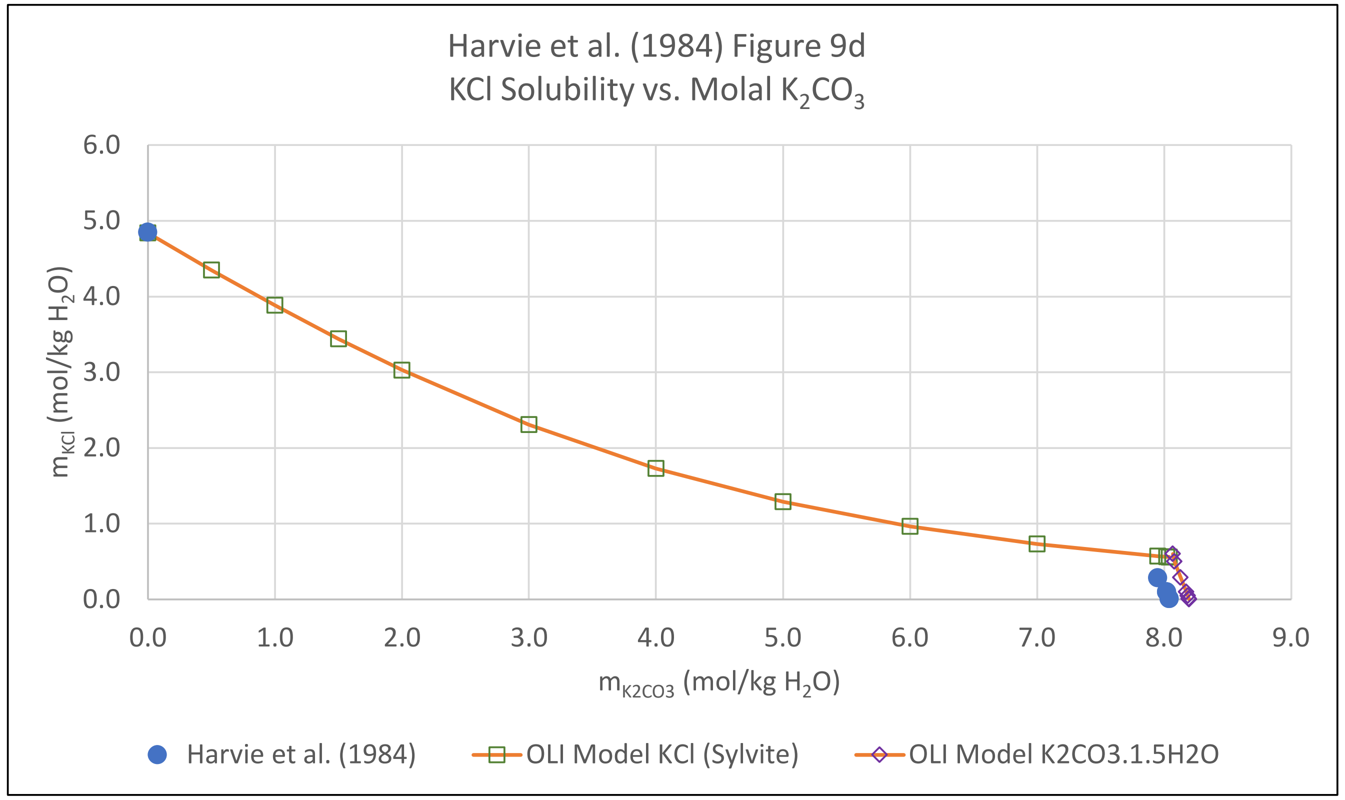


FIG. 9. Salt solubilities in potassium carbonate systems. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 9d

Harvie et al (1984)		OLI Prediction		Residual
m_{K2CO3} (mol/kg H_2O)	m_{KCl} (mol/kg H_2O)	KCl (Sylvite) (mol/kg H_2O)	K_2CO_3.1.5H_2O (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.0	4.85	4.84	na	-0.2
0.5		4.35	na	na
1.0		3.88	na	na
1.5		3.44	na	na
2.0		3.03	na	na
3.0		2.31	na	na
4.0		1.73	na	na
5.0		1.29	na	na
6.0		0.96	na	na
7.0		0.73	na	na
7.95	0.29	0.57	na	na
8.02	0.10	0.56	na	na
8.04	0.01	0.56	na	na
	0.00	na	8.20	na
8.04	0.01	na	8.19	1.9
	0.05	na	8.18	na
8.02	0.10	na	8.17	1.9
7.95	0.29	na	8.13	2.3
	0.50	na	8.08	na
	0.60	na	8.07	na
Mean	na	na	8.17	na
Std. Dev.	na	na	0.05	na
Mean of absolute values of residuals				1.6
Std. Dev. of absolute values of residuals				0.9
Minimum of absolute values of residuals				0.2
Maximum of absolute values of residuals				2.3
K2CO3.1.5H2O Only	Pearson Correlation Coefficient (Precision)			0.994
	Bias (Location)			7.69922
	Scale Differential			0.00953
	Imprecision (1 - r)			0.00586
	Deviance (Bias + Scale Diff. + Imprecision)			7.71461
	Accuracy = 1/(1 + Bias + Scale Diff.)			0.115
	Concordance (Accuracy * Precision)			0.114



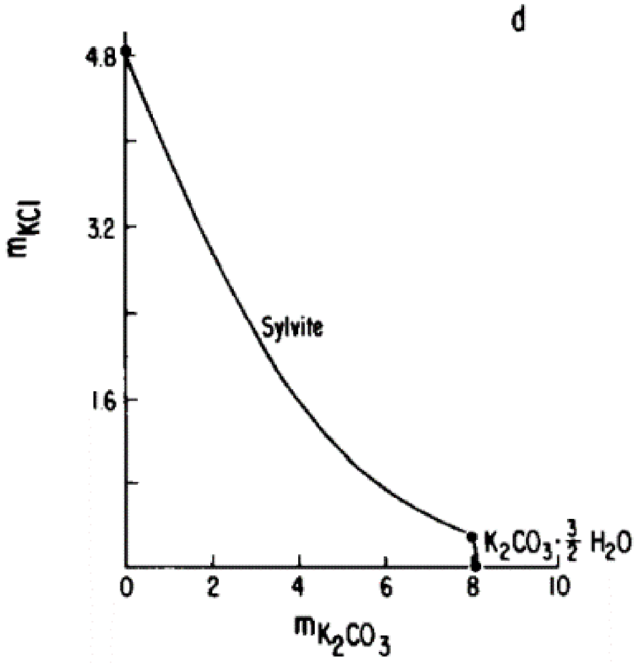
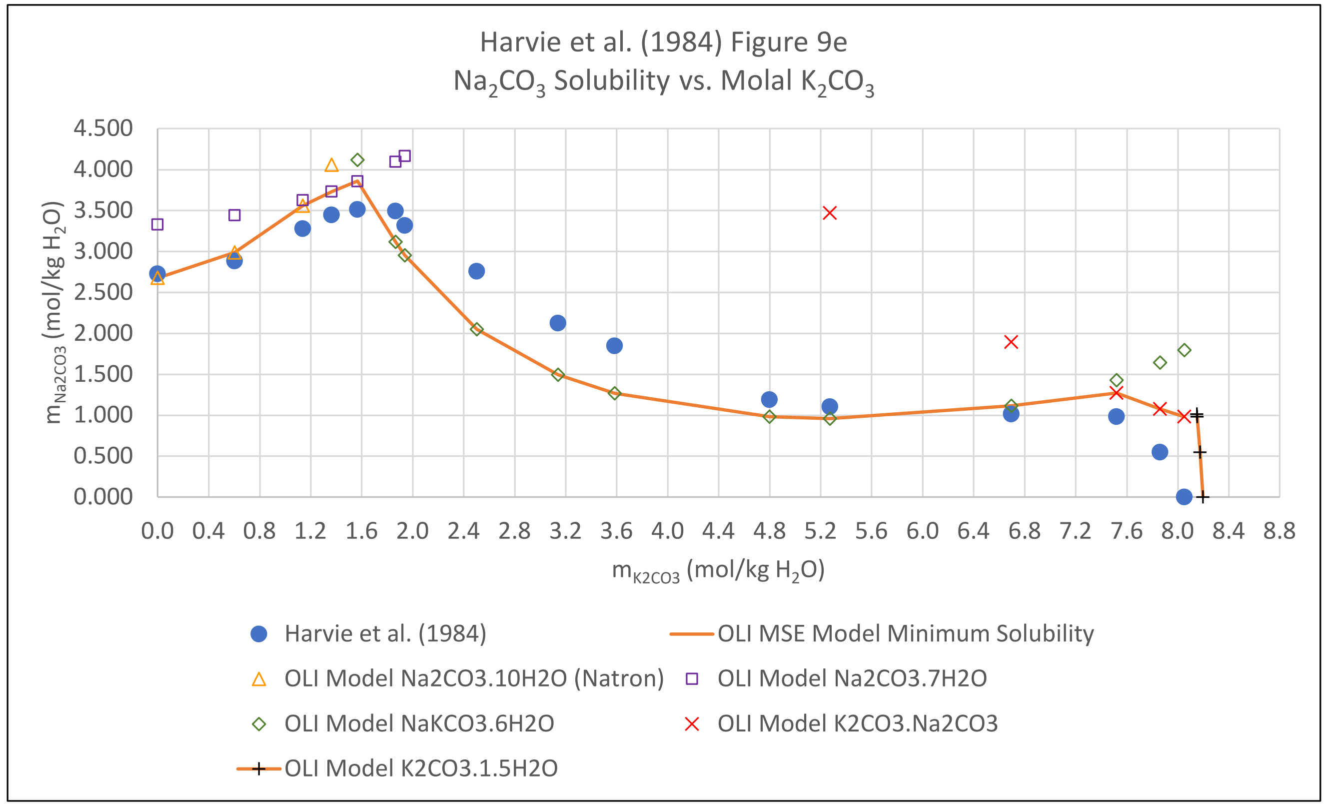


FIG. 9. Salt solubilities in potassium carbonate systems. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 9e

Harvie et al (1984)		OLI Prediction						Residual
m_{K2CO3} (mol/kg H_2O)	m_{Na2CO3} (mol/kg H_2O)	$Na_2CO_3.10H_2O$ (Natron) (mol/kg H_2O)	$Na_2CO_3.7H_2O$ (mol/kg H_2O)	$NaKCO_3.6H_2O$ (mol/kg H_2O)	$K_2CO_3.Na_2CO_3$ (mol/kg H_2O)	$K_2CO_3.1.5H_2O$ (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	2.73	2.68	3.33				2.68	-1.8
0.60	2.88	2.99	3.44				2.99	3.7
1.14	3.28	3.56	3.62				3.56	8.6
1.36	3.44	4.06	3.73				3.73	8.3
1.57	3.51		3.86	4.12			3.86	9.8
1.87	3.49		4.10	3.12			3.12	-10.7
1.94	3.31		4.16	2.95			2.95	-10.9
2.50	2.76			2.05			2.05	-25.7
3.14	2.12			1.50			1.50	-29.6
3.58	1.84			1.27			1.27	-31.3
4.80	1.19			0.98			0.98	-17.5
5.27	1.10			0.96	3.47		0.96	-13.2
6.69	1.01			1.12	1.89	8.15	1.12	10.3
7.52	0.98			1.43	1.27	8.15	1.27	29.6
7.86	0.55			1.64	1.08	8.17	1.08	4.0
8.05	0.00			1.80	0.98	8.20	0.98	1.8
Mean	2.14	na	na	na	na	na	2.13	na
Std. Dev.	1.19	na	na	na	na	na	1.11	na
Mean of absolute values of residuals								13.5
Std. Dev. of absolute values of residuals								10.2
Minimum of absolute values of residuals								1.8
Maximum of absolute values of residuals								31.3
Pearson Correlation Coefficient (Precision)								0.921
Bias (Location)								0.00002
Scale Differential								0.00259
Imprecision (1 - r)								0.07857
Deviance (Bias + Scale Diff. + Imprecision)								0.08119
Accuracy = 1/(1 + Bias + Scale Diff.)								0.997
Concordance (Accuracy * Precision)								0.919



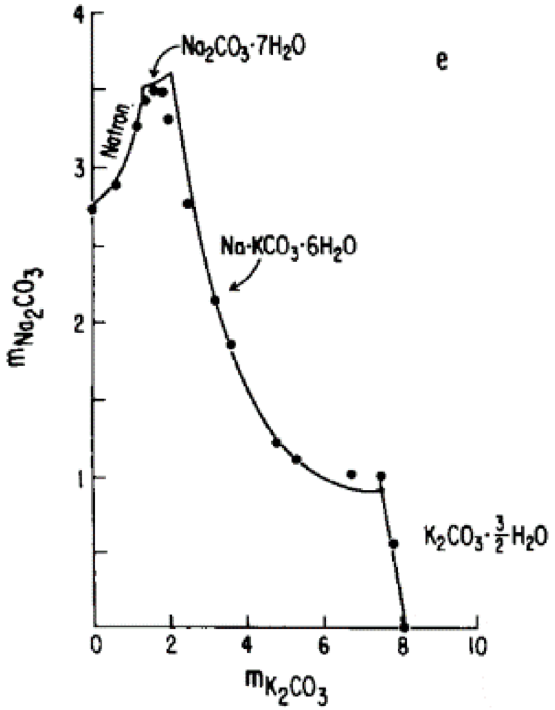
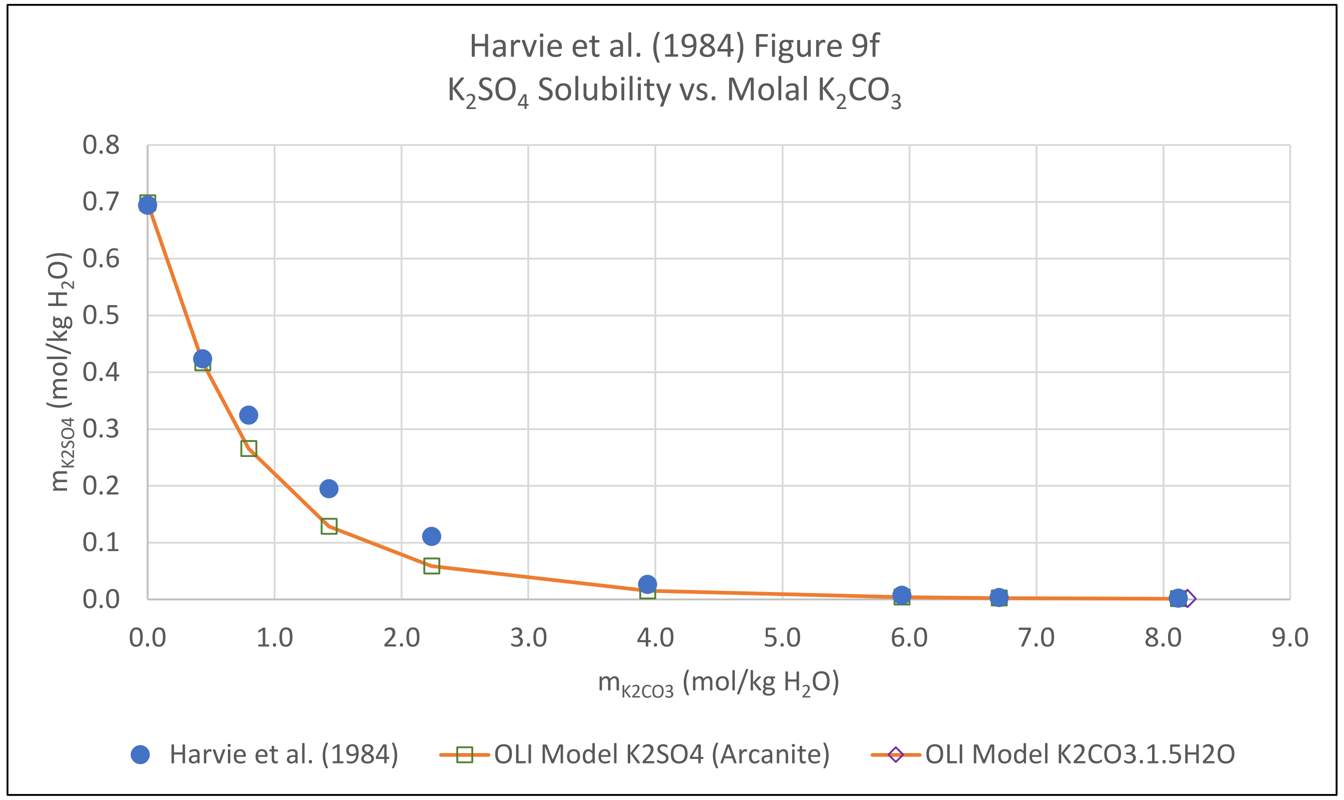


FIG. 9. Salt solubilities in potassium carbonate systems. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 9f

Harvie et al (1984)		OLI Prediction		Residual
m_{K2CO3} (mol/kg H_2O)	m_{K2SO4} (mol/kg H_2O)	K_2SO_4 (Arcanite) (mol/kg H_2O)	K_2CO_3.1.5H_2O (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	0.69	0.70		0.7
0.44	0.42	0.42		-1.6
0.80	0.32	0.27		-18.2
1.43	0.19	0.13		-34.0
2.24	0.11	0.06		-46.9
3.94	0.026	0.015		-42.9
5.94	0.007	3.92E-03		-45.3
6.71	0.003	2.49E-03		-24.0
8.12	0.002	1.18E-03		-30.4
8.12	1.14E-03	na	8.19	0.9
Mean	0.20	0.18	na	na
Std. Dev.	0.24	0.24	na	na
Mean of absolute values of residuals				24.5
Std. Dev. of absolute values of residuals				18.5
Minimum of absolute values of residuals				0.7
Maximum of absolute values of residuals				46.9
Pearson Correlation Coefficient (Precision)				0.993
Bias (Location)				0.00453
Scale Differential				0.00004
Imprecision (1 - r)				0.00697
Deviance (Bias + Scale Diff. + Imprecision)				0.01155
Accuracy = 1/(1 + Bias + Scale Diff.)				0.995
Concordance (Accuracy * Precision)				0.989



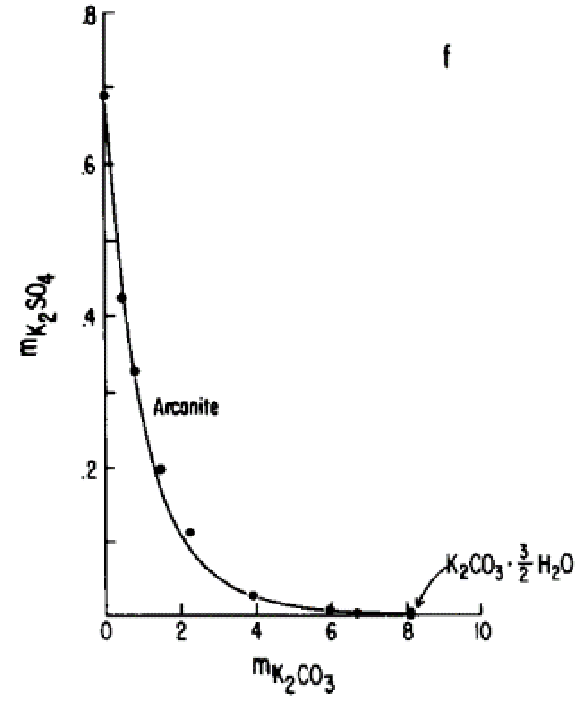
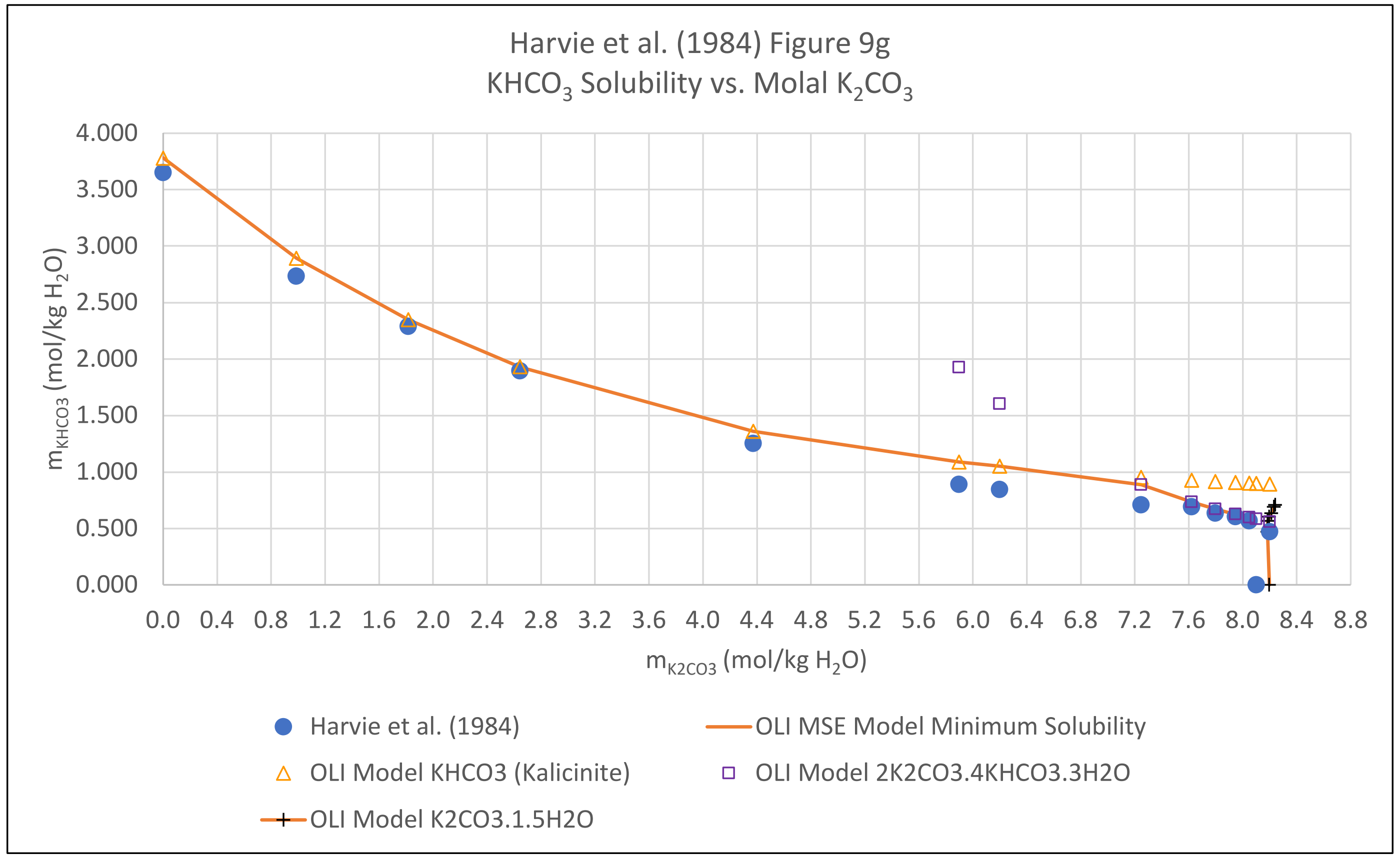


FIG. 9. Salt solubilities in potassium carbonate systems. Closed systems.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 9g

Harvie et al (1984)		OLI Prediction				Residual
m_{K2CO3} (mol/kg H_2O)	m_{KHCO3} (mol/kg H_2O)	$KHCO_3$ (Kalicinite) (mol/kg H_2O)	$2K_2CO_3.4KHCO_3.3H_2O$ (mol/kg H_2O)	$K_2CO_3.1.5H_2O$ (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	3.65	3.78			3.78	3.6
0.99	2.73	2.89			2.89	5.8
1.82	2.29	2.35			2.35	2.7
2.64	1.89	1.93			1.93	2.0
4.37	1.25	1.36			1.36	8.7
5.90	0.89	1.09	1.93		1.09	22.5
6.20	0.85	1.05	1.60		1.05	24.4
7.25	0.71	0.95	0.89	8.24	0.89	25.1
7.62	0.69	0.93	0.73	8.23	0.73	6.3
7.80	0.64	0.92	0.67	8.21	0.67	5.9
7.95	0.60	0.91	0.63	8.20	0.63	3.6
8.05	0.57	0.90	0.60	8.18	0.60	5.3
8.20	0.47	0.89	0.56	8.18		-0.2
8.10	0.00	0.90	0.58	8.20		1.2
Mean	1.40	na	na	8.19	1.50	na
Std. Dev.	1.02	na	na	0.01	1.03	na
					Mean of absolute values of residuals	8.4
					Std. Dev. of absolute values of residuals	8.8
					Minimum of absolute values of residuals	0.2
					Maximum of absolute values of residuals	25.1
Kalicinite and mixed salt					Pearson Correlation Coefficient (Precision)	0.998
					Bias (Location)	0.00533
					Scale Differential	0.00009
					Imprecision (1 - r)	0.00232
					Deviance (Bias + Scale Diff. + Imprecision)	0.00773
					Accuracy = 1/(1 + Bias + Scale Diff.)	0.995
					Concordance (Accuracy * Precision)	0.992
K2CO3.1.5H2O Only					Pearson Correlation Coefficient (Precision)	-1.000
					Bias (Location)	2.46282
					Scale Differential	2.91406
					Imprecision (1 - r)	2.00000
					Deviance (Bias + Scale Diff. + Imprecision)	7.37688
					Accuracy = 1/(1 + Bias + Scale Diff.)	0.157
					Concordance (Accuracy * Precision)	-0.157



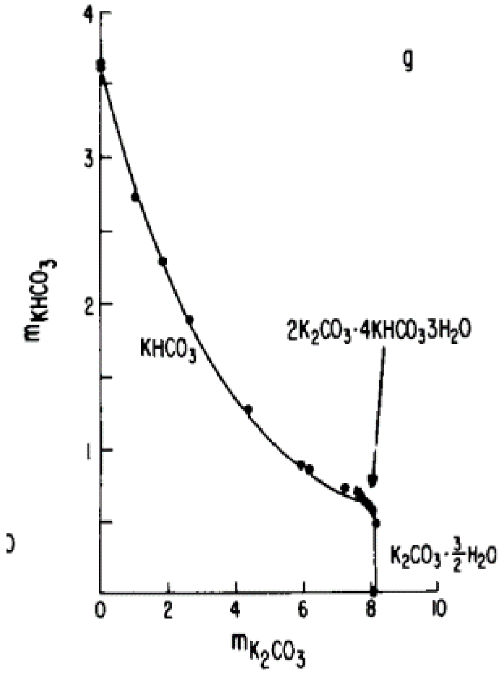


FIG. 9. Salt solubilities in potassium carbonate systems. Closed systems.

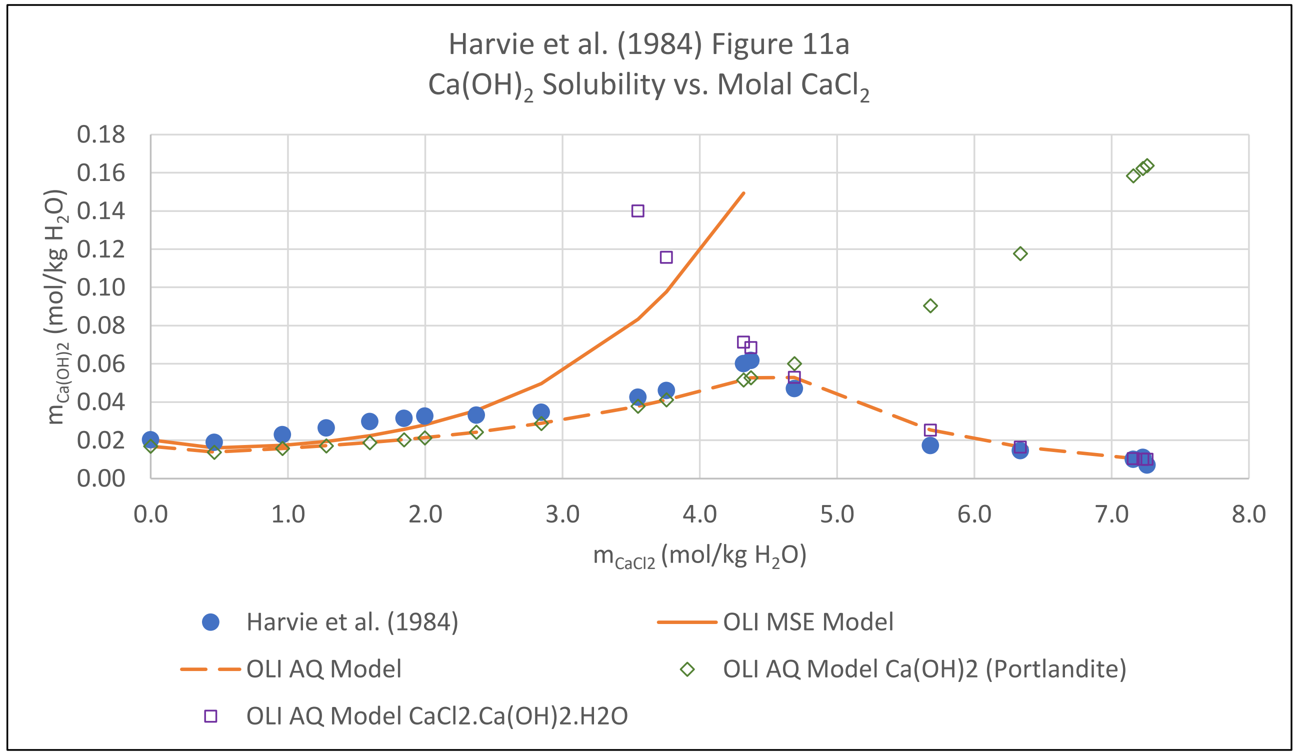
Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 11a

Harvie et al (1984)		OLI MSE Model*	Residual	OLI AQ Model*			Residual
m_{CaCl2} (mol/kg H_2O)	$m_{Ca(OH)2}$ (mol/kg H_2O)	$Ca(OH)_2$ (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)	$Ca(OH)_2$ (mol/kg H_2O)	$CaCl_2$.$Ca(OH)_2$.H_2O** (mol/kg H2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	0.020	0.020	-0.2	0.017		0.017	-16.9
0.46	0.019	0.016	-15.3	0.014	4.69	0.014	-26.9
0.96	0.023	0.017	-24.5	0.016	2.76	0.016	-31.7
1.28	0.026	0.019	-26.6	0.017	1.92	0.017	-35.2
1.60	0.030	0.022	-24.7	0.019	1.26	0.019	-37.0
1.85	0.031	0.026	-18.3	0.020	0.90	0.020	-35.5
2.00	0.033	0.028	-14.1	0.021	0.74	0.021	-34.8
2.37	0.033	0.036	7.0	0.024	0.47	0.024	-27.1
2.85	0.035	0.050	43.1	0.029	0.28	0.029	-16.8
3.55	0.042	0.083	96.1	0.038	0.14	0.038	-11.0
3.76	0.046	0.098	112.1	0.041	0.12	0.041	-10.7
4.32	0.060	0.15	148.8	0.05	0.071	0.052	-14.0
4.37	0.062	0.16	151.4	0.05	0.068	0.053	-14.6
4.69	0.047	0.20	**	0.06	0.053	0.053	12.3
5.68	0.017	0.40	**	0.09	0.025	0.025	46.7
6.34	0.015	0.61	**	0.12	0.016	0.016	12.5
7.16	0.010	0.97	**	0.16	0.010	0.010	4.5
7.23	0.011	1.01	**	0.16	0.010	0.010	-7.8
7.26	0.007	1.02	**	0.16	0.010	0.010	40.4
Mean	0.03	0.26	na	na	na	0.03	na
Std. Dev.	0.02	0.36	na	na	na	0.01	na
Mean of absolute values of residuals			52.5	Mean of absolute values of residuals			23.0
Std. Dev. of absolute values of residuals			54.5	Std. Dev. of absolute values of residuals			12.8
Minimum of absolute values of residuals			0.2	Minimum of absolute values of residuals			4.5
Maximum of absolute values of residuals			151.4	Maximum of absolute values of residuals			46.7
Pearson Correlation Coefficient (Precision)			-0.579	Pearson Correlation Coefficient (Precision)			0.931
Bias (Location)			4.77407	Bias (Location)			0.04232
Scale Differential			10.31680	Scale Differential			0.00434
Imprecision (1 - r)			1.57918	Imprecision (1 - r)			0.06911
Deviance (Bias + Scale Diff. + Imprecision)			16.67006	Deviance (Bias + Scale Diff. + Imprecision)			0.11576
Accuracy = 1/(1 + Bias + Scale Diff.)			0.062	Accuracy = 1/(1 + Bias + Scale Diff.)			0.955
Concordance (Accuracy * Precision)			-0.036	Concordance (Accuracy * Precision)			0.889

* $CaCl_2$.3$Ca(OH)_2$.13H_2O solid species is not included in either the OLI MSE or AQ databank.

** CaCl2.Ca(OH)2.H2O solid species is included in the OLI AQ databank but not the MSE databank.



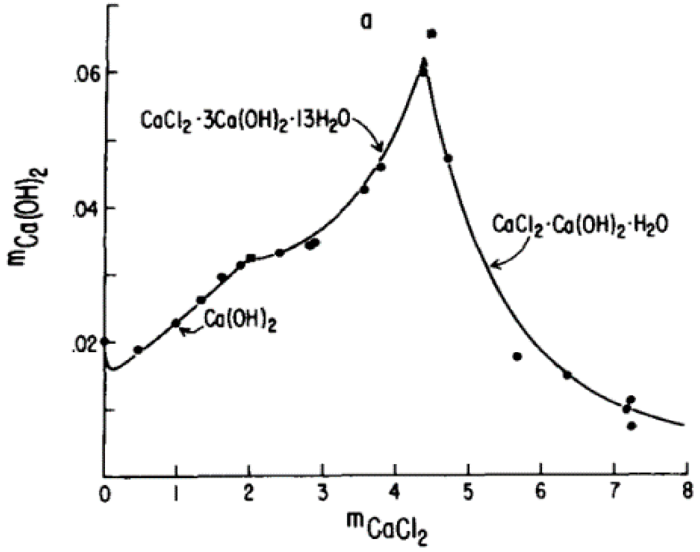


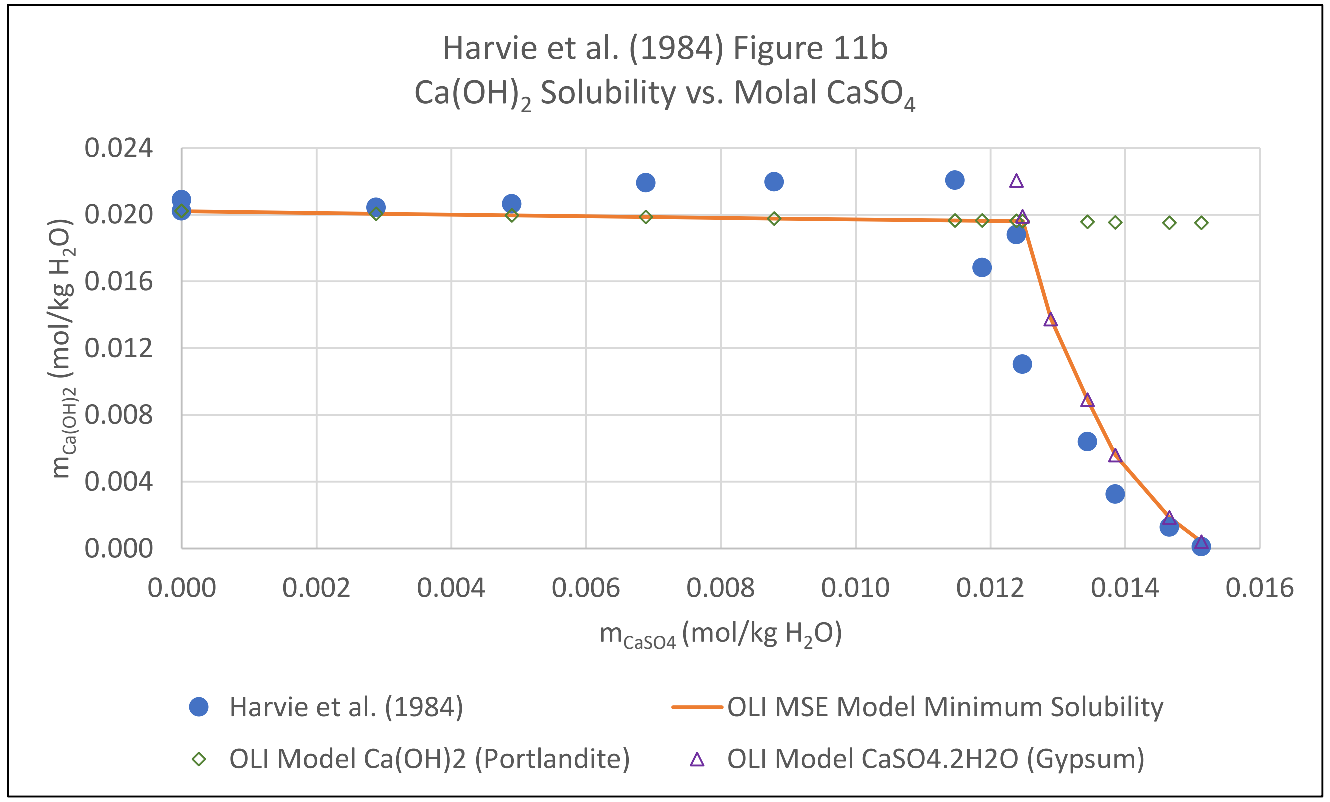
FIG. 11. $Ca(OH)_2$ salt solubilities in various salt solutions. In (a) and (b) solubility and emf data are used in parameterization. (c)–(f) are predicted using fully parameterized model.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 11b

Harvie et al (1984)		OLI Prediction			Residual
m_{CaSO4} (mol/kg H_2O)	$m_{Ca(OH)2}$ (mol/kg H_2O)	$Ca(OH)_2$ (mol/kg H_2O)	$CaSO_4.2H_2O$ (mol/kg H_2O)	Minimum Solubility (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00E+00	2.09E-02	0.0202		0.0202	-3.2
0.00E+00	2.02E-02	0.0202		0.0202	0.0
2.89E-03	2.04E-02	0.0201		0.0201	-1.9
4.90E-03	2.07E-02	0.0200		0.0200	-3.4
6.89E-03	2.19E-02	0.0199		0.0199	-9.4
8.79E-03	2.20E-02	0.0198		0.0198	-10.0
1.15E-02	2.21E-02	0.0197		0.0197	-10.9
1.19E-02	1.68E-02	0.0196		0.0196	16.7
1.24E-02	1.88E-02	0.0196	0.0220	0.0196	4.3
1.25E-02	1.10E-02	0.0196	0.0199	0.0196	77.8
1.29E-02			0.0137	0.0137	na
1.34E-02	6.40E-03	0.0196	8.92E-03	8.92E-03	39.3
1.39E-02	3.26E-03	0.0195	5.60E-03	5.60E-03	71.8
1.47E-02	1.27E-03	0.0195	1.86E-03	1.86E-03	45.8
1.51E-02	1.13E-04	0.0195	4.05E-04	4.05E-04	**
Mean	1.47E-02	na	na	1.53E-02	na
Std. Dev.	8.43E-03	na	na	7.31E-03	na
Mean of absolute values of residuals					22.7
Std. Dev. of absolute values of residuals					27.1
Minimum of absolute values of residuals					0.0
Maximum of absolute values of residuals					77.8
Pearson Correlation Coefficient (Precision)					0.943
Bias (Location)					0.00287
Scale Differential					0.01016
Imprecision (1 - r)					0.05687
Deviance (Bias + Scale Diff. + Imprecision)					0.06989
Accuracy = 1/(1 + Bias + Scale Diff.)					0.987
Concordance (Accuracy * Precision)					0.931

** Not included in residual calculations because of large uncertainty in digitized values located at x axis



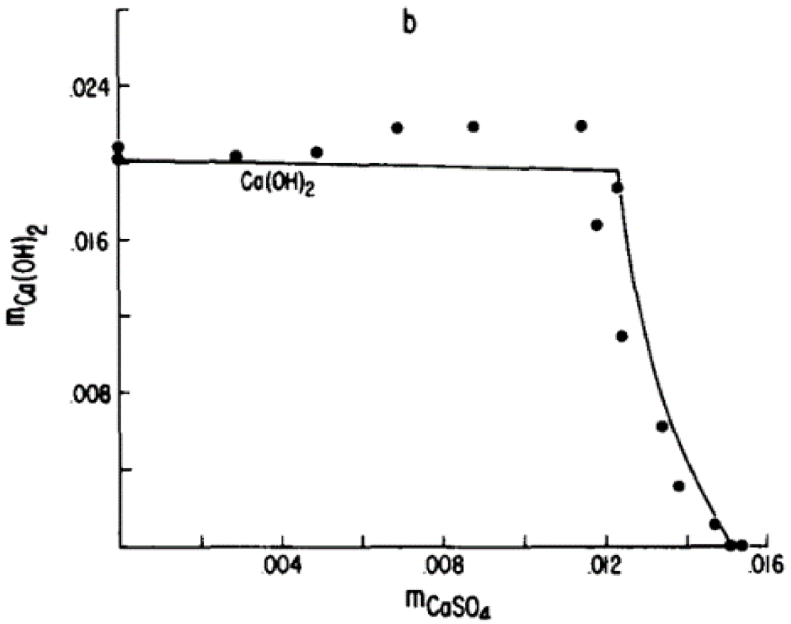
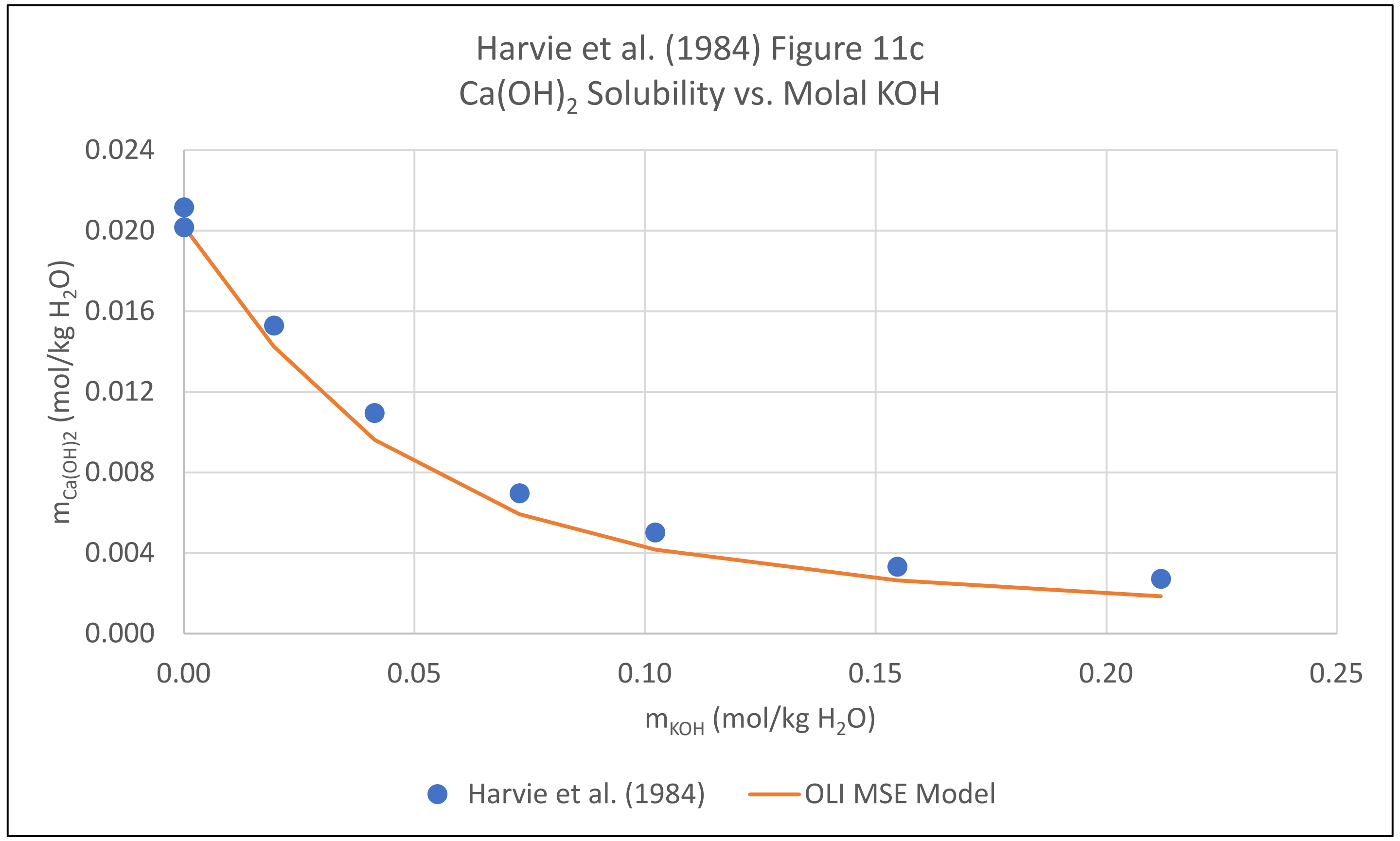


FIG. 11. $Ca(OH)_2$ salt solubilities in various salt solutions. In (a) and (b) solubility and emf data are used in parameterization. (c)–(f) are predicted using fully parameterized model.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 11c

Harvie et al (1984)		OLI Prediction	Residual
m_{KOH} (mol/kg H_2O)	$m_{Ca(OH)2}$ (mol/kg H_2O)	$Ca(OH)_2$ (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.0000	0.0212	0.0202	-4.4
0.0000	0.0202	0.0202	0.2
0.0195	0.0153	0.0143	-6.7
0.0413	0.0109	0.0096	-12.0
0.0728	0.0070	0.0059	-14.9
0.1022	0.0050	0.0042	-17.0
0.1547	0.0033	0.0026	-20.4
0.2118	0.0027	0.0019	-31.3
Mean	0.0107	0.0099	na
Std. Dev.	0.0074	0.0075	na
Mean of absolute values of residuals			13.4
Std. Dev. of absolute values of residuals			9.9
Minimum of absolute values of residuals			0.2
Maximum of absolute values of residuals			31.3
Pearson Correlation Coefficient (Precision)			0.999
Bias (Location)			0.00707
Scale Differential			0.00014
Imprecision (1 - r)			0.00129
Deviance (Bias + Scale Diff. + Imprecision)			0.00851
Accuracy = 1/(1 + Bias + Scale Diff.)			0.993
Concordance (Accuracy * Precision)			0.992



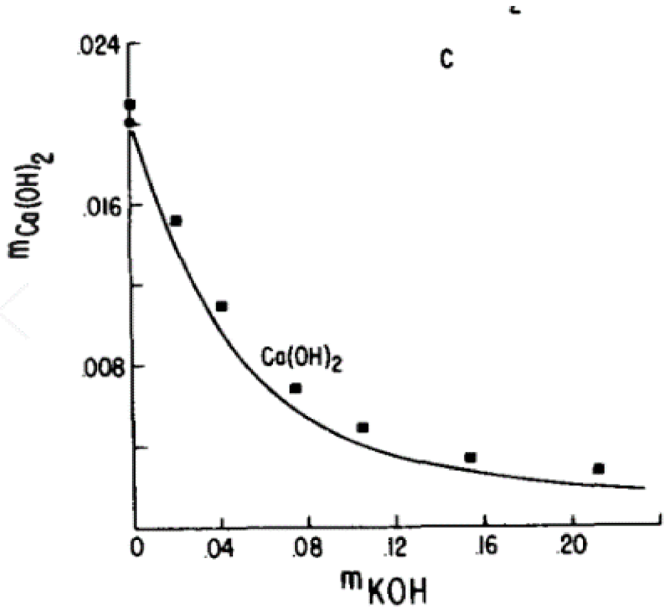
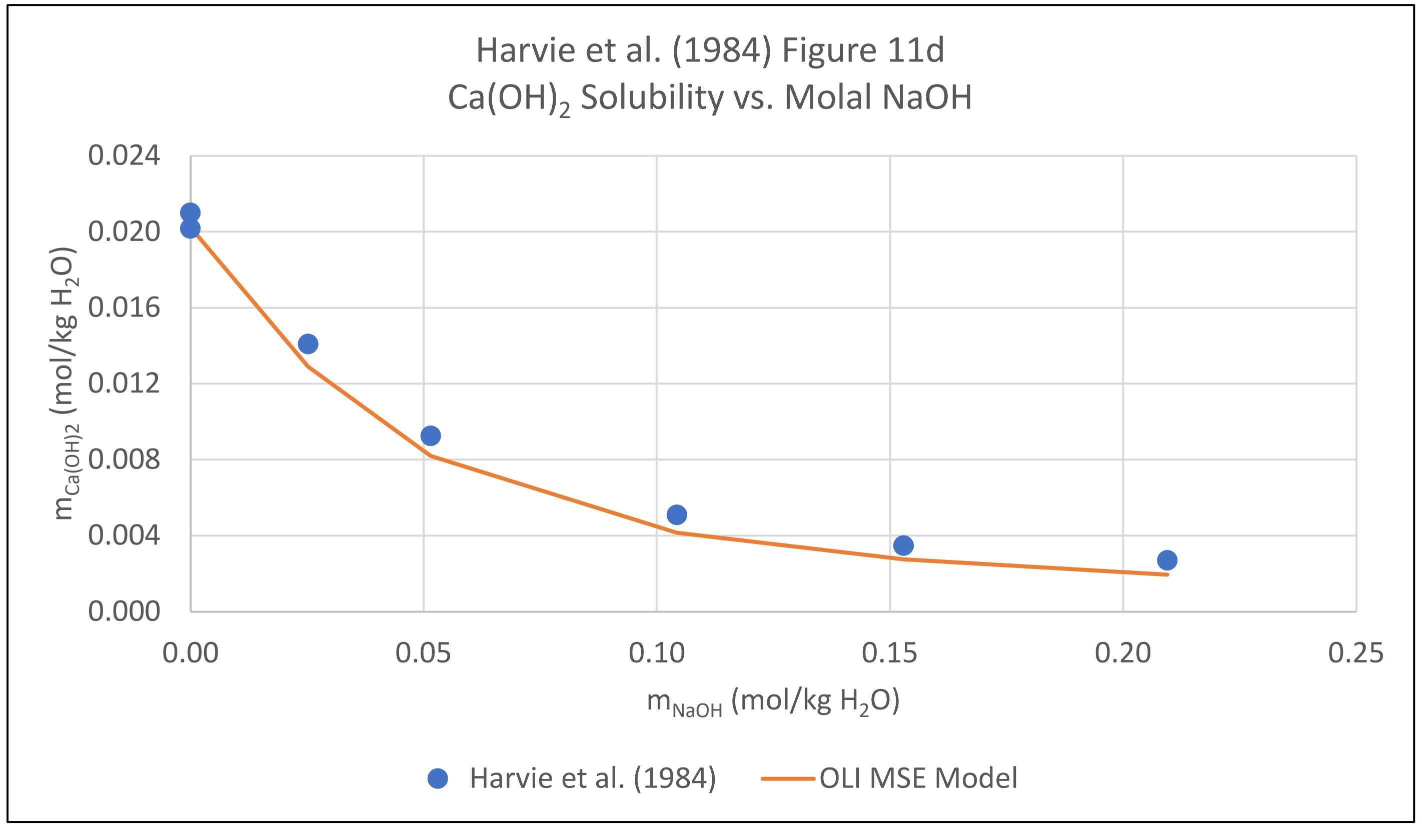


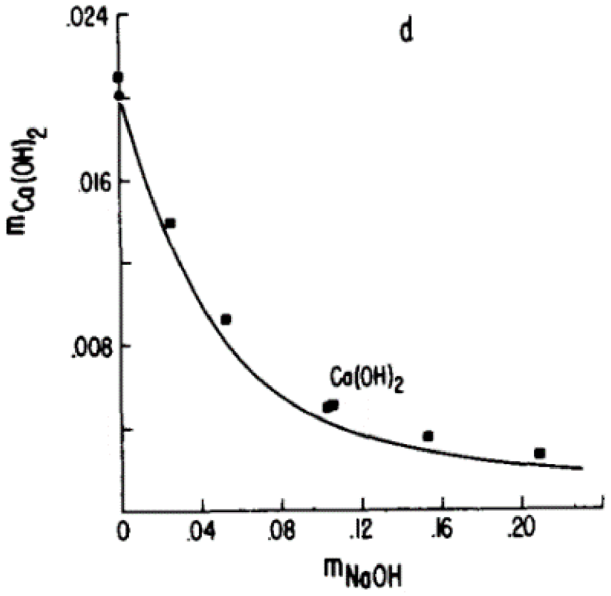
FIG. 11. $Ca(OH)_2$ salt solubilities in various salt solutions. In (a) and (b) solubility and emf data are used in parameterization. (c)–(f) are predicted using fully parameterized model.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 11d

Harvie et al (1984)		OLI Prediction	Residual
m_{NaOH} (mol/kg H_2O)	$m_{Ca(OH)2}$ (mol/kg H_2O)	$Ca(OH)_2$ (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.0000	0.0210	0.0202	-3.7
0.0000	0.0202	0.0202	0.2
0.0252	0.0141	0.0129	-8.5
0.0515	0.0092	0.0082	-11.5
0.1043	0.0051	0.0042	-18.5
0.1529	0.0035	0.0027	-20.7
0.2095	0.0027	0.0019	-28.0
Mean	0.011	0.010	na
Std. Dev.	0.008	0.008	na
Mean of absolute values of residuals			13.0
Std. Dev. of absolute values of residuals			9.9
Minimum of absolute values of residuals			0.2
Maximum of absolute values of residuals			28.0
Pearson Correlation Coefficient (Precision)			0.999
Bias (Location)			0.00571
Scale Differential			0.00023
Imprecision (1 - r)			0.00110
Deviance (Bias + Scale Diff. + Imprecision)			0.00703
Accuracy = 1/(1 + Bias + Scale Diff.)			0.994
Concordance (Accuracy * Precision)			0.993





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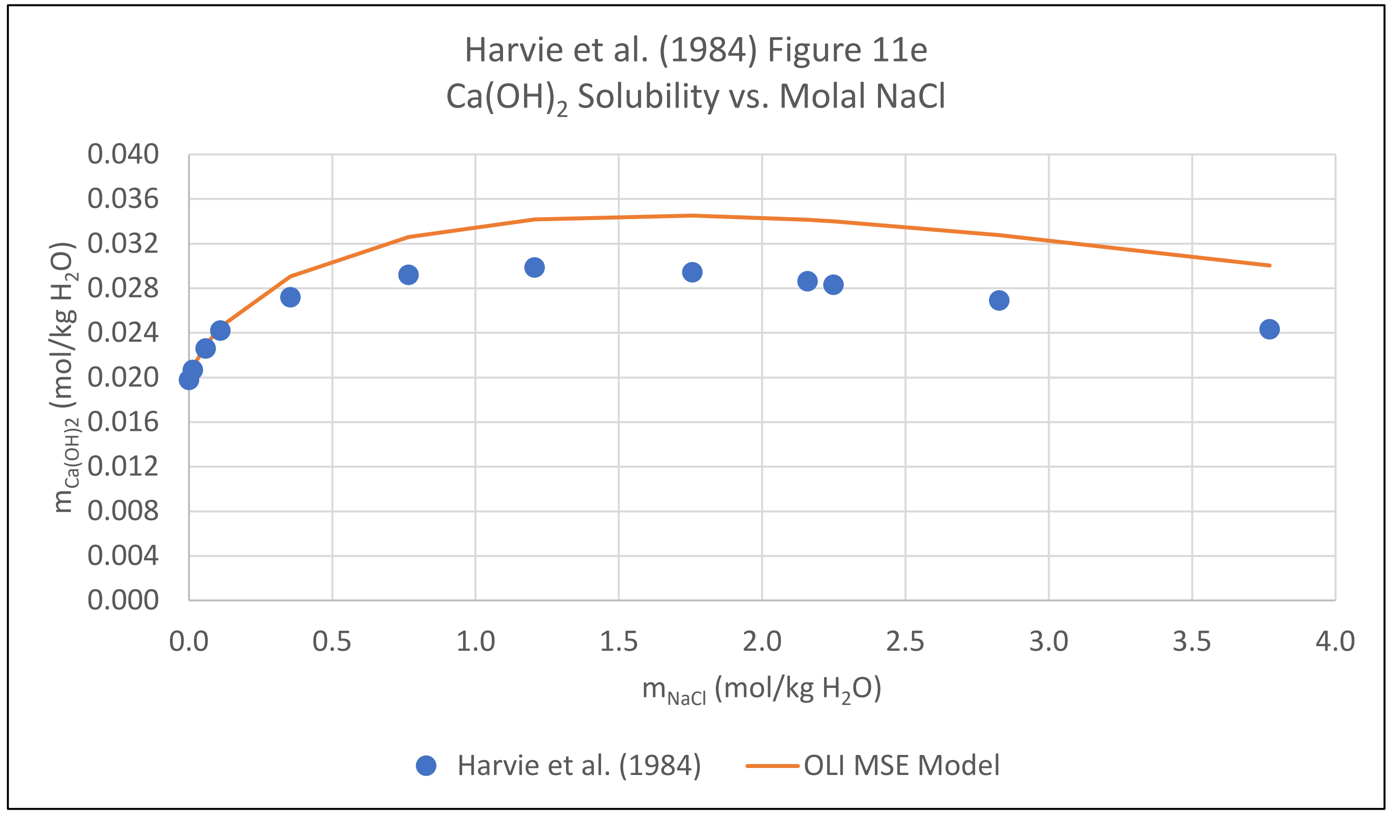
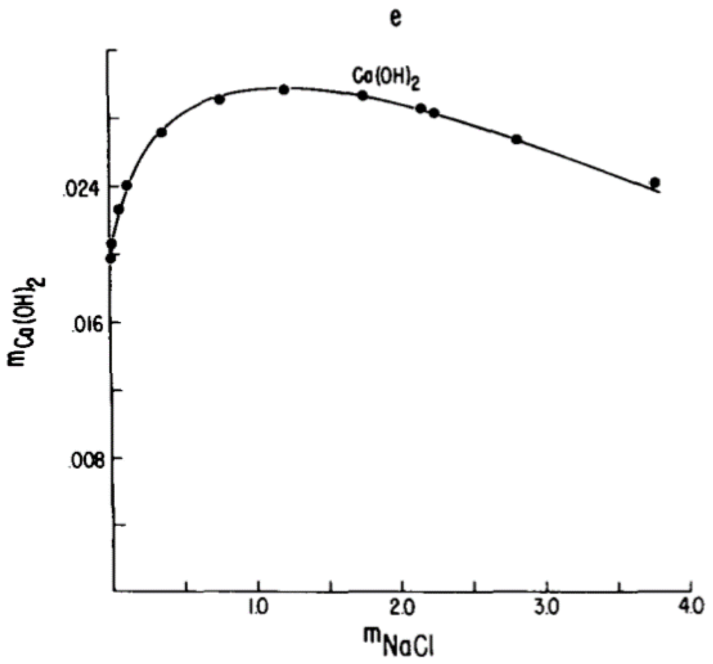
Harvie et al (1984) Figure 11e

Harvie et al (1984)		OLI Prediction	Residual
m_{NaCl} (mol/kg H_2O)	$m_{Ca(OH)2}$ (mol/kg H_2O)	$Ca(OH)_2$ (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.000	0.020	0.020	2.2
0.013	0.021	0.021	1.4
0.058	0.023	0.023	1.5
0.110	0.024	0.025	1.4
0.354	0.027	0.029	6.9
0.767	0.029	0.033	11.7
1.206	0.030	0.034	14.4
1.756	0.029	0.035	17.4
2.158	0.029	0.034	19.2
2.250	0.028	0.034	20.1
2.827	0.027	0.033	21.8
3.771	0.024	0.030	23.6
Mean	0.026	0.029	na
Std. Dev.	0.004	0.006	na
Mean of absolute values of residuals			11.8
Std. Dev. of absolute values of residuals			8.7
Minimum of absolute values of residuals			1.4
Maximum of absolute values of residuals			23.6
Pearson Correlation Coefficient (Precision)			0.953
Bias (Location)			0.29510
Scale Differential			0.10342
Imprecision (1 - r)			0.04686
Deviance (Bias + Scale Diff. + Imprecision)			0.44538
Accuracy = 1/(1 + Bias + Scale Diff.)			0.715
Concordance (Accuracy * Precision)			0.682





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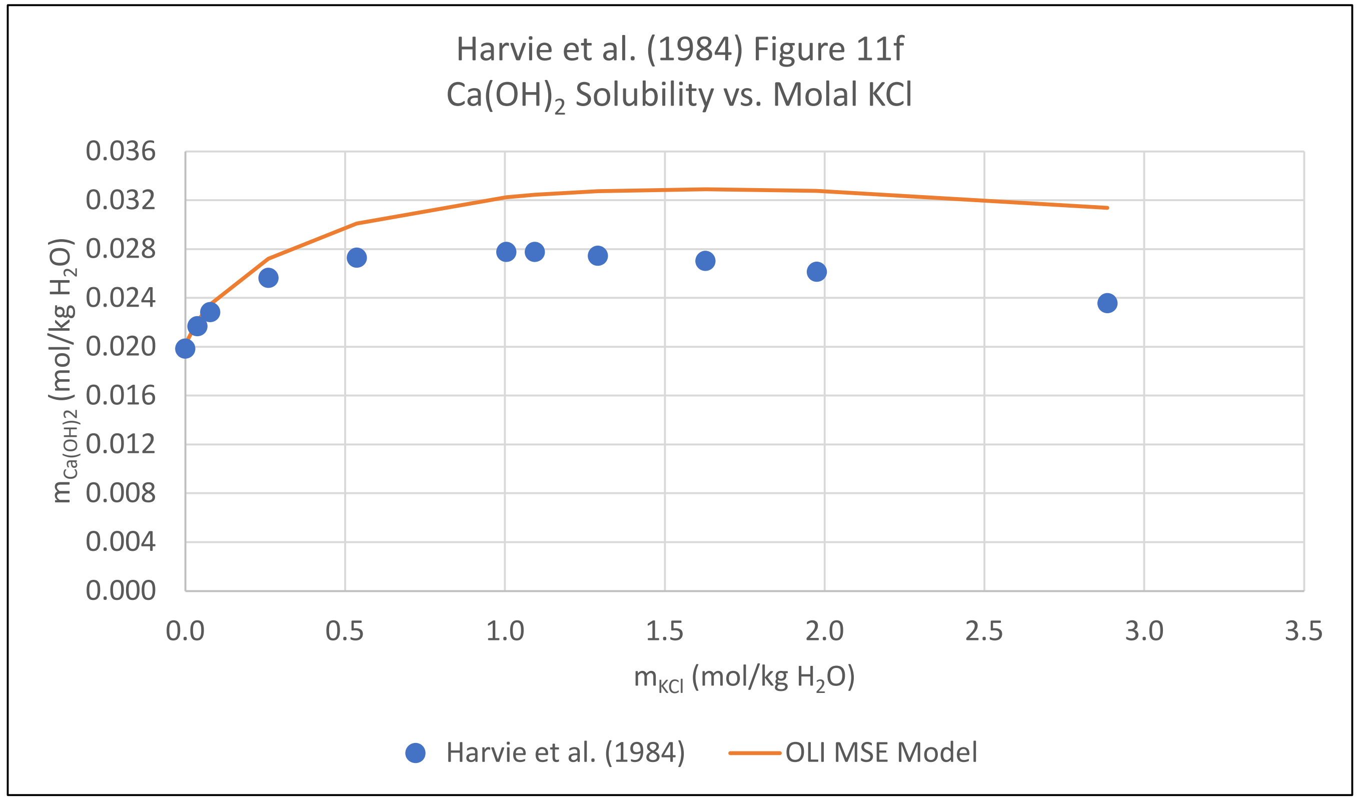
Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 11f

Harvie et al (1984)		OLI Prediction	Residual
m_{KCl} (mol/kg H_2O)	$m_{Ca(OH)2}$ (mol/kg H_2O)	$Ca(OH)_2$ (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.000	0.020	0.020	1.9
0.038	0.022	0.022	1.8
0.078	0.023	0.023	2.7
0.260	0.026	0.027	6.0
0.537	0.027	0.030	10.2
1.004	0.028	0.032	16.0
1.094	0.028	0.032	16.8
1.290	0.027	0.033	19.2
1.627	0.027	0.033	21.8
1.976	0.026	0.033	25.2
2.885	0.024	0.031	33.1
Mean	0.025	0.029	na
Std. Dev.	0.003	0.005	na
Mean of absolute values of residuals			14.0
Std. Dev. of absolute values of residuals			10.5
Minimum of absolute values of residuals			1.8
Maximum of absolute values of residuals			33.1
Pearson Correlation Coefficient (Precision)			0.890
Bias (Location)			0.55540
Scale Differential			0.15654
Imprecision (1 - r)			0.11034
Deviance (Bias + Scale Diff. + Imprecision)			0.82228
Accuracy = 1/(1 + Bias + Scale Diff.)			0.584
Concordance (Accuracy * Precision)			0.520



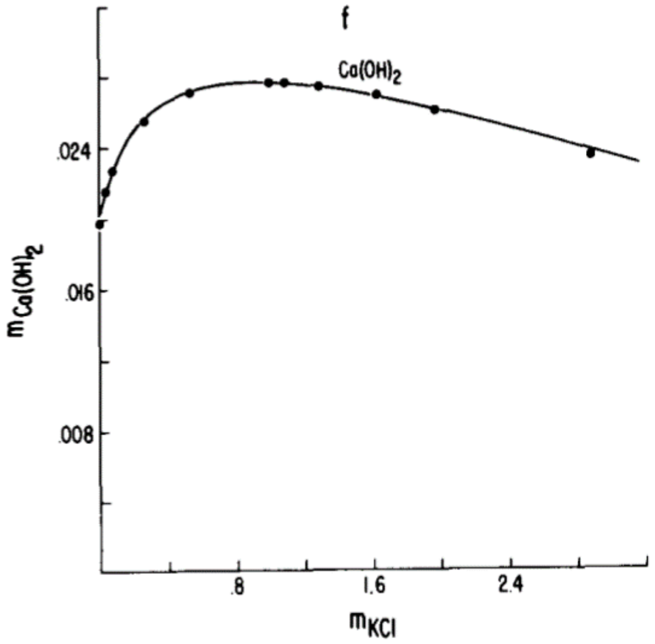


FIG. 11. $Ca(OH)_2$ salt solubilities in various salt solutions. In (a) and (b) solubility and emf data are used in parameterization. (c)–(f) are predicted using fully parameterized model.

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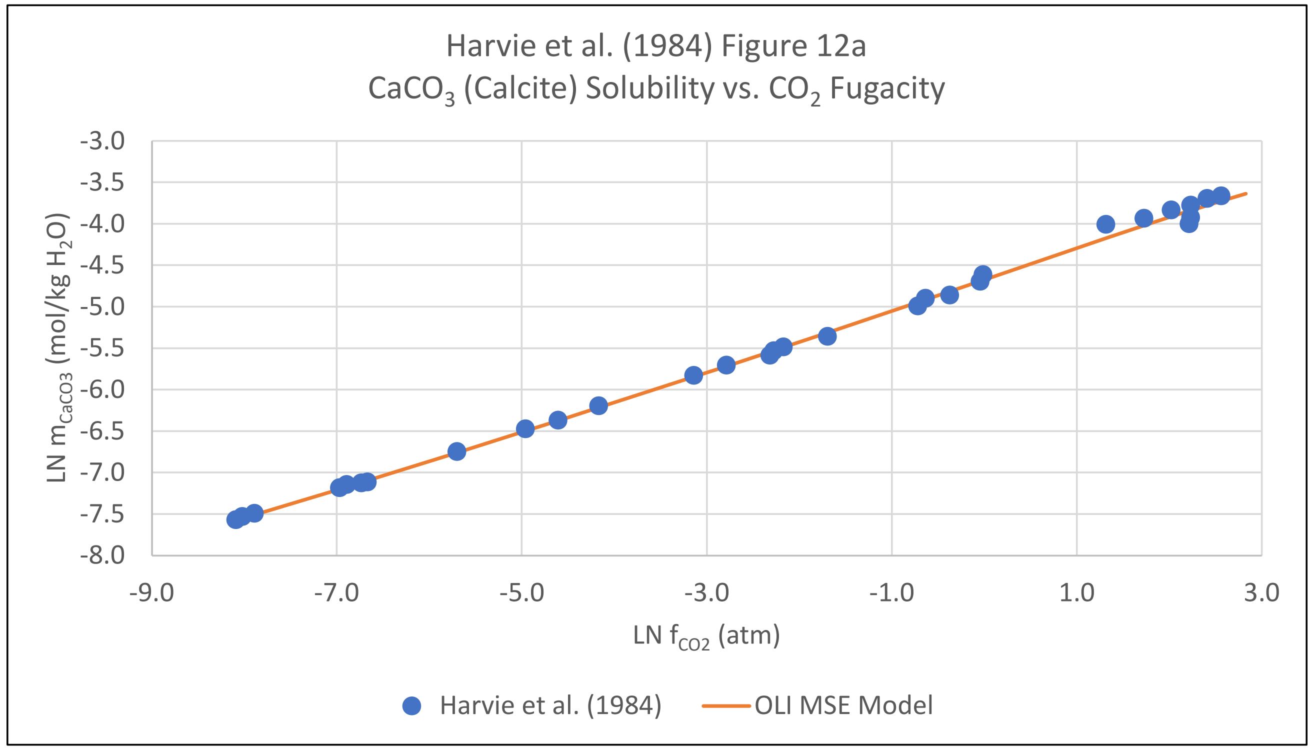
Harvie et al (1984) Figure 12a

Harvie et al (1984)		OLI Prediction					Residual
LN f_{CO2}	LN m_{CaCO3} (mol/kg H_2O)	Assumed P_{total} (atm)	f_{CO2} (atm)	LN f_{CO2}	$CaCO_3$ (Calcite) (mol/kg H_2O)	LN m_{CaCO3} (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
-8.0934	-7.5684	1.0	3.08E-04	-8.0852	5.13E-04	-7.5759	0.1
-8.0261	-7.5286	1.0	3.28E-04	-8.0227	5.23E-04	-7.5551	0.4
-7.8914	-7.4888	1.0	3.68E-04	-7.9083	5.44E-04	-7.5170	0.4
-6.9738	-7.1833	1.0	9.34E-04	-6.9759	7.45E-04	-7.2017	0.3
-6.8980	-7.1435	1.0	1.00E-03	-6.9041	7.64E-04	-7.1771	0.5
-6.7380	-7.1234	1.0	1.18E-03	-6.7400	8.08E-04	-7.1208	0.0
-6.6706	-7.1101	1.0	1.26E-03	-6.6750	8.26E-04	-7.0985	-0.2
-5.7026	-6.7450	1.0	3.32E-03	-5.7080	1.16E-03	-6.7628	0.3
-4.9619	-6.4728	1.0	6.96E-03	-4.9681	1.50E-03	-6.5022	0.5
-4.6082	-6.3665	1.0	9.91E-03	-4.6144	1.70E-03	-6.3767	0.2
-4.1706	-6.1939	1.0	1.53E-02	-4.1770	1.99E-03	-6.2204	0.4
-3.1436	-5.8287	1.0	4.29E-02	-3.1497	2.88E-03	-5.8494	0.4
-2.7900	-5.7025	1.0	6.10E-02	-2.7961	3.28E-03	-5.7203	0.3
-2.3185	-5.5829	1.0	9.78E-02	-2.3245	3.90E-03	-5.5471	-0.6
-2.2765	-5.5299	1.0	1.02E-01	-2.2826	3.96E-03	-5.5316	0.0
-2.1755	-5.4834	1.0	1.13E-01	-2.1815	4.11E-03	-5.4943	0.2
-1.6956	-5.3551	1.0	1.82E-01	-1.7015	4.91E-03	-5.3162	-0.7
-0.7204	-4.9895	1.0	4.84E-01	-0.7258	7.08E-03	-4.9503	-0.8
-0.6364	-4.8964	1.0	5.26E-01	-0.6417	7.31E-03	-4.9186	0.5
-0.3757	-4.8565	1.0	6.83E-01	-0.3809	8.07E-03	-4.8199	-0.8
-0.0479	-4.6903	1.0	9.48E-01	-0.0529	9.14E-03	-4.6954	0.1
-0.0143	-4.6105	1.038	1.00E+00	0.0001	9.32E-03	-4.6758	1.4
1.3138	-4.0055	3.916	3.80E+00	1.3359	1.55E-02	-4.1681	4.1
1.7259	-3.9324	5.913	5.70E+00	1.7404	1.80E-02	-4.0173	2.2
2.0201	-3.8327	7.936	7.58E+00	2.0256	2.00E-02	-3.9133	2.1
2.2137	-3.9989	9.631	9.12E+00	2.2110	2.13E-02	-3.8470	-3.8
2.2303	-3.7729	9.792	9.27E+00	2.2268	2.15E-02	-3.8414	1.8
2.2304	-3.9191	9.793	9.27E+00	2.2269	2.15E-02	-3.8413	-2.0
2.4068	-3.6931	11.683	1.10E+01	2.3940	2.28E-02	-3.7829	2.4
2.5582	-3.6598	13.592	1.26E+01	2.5356	2.39E-02	-3.7344	2.0
2.8779	-3.7862	18.713	1.69E+01	2.8283	2.63E-02	-3.6378	-3.9
Mean	-5.45	na	na	na	na	-5.46	na
Std. Dev.	1.34	na	na	na	na	1.34	na
Mean of absolute values of residuals							1.1
Std. Dev. of absolute values of residuals							1.2
Minimum of absolute values of residuals							0.0
Maximum of absolute values of residuals							4.1
Pearson Correlation Coefficient (Precision)							0.999
Bias (Location)							0.00004
Scale Differential							0.00000
Imprecision (1 - r)							0.00112
Deviance (Bias + Scale Diff. + Imprecision)							0.00116
Accuracy = 1/(1 + Bias + Scale Diff.)							1.000
Concordance (Accuracy * Precision)							0.999



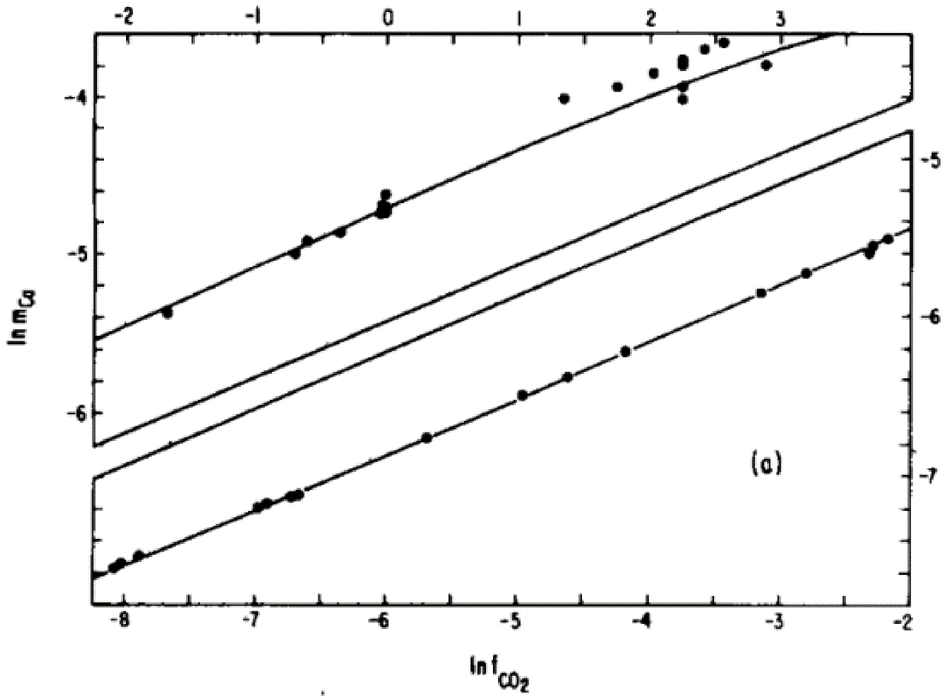


FIG. 12. The solubility of calcite in water (a) and the predicted solubilities of calcite in NaCl solutions (b)–(f).

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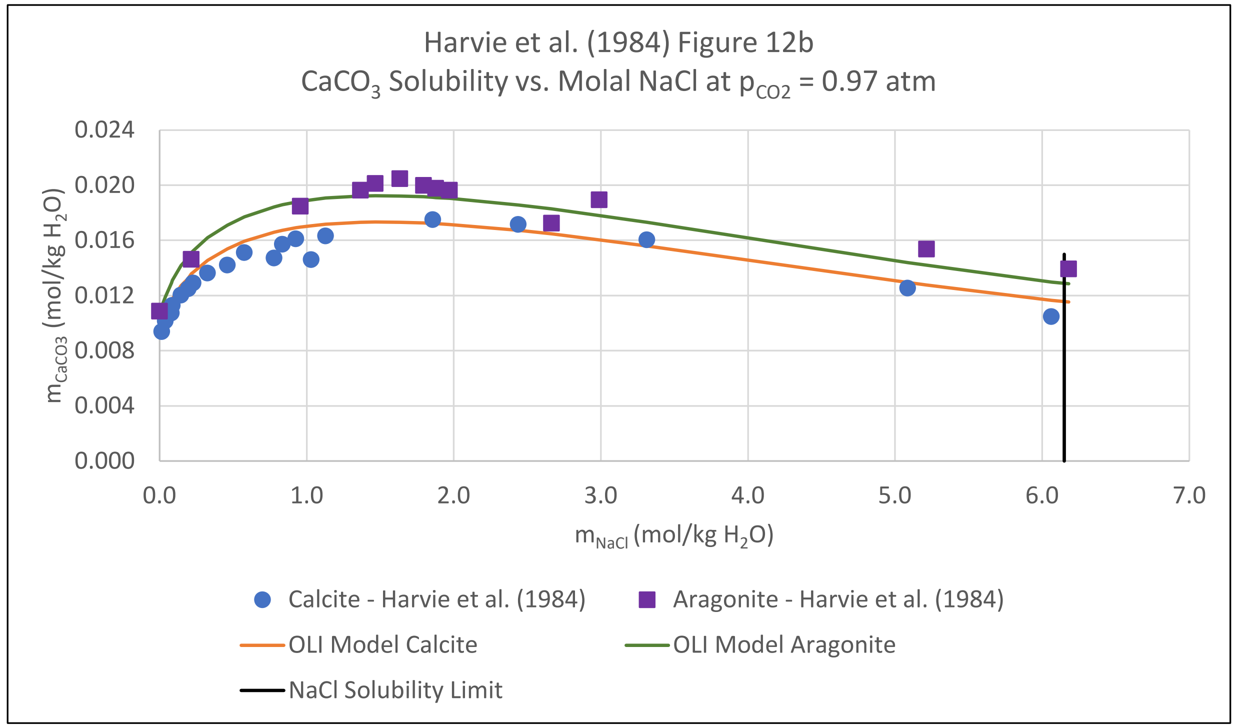
Harvie et al (1984) Figure 12b

Harvie et al (1984)			OLI Prediction			Residual
m_{NaCl} (mol/kg H_2O)	m_{Ca} (mol/kg H_2O) Calcite	m_{Ca} (mol/kg H_2O) Aragonite	$CaCO_3$ (Calcite) (mol/kg H_2O)	$CaCO_3$ (Argonite) (mol/kg H_2O)	NaCl (Halite) (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00		0.011	0.0092	0.0104		-4.6
0.02	0.009		0.0100	0.0112		6.8
0.04	0.010		0.0106	0.0119		4.9
0.08	0.011		0.0116	0.0129		7.7
0.09	0.011		0.0118	0.0131		4.1
0.15	0.012		0.0127	0.0142		5.8
0.19	0.012		0.0132	0.0147		6.0
0.22		0.015	0.0136	0.0151		3.3
0.23	0.013		0.0137	0.0152		5.9
0.33	0.014		0.0146	0.0162		6.7
0.46	0.014		0.0154	0.0171		8.3
0.58	0.015		0.0159	0.0177		5.4
0.78	0.015		0.0166	0.0184		12.6
0.84	0.016		0.0167	0.0186		6.4
0.93	0.016		0.0169	0.0188		4.9
0.96		0.018	0.0170	0.0188		1.8
1.03	0.015		0.0171	0.0189		16.8
1.13	0.016		0.0172	0.0191		5.2
1.37		0.020	0.0173	0.0192		-2.2
1.47		0.020	0.0173	0.0192		-4.5
1.63		0.020	0.0173	0.0192		-6.1
1.79		0.020	0.0173	0.0192		-4.1
1.86	0.018		0.0172	0.0191		-1.6
1.88		0.020	0.0172	0.0191		-3.4
1.97		0.020	0.0172	0.0190		-3.1
2.44	0.017		0.0167	0.0186		-2.5
2.66		0.017	0.0165	0.0183		5.9
2.99		0.019	0.0160	0.0178		-6.0
3.31	0.016		0.0156	0.0173		-2.9
5.09	0.013		0.0129	0.0144		3.2
5.21		0.015	0.0128	0.0142		-7.6
6.06	0.010		0.0116	0.0130		11.1
6.18		0.014	0.0115	0.0129	NaCl PPT	-7.7
6.15				0.0000	NaCl PPT	na
6.15				0.0150	NaCl PPT	na
Mean	0.0137	0.0176	0.0144	0.0171	na	na
Std. Dev.	0.0025	0.0030	0.0024	0.0030	na	na
Mean of absolute values of residuals						5.7
Std. Dev. of absolute values of residuals						3.2
Minimum of absolute values of residuals						1.6
Maximum of absolute values of residuals						16.8
Pearson Correlation Coefficient (Precision)			0.961	0.972		
Bias (Location)			0.04902	0.01615		
Scale Differential			0.00009	0.00007		
Imprecision (1 - r)			0.03873	0.02799		
Deviance (Bias + Scale Diff. + Imprecision)			0.08784	0.04421		
Accuracy = 1/(1 + Bias + Scale Diff.)			0.953	0.984		
Concordance (Accuracy * Precision)			0.916	0.956		



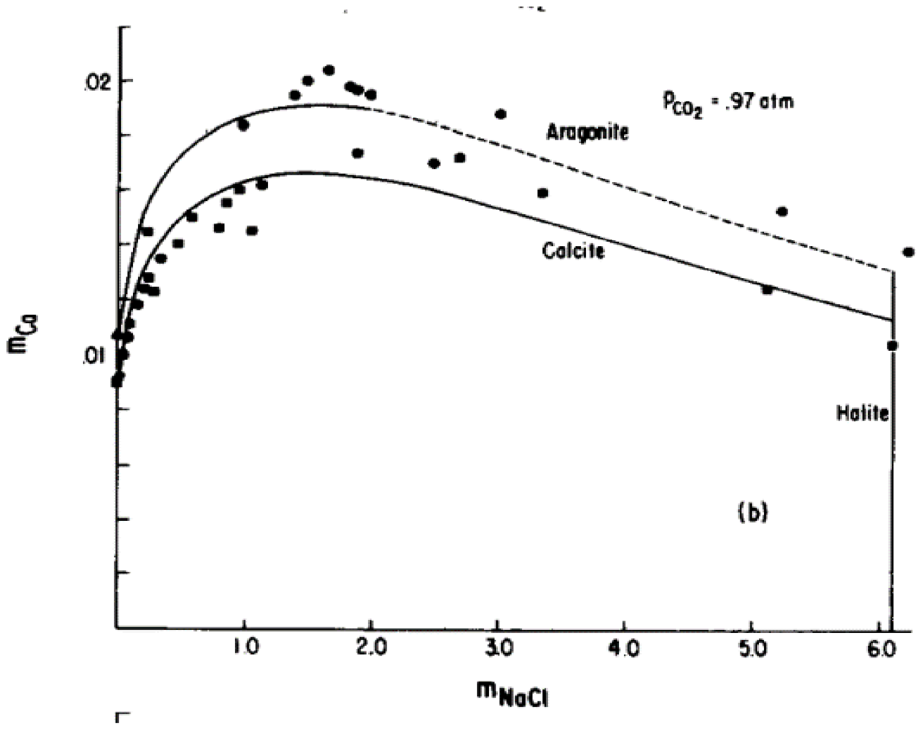


FIG. 12. The solubility of calcite in water (a) and the predicted solubilities of calcite in NaCl solutions (b)–(f).

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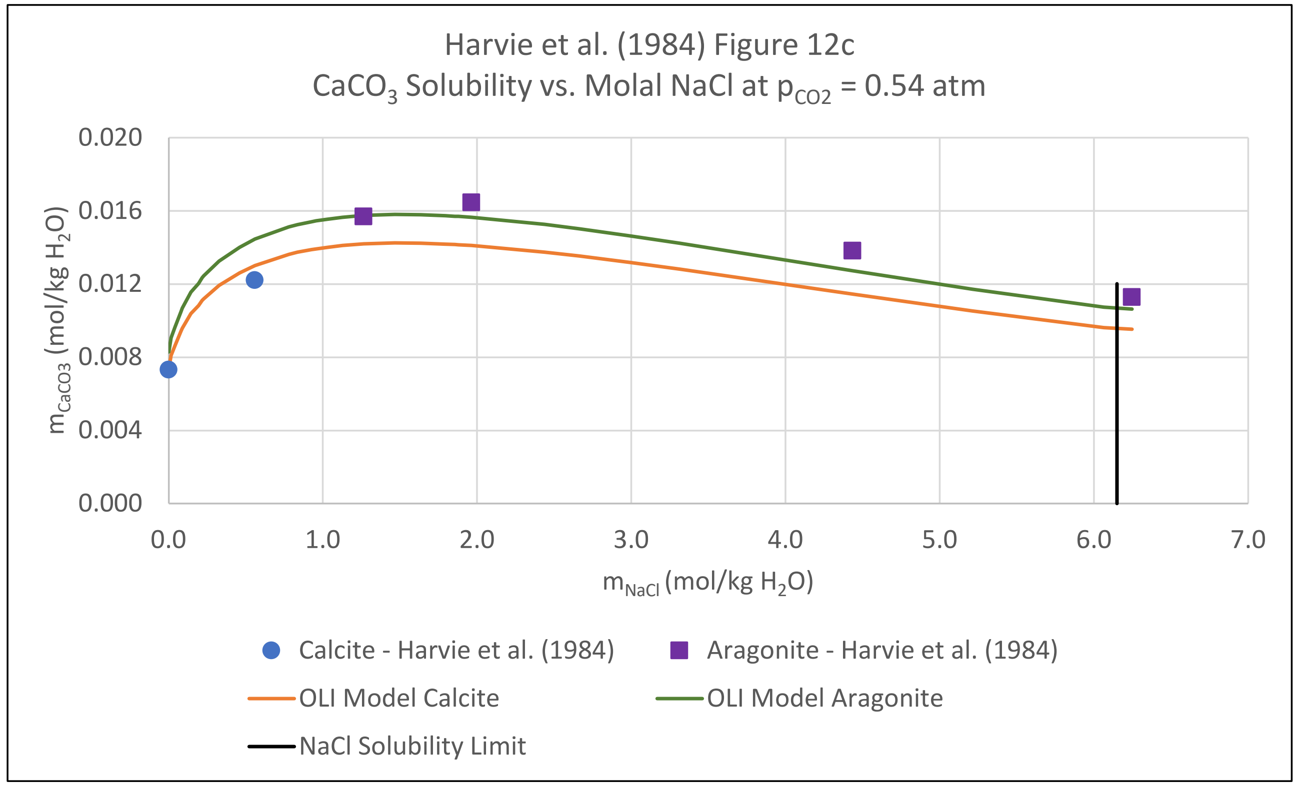
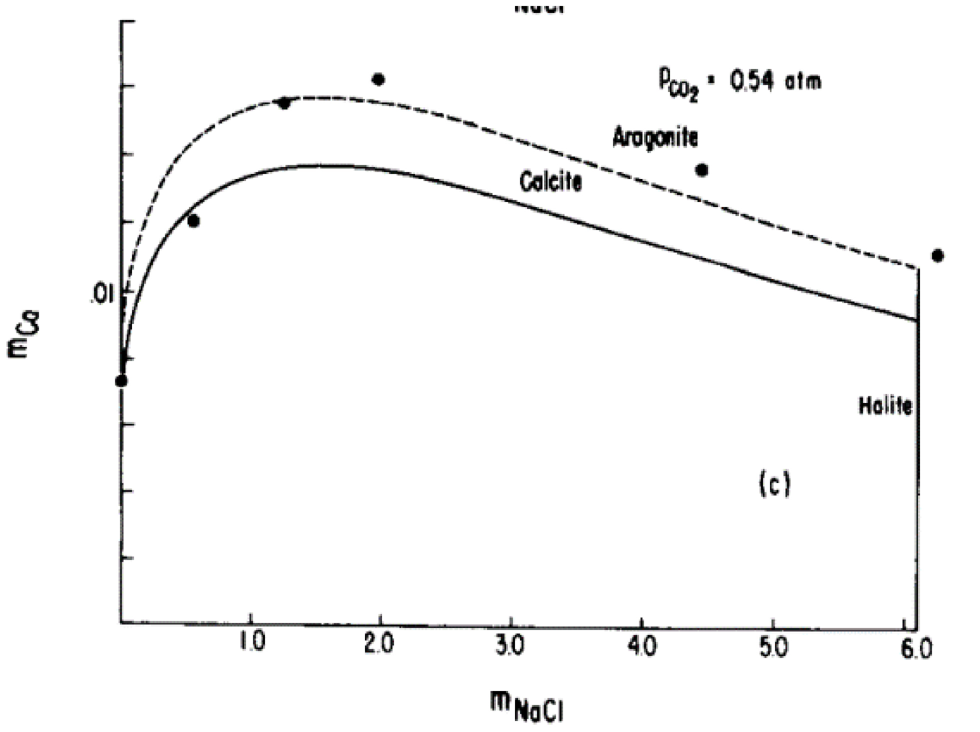
Harvie et al (1984) Figure 12c

Harvie et al (1984)			OLI Prediction			Residual
m_{NaCl} (mol/kg H_2O)	m_{Ca} (mol/kg H_2O) Calcite	m_{Ca} (mol/kg H_2O) Aragonite	$CaCO_3$ (Calcite) (mol/kg H_2O)	$CaCO_3$ (Argonite) (mol/kg H_2O)	NaCl (Halite) (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	0.0073		0.0074	0.0083		0.8
0.02			0.0081	0.0091		na
0.04			0.0086	0.0096		na
0.08			0.0094	0.0105		na
0.09			0.0096	0.0107		na
0.15			0.0104	0.0116		na
0.19			0.0108	0.0120		na
0.22			0.0111	0.0123		na
0.23			0.0112	0.0124		na
0.33			0.0119	0.0133		na
0.46			0.0126	0.0140		na
0.56	0.012		0.0130	0.0145		6.7
0.78			0.0136	0.0151		na
0.84			0.0137	0.0152		na
0.93			0.0139	0.0154		na
0.96			0.0139	0.0155		na
1.03			0.0140	0.0156		na
1.13			0.0141	0.0157		na
1.27		0.0157	0.0142	0.0158		0.5
1.47			0.0142	0.0158		na
1.63			0.0142	0.0158		na
1.79			0.0142	0.0157		na
1.86			0.0142	0.0157		na
1.88			0.0141	0.0157		na
1.96		0.0164	0.0141	0.0157		-4.8
2.44			0.0137	0.0153		na
2.66			0.0135	0.0150		na
2.99			0.0132	0.0146		na
3.31			0.0128	0.0142		na
4.43		0.014	0.0115	0.0127		-7.8
5.21			0.0105	0.0117		na
6.06			0.0096	0.0107		na
6.25		0.011	0.0095	0.01063	NaCl PPT	-5.7
6.15				0.0000	NaCl PPT	na
6.15				0.0120	NaCl PPT	na
Mean	0.0097	0.0143	0.0102	0.0137	na	na
Std. Dev.	0.0035	0.0023	0.0040	0.0025	na	na
Mean of absolute values of residuals						4.4
Std. Dev. of absolute values of residuals						3.1
Minimum of absolute values of residuals						0.5
Maximum of absolute values of residuals						7.8
Pearson Correlation Coefficient (Precision)			1.000	0.981		
Bias (Location)			0.01404	0.04347		
Scale Differential			0.01056	0.00260		
Imprecision (1 - r)			0.00000	0.01853		
Deviance (Bias + Scale Diff. + Imprecision)			0.02459	0.06459		
Accuracy = 1/(1 + Bias + Scale Diff.)			0.976	0.956		
Concordance (Accuracy * Precision)			0.976	0.938		





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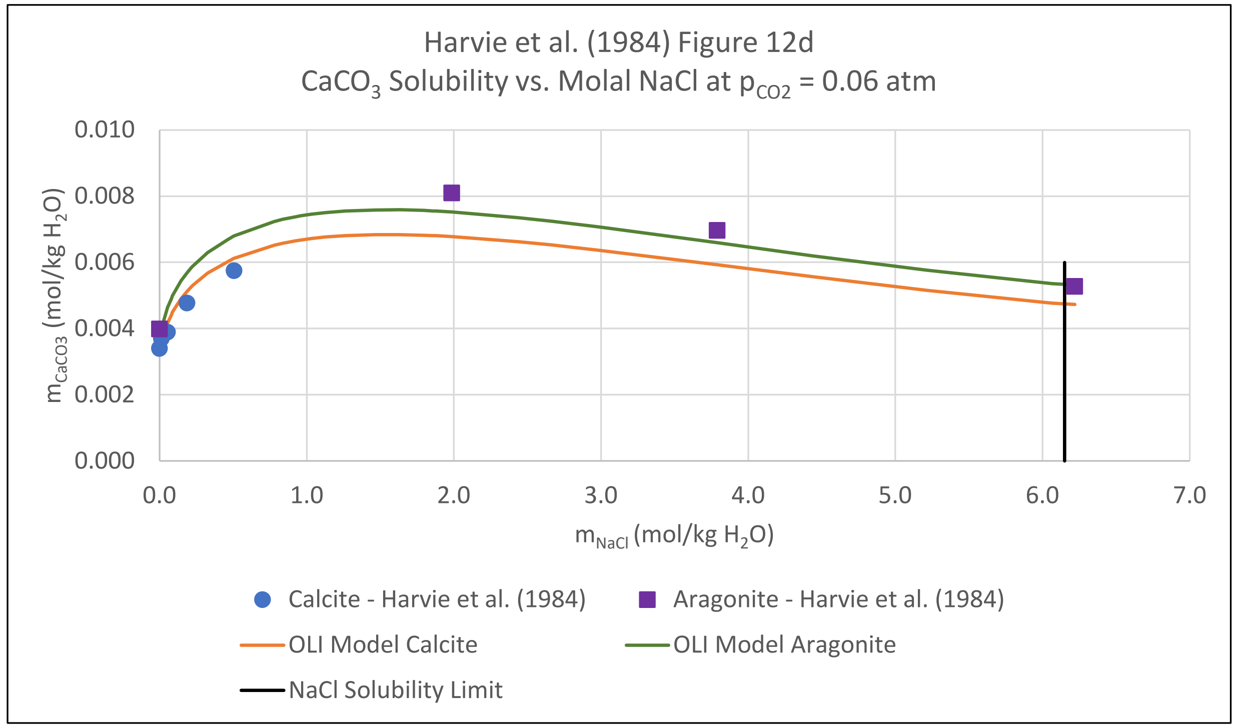
Harvie et al (1984) Figure 12d

Harvie et al (1984)			OLI Prediction			Residual
m_{NaCl} (mol/kg H_2O)	m_{Ca} (mol/kg H_2O) Calcite	m_{Ca} (mol/kg H_2O) Aragonite	$CaCO_3$ (Calcite) (mol/kg H_2O)	$CaCO_3$ (Argonite) (mol/kg H_2O)	NaCl (Halite) (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00	0.0034		0.0033			-4.2
0.00		0.004		0.0036		-8.8
0.014	0.0037		0.0036	0.0040		-2.6
0.055	0.0039		0.0042	0.0046		7.1
0.08			0.0044	0.0049		na
0.09			0.0045	0.0050		na
0.15			0.0049	0.0054		na
0.19	0.005		0.0051	0.0057		7.2
0.22			0.0053	0.0058		na
0.23			0.0053	0.0059		na
0.33			0.0057	0.0063		na
0.46			0.0060	0.0067		na
0.51	0.006		0.0061	0.0068		6.6
0.78			0.0065	0.0072		na
0.84			0.0066	0.0073		na
0.93			0.0067	0.0074		na
0.96			0.0067	0.0074		na
1.03			0.0067	0.0075		na
1.13			0.0068	0.0075		na
1.27			0.0068	0.0076		na
1.47			0.0068	0.0076		na
1.63			0.0068	0.0076		na
1.79			0.0068	0.0076		na
1.86			0.0068	0.0076		na
1.88			0.0068	0.0075		na
1.99		0.0081	0.0068	0.0075		-7.2
2.44			0.0066	0.0074		na
2.66			0.0065	0.0072		na
2.99			0.0064	0.0071		na
3.79		0.007	0.0059	0.0066		-5.4
4.43			0.0056	0.0062		na
5.21			0.0052	0.0058		na
6.06			0.0048	0.0054		na
6.22		0.005	0.0047	0.00532	NaCl PPT	0.9
6.15				0.0000	NaCl PPT	na
6.15				0.0060	NaCl PPT	na
Mean	0.0043	0.0061	0.0045	0.0058	na	na
Std. Dev.	0.0010	0.0018	0.0012	0.0017	na	na
Mean of absolute values of residuals						5.5
Std. Dev. of absolute values of residuals						2.5
Minimum of absolute values of residuals						0.9
Maximum of absolute values of residuals						8.8
Pearson Correlation Coefficient (Precision)			0.992	0.992		
Bias (Location)			0.01289	0.02174		
Scale Differential			0.02052	0.00295		
Imprecision (1 - r)			0.00761	0.00825		
Deviance (Bias + Scale Diff. + Imprecision)			0.04102	0.03294		
Accuracy = 1/(1 + Bias + Scale Diff.)			0.968	0.976		
Concordance (Accuracy * Precision)			0.960	0.968		



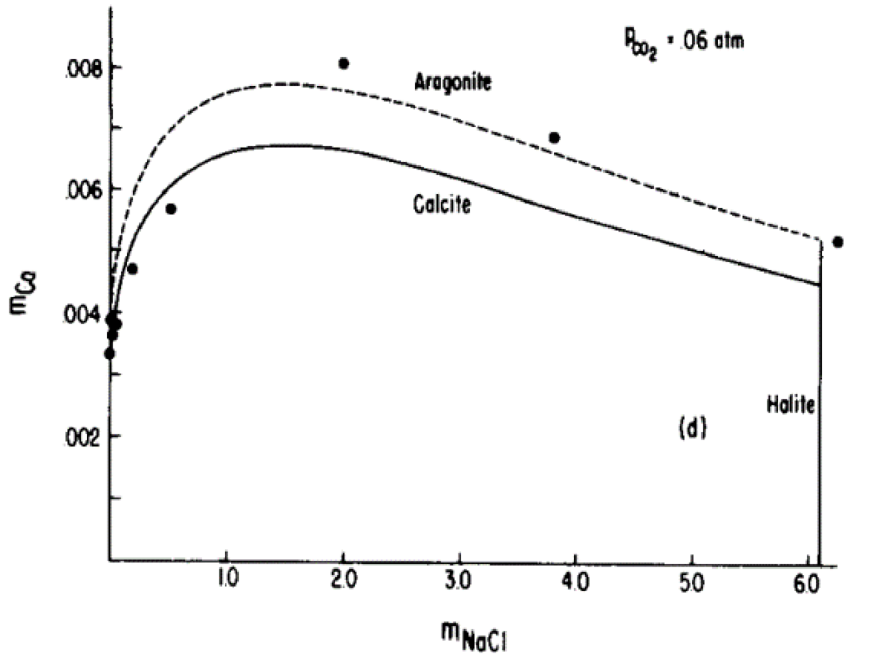
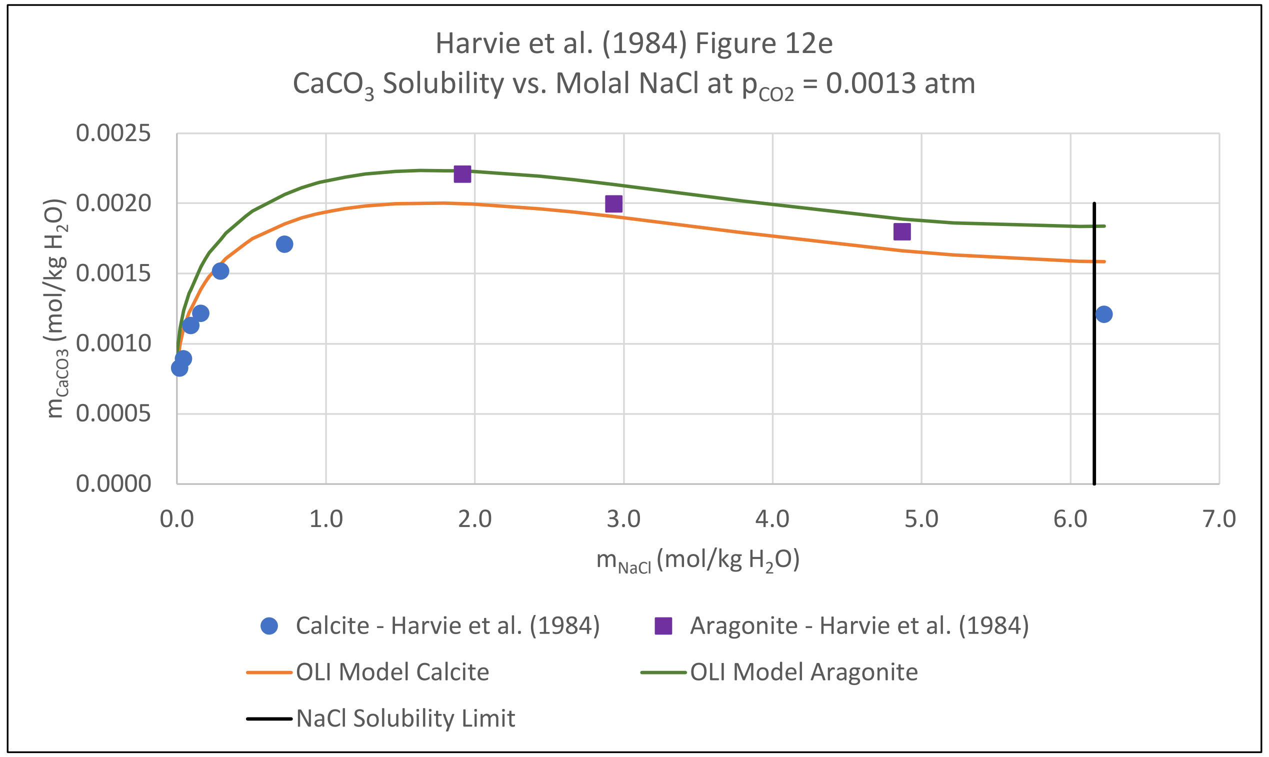


FIG. 12. The solubility of calcite in water (a) and the predicted solubilities of calcite in NaCl solutions (b)–(f).

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 12e

Harvie et al (1984)			OLI Prediction			Residual
m_{NaCl} (mol/kg H_2O)	m_{Ca} (mol/kg H_2O) Calcite	m_{Ca} (mol/kg H_2O) Aragonite	$CaCO_3$ (Calcite) (mol/kg H_2O)	$CaCO_3$ (Argonite) (mol/kg H_2O)	NaCl (Halite) (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.00			8.33E-04	9.31E-04		na
0.019	8.25E-04		9.99E-04	1.11E-03		21.1
0.044	8.91E-04		1.11E-03	1.24E-03		24.8
0.08			1.22E-03	1.36E-03		na
0.09	1.13E-03		1.25E-03	1.39E-03		10.6
0.16	1.22E-03		1.39E-03	1.55E-03		14.4
0.19			1.44E-03	1.60E-03		na
0.22			1.48E-03	1.65E-03		na
0.29	1.51E-03		1.57E-03	1.74E-03		3.3
0.33			1.61E-03	1.79E-03		na
0.46			1.71E-03	1.91E-03		na
0.51			1.75E-03	1.94E-03		na
0.72	1.71E-03		1.85E-03	2.06E-03		8.4
0.84			1.89E-03	2.11E-03		na
0.93			1.92E-03	2.14E-03		na
0.96			1.93E-03	2.15E-03		na
1.03			1.94E-03	2.17E-03		na
1.13			1.96E-03	2.19E-03		na
1.27			1.98E-03	2.21E-03		na
1.47			2.00E-03	2.23E-03		na
1.63			2.00E-03	2.23E-03		na
1.79			2.00E-03	2.23E-03		na
1.86			2.00E-03	2.23E-03		na
1.92		2.21E-03	2.00E-03	2.23E-03		1.0
1.99			1.99E-03	2.23E-03		na
2.44			1.96E-03	2.19E-03		na
2.66			1.94E-03	2.17E-03		na
2.93		1.99E-03	1.90E-03	2.13E-03		7.0
3.79			1.79E-03	2.02E-03		na
4.87		1.80E-03	1.66E-03	1.89E-03		5.1
5.21			1.63E-03	1.86E-03		na
6.06			1.59E-03	1.83E-03		na
6.23	1.21E-03		1.58E-03	1.84E-03	NaCl PPT	31.2
6.16				0.00E+00	NaCl PPT	na
6.16				2.00E-03	NaCl PPT	na
Mean	0.0012	0.0020	0.0014	0.0021	na	na
Std. Dev.	0.0003	0.0002	0.0003	0.0002	na	na
Mean of absolute values of residuals						12.7
Std. Dev. of absolute values of residuals						10.0
Minimum of absolute values of residuals						1.0
Maximum of absolute values of residuals						31.2
Pearson Correlation Coefficient (Precision)			0.947	0.964		
Bias (Location)			0.20166	0.14655		
Scale Differential			0.00170	0.01139		
Imprecision (1 - r)			0.05350	0.03596		
Deviance (Bias + Scale Diff. + Imprecision)			0.25686	0.19390		
Accuracy = 1/(1 + Bias + Scale Diff.)			0.831	0.864		
Concordance (Accuracy * Precision)			0.787	0.833		



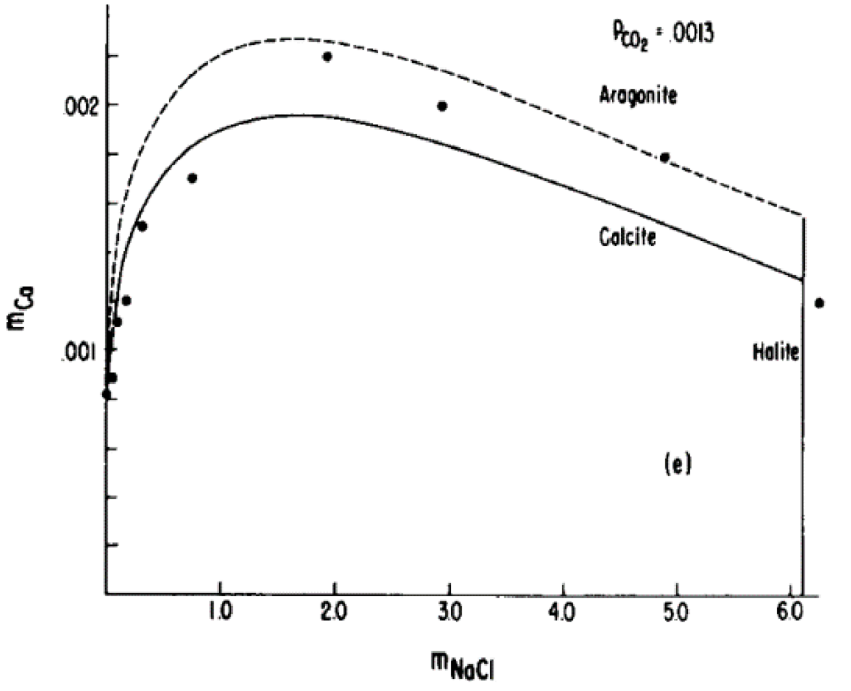
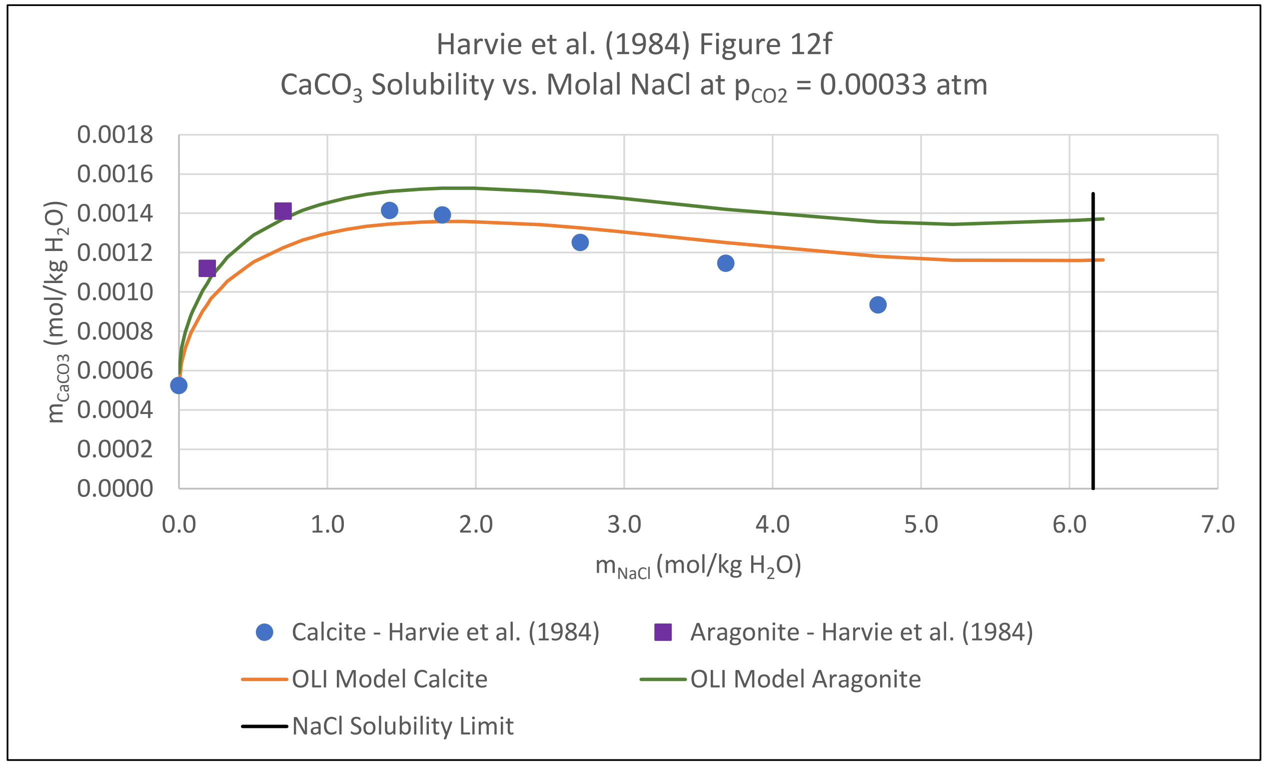


FIG. 12. The solubility of calcite in water (a) and the predicted solubilities of calcite in NaCl solutions (b)–(f).

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 12f

Harvie et al (1984)			OLI Prediction			Residual
m_{NaCl} (mol/kg H_2O)	m_{Ca} (mol/kg H_2O) Calcite	m_{Ca} (mol/kg H_2O) Aragonite	$CaCO_3$ (Calcite) (mol/kg H_2O)	$CaCO_3$ (Argonite) (mol/kg H_2O)	NaCl (Halite) (mol/kg H_2O)	(OLI - Harvie)/Harvie (%)
0.0002	5.23E-04		5.26E-04	5.88E-04		0.6
0.019			6.40E-04	7.13E-04		na
0.044			7.15E-04	7.97E-04		na
0.08			7.90E-04	8.80E-04		na
0.09			8.07E-04	8.99E-04		na
0.16			9.03E-04	1.01E-03		na
0.19		1.12E-03	9.36E-04	1.04E-03		-6.8
0.22			9.65E-04	1.08E-03		na
0.29			1.02E-03	1.14E-03		na
0.33			1.05E-03	1.18E-03		na
0.46			1.13E-03	1.26E-03		na
0.51			1.15E-03	1.29E-03		na
0.70		1.41E-03	1.23E-03	1.37E-03		-2.8
0.84			1.26E-03	1.42E-03		na
0.93			1.28E-03	1.44E-03		na
0.96			1.29E-03	1.45E-03		na
1.03			1.30E-03	1.46E-03		na
1.13			1.32E-03	1.48E-03		na
1.27			1.33E-03	1.50E-03		na
1.42	1.41E-03		1.35E-03	1.51E-03		-4.8
1.63			1.36E-03	1.52E-03		na
1.78	1.39E-03		1.36E-03	1.53E-03		-2.4
1.86			1.36E-03	1.53E-03		na
1.92			1.36E-03	1.53E-03		na
1.99			1.36E-03	1.53E-03		na
2.44			1.34E-03	1.51E-03		na
2.71	1.25E-03		1.33E-03	1.50E-03		5.9
2.93			1.31E-03	1.48E-03		na
3.69	1.15E-03		1.25E-03	1.42E-03		9.2
4.71	9.34E-04		1.18E-03	1.36E-03		26.5
5.21			1.16E-03	1.34E-03		na
6.06			1.16E-03	1.37E-03		na
6.23			1.16E-03	1.37E-03	NaCl PPT	na
6.16				0.00E+00	NaCl PPT	na
6.16				1.50E-03	NaCl PPT	na
Mean	0.0011	0.0013	0.0012	0.0012	na	na
Std. Dev.	0.0003	0.0002	0.0003	0.0002	na	na
Mean of absolute values of residuals						7.4
Std. Dev. of absolute values of residuals						8.2
Minimum of absolute values of residuals						0.6
Maximum of absolute values of residuals						26.5
Pearson Correlation Coefficient (Precision)			0.941	1.000		
Bias (Location)			0.01661	0.07005		
Scale Differential			0.00138	0.00678		
Imprecision (1 - r)			0.05940	0.00000		
Deviance (Bias + Scale Diff. + Imprecision)			0.07739	0.07683		
Accuracy = 1/(1 + Bias + Scale Diff.)			0.982	0.929		
Concordance (Accuracy * Precision)			0.924	0.929		



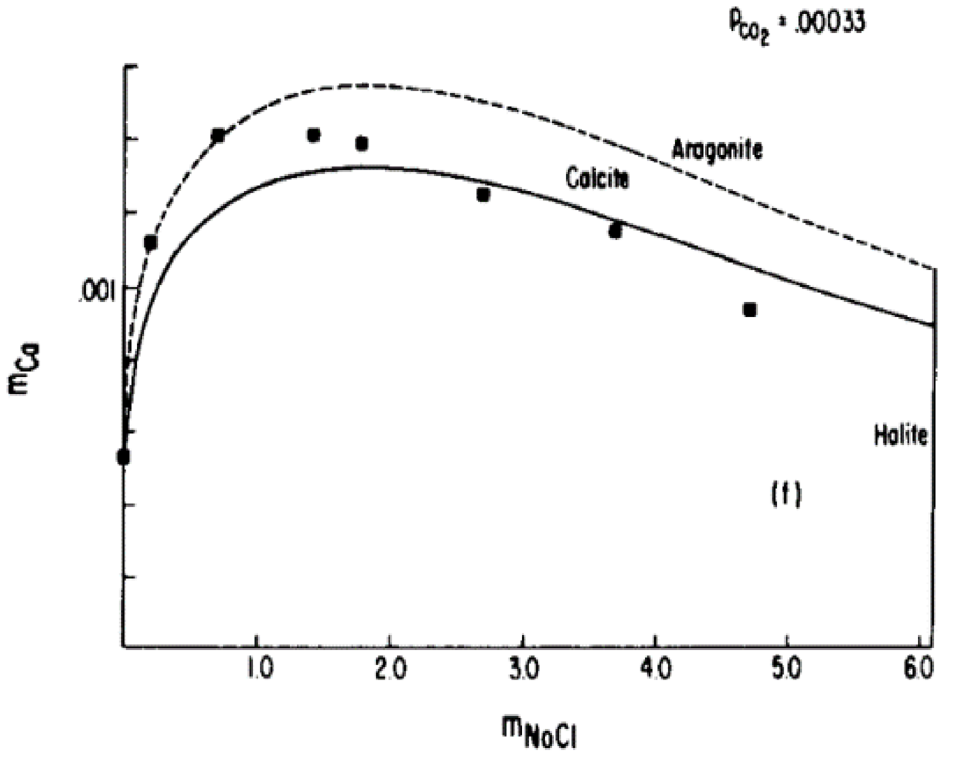


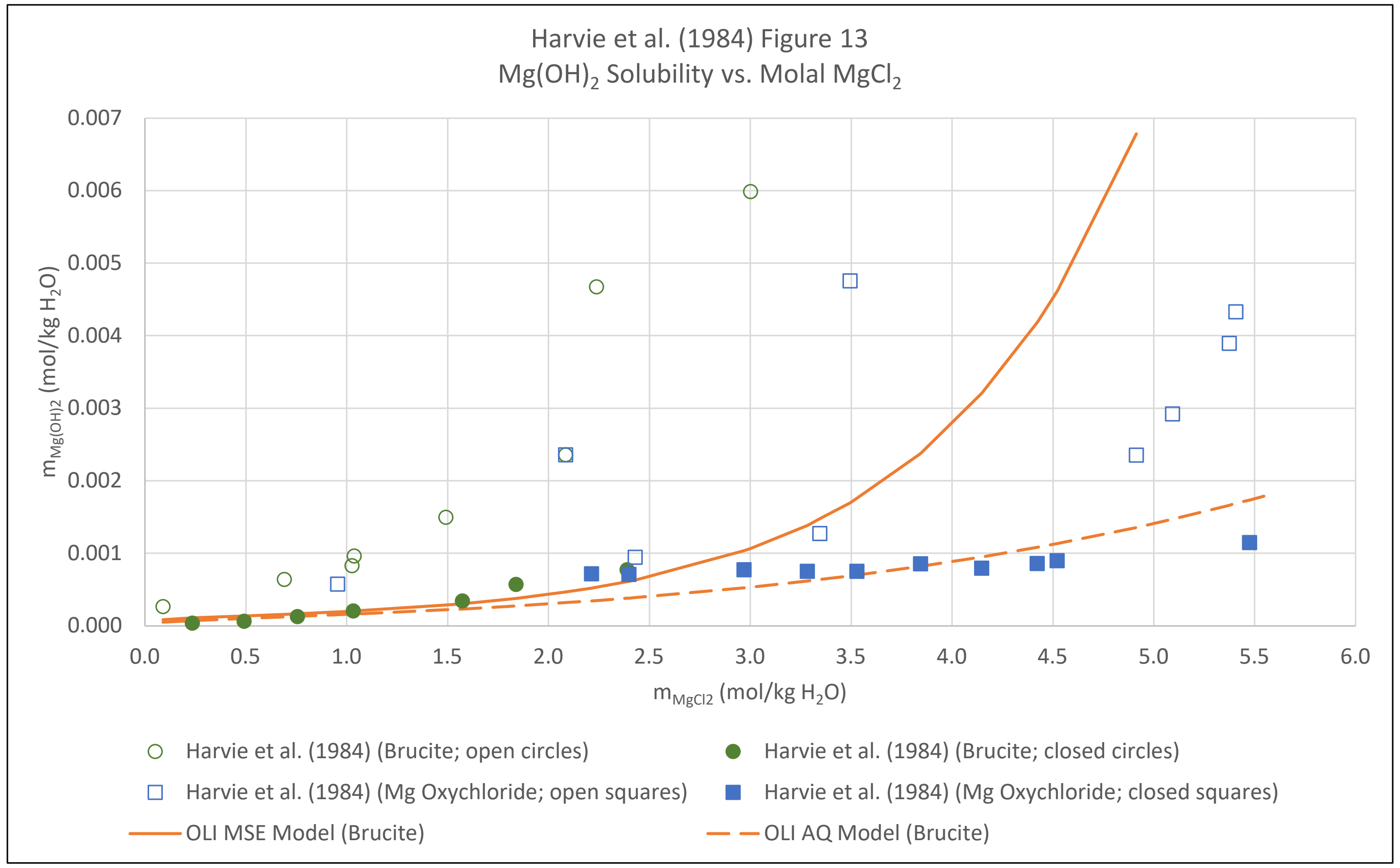
FIG. 12. The solubility of calcite in water (a) and the predicted solubilities of calcite in NaCl solutions (b)–(f).

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 13

Harvie et al (1984)					OLI MSE Model		OLI AQ Model	
m_{MgCl2} (mol/kg H_2O)	Brucite (mol/kg H_2O)		Magnesium Oxychloride* (mol/kg H_2O)		Mg(OH)2 (mol/kg H_2O)	Residual (Closed Circles Only) (OLI - Harvie)/Harvie (%)	Mg(OH)2 (mol/kg H_2O)	Residual (Closed Circles and Squares) (OLI - Harvie)/Harvie (%)
	Open Circles	Closed Circles	Open Squares	Closed Squares				
0.09	2.65E-04				8.45E-05	na	4.87E-05	na
0.24		3.68E-05			1.09E-04	195.9	7.07E-05	92.0
0.49		6.41E-05			1.36E-04	112.1	9.95E-05	55.3
0.69	6.41E-04				1.57E-04	na	1.21E-04	na
0.76		1.29E-04			1.65E-04	27.8	1.29E-04	-0.4
0.96			5.73E-04		1.90E-04	na	1.51E-04	na
1.03	8.29E-04				2.00E-04	na	1.59E-04	na
1.03		2.04E-04			2.00E-04	-1.6	1.59E-04	-21.9
1.04	9.61E-04				2.02E-04	na	1.60E-04	na
1.49	1.50E-03				2.84E-04	na	2.19E-04	na
1.57		3.43E-04			3.03E-04	-11.7	2.31E-04	-32.8
1.84		5.69E-04			3.78E-04	-33.6	2.73E-04	-52.0
2.09	2.36E-03		2.36E-03		4.68E-04	na	3.18E-04	na
2.21				7.19E-04	5.19E-04	na	3.41E-04	-52.6
2.24	4.68E-03				5.33E-04	na	3.47E-04	na
2.39		7.75E-04			6.09E-04	-21.5	3.79E-04	-51.2
2.40				7.09E-04	6.14E-04	na	3.81E-04	-46.3
2.43			9.45E-04		6.31E-04	na	3.87E-04	na
2.97				7.73E-04	1.03E-03	na	5.22E-04	-32.4
3.00	5.99E-03				1.06E-03	na	5.31E-04	na
3.28				7.52E-04	1.38E-03	na	6.15E-04	-18.2
3.35			1.27E-03		1.48E-03	na	6.38E-04	na
3.49			4.76E-03		1.69E-03	na	6.85E-04	na
3.53				7.51E-04	1.76E-03	na	7.00E-04	-6.9
3.84				8.54E-04	2.37E-03	na	8.17E-04	-4.3
4.15				7.96E-04	3.21E-03	na	9.51E-04	19.5
4.42				8.61E-04	4.18E-03	na	1.08E-03	25.6
4.52				8.98E-04	4.62E-03	na	1.13E-03	26.1
4.91			2.35E-03		6.78E-03	na	1.35E-03	na
5.09			2.92E-03			na	1.47E-03	na
5.37			3.90E-03			na	1.66E-03	na
5.41			4.33E-03			na	1.69E-03	na
5.47				1.15E-03		na	1.73E-03	50.7
5.59			4.44E-03			na	1.82E-03	na
Mean	1.58E-03				1.22E-03	na	6.29E-04	na
Std. Dev.	1.60E-03				1.61E-03	na	5.48E-04	na
Mean of absolute values of residuals						57.8		34.6
Std. Dev. of absolute values of residuals						70.8		23.3
Minimum of absolute values of residuals						1.6		0.4
Maximum of absolute values of residuals						195.9		92.0
Pearson Correlation Coefficient (Precision)						0.157		0.502
Bias (Location)						0.02686		0.53820
Scale Differential						0.00003		0.62863
Imprecision (1 - r)						0.84324		0.49821
Deviance (Bias + Scale Diff. + Imprecision)						0.87013		1.66503
Accuracy = 1/(1 + Bias + Scale Diff.)						0.974		0.462
Concordance (Accuracy * Precision)						0.153		0.232

* Magnesium oxychloride is not included in the OLI MSE databank



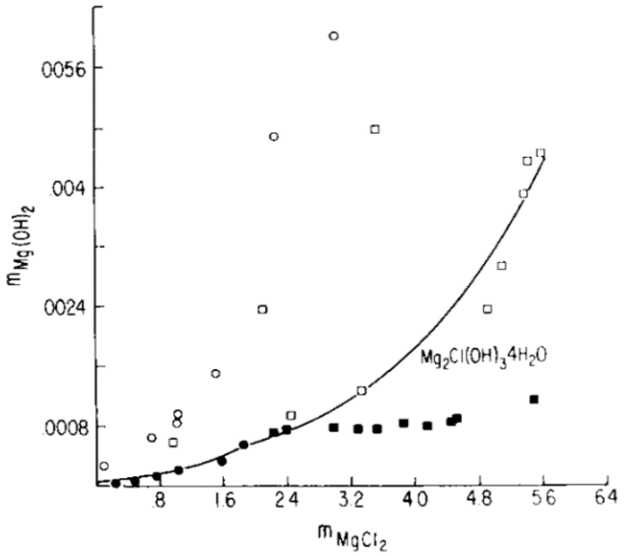


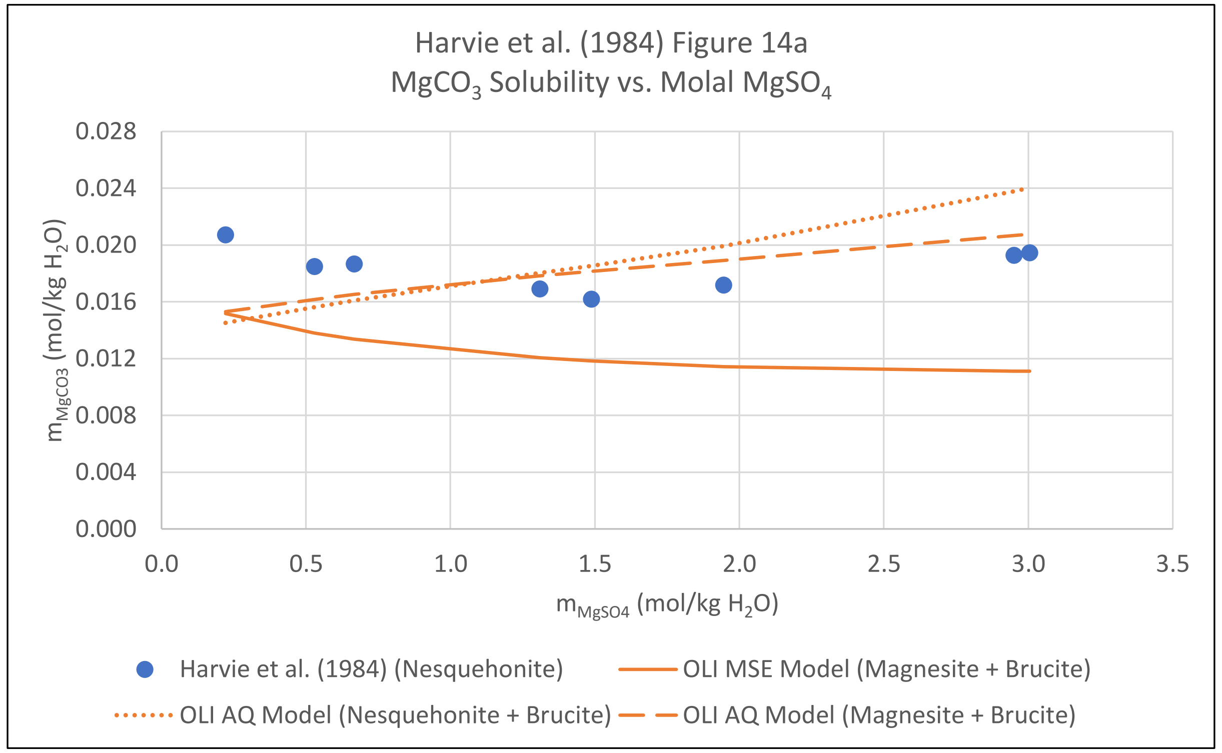
FIG. 13. The predicted solubility of brucite and magnesium oxychloride in Mg-OH-Cl-H_2O solutions *versus* the available data.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 14a

Harvie et al (1984)		OLI MSE Model	OLI AQ Model		Residual MSE Model	Residual AQ Model	
m_{MgSO4} (mol/kg H_2O)	m_{MgCO3} (mol/kg H_2O)	$MgCO_3$ (Magnesite+Brucite)* (mol/kg H_2O)	$MgCO_3.3H_2O$ (Nesquehonite+Brucite)* (mol/kg H_2O)	$MgCO_3$ (Magnesite+Brucite)* (mol/kg H_2O)	$MgCO_3$ (OLI - Harvie)/Harvie (%)	$MgCO_3.3H_2O$ (OLI - Harvie)/Harvie (%)	$MgCO_3$ (OLI - Harvie)/Harvie (%)
0.22	0.021	0.015	0.015	0.015	-26.8	-29.9	-26.2
0.53	0.018	0.014	0.016	0.016	-25.3	-15.5	-12.5
0.67	0.019	0.013	0.016	0.017	-28.4	-13.8	-11.5
1.31	0.017	0.012	0.018	0.018	-28.6	6.7	5.6
1.49	0.016	0.012	0.019	0.018	-26.8	14.5	12.1
1.95	0.017	0.011	0.020	0.019	-33.5	16.0	10.1
2.95	0.019	0.011	0.024	0.021	-42.4	23.4	7.2
3.01	0.019	0.011	0.024	0.021	-42.9	23.5	6.8
Mean	0.018	0.012	0.019	0.018	na	na	na
Std. Dev.	0.002	0.001	0.004	0.002	na	na	na
Mean of absolute values of residuals					31.8	17.9	11.5
Std. Dev. of absolute values of residuals					7.1	7.3	6.5
Minimum of absolute values of residuals					25.3	6.7	5.6
Maximum of absolute values of residuals					42.9	29.9	26.2
Pearson Correlation Coefficient (Precision)					0.467	-0.019	
Bias (Location)					7.74229	0.01951	
Scale Differential					0.00033	0.39565	
Imprecision (1 - r)					0.53318	1.01851	
Deviance (Bias + Scale Diff. + Imprecision)					8.27580	1.43368	
Accuracy = 1/(1 + Bias + Scale Diff.)					0.114	0.707	
Concordance (Accuracy * Precision)					0.053	-0.013	

* Nesquehonite is included in OLI's AQ databank but not the MSE databank. Magnesite solubility is simulated instead in the MSE model case. $Mg(OH)_2$ (Brucite) is also allowed to form.



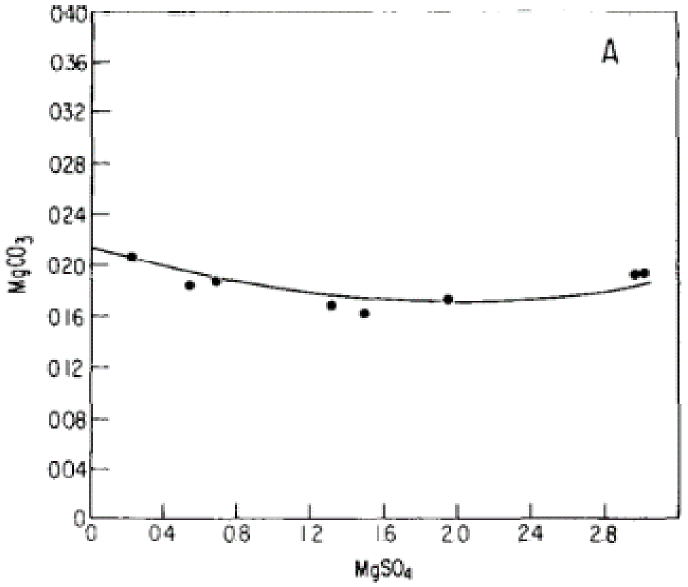


FIG. 14. Predicted solubility of nesquehonite in $MgSO_4$ (a) and $MgCl_2$ (b) solutions.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.

Harvie et al (1984) Figure 14b

Harvie et al (1984)		OLI MSE Model			OLI AQ Model			Residual MSE Model	Residual AQ Model
m_{MgCl2} (mol/kg H_2O)	m_{MgCO3} (mol/kg H_2O)	$MgCO_3$ (Magnesite)* (mol/kg H_2O)	$MgCO_3$ (Magnesite+Brucite)* (mol/kg H_2O)	Hydromagnesite (mol/kg H_2O)	$MgCO_3.3H_2O$ (Nesquehonite)* (mol/kg H_2O)	$MgCO_3.3H_2O$ (Nesquehonite+Brucite)* (mol/kg H_2O)	Hydromagnesite + Artinite (mol/kg H_2O)	$MgCO_3$ + $Mg(OH)_2$ (OLI - Harvie)/Harvie (%)	$MgCO_3.3H_2O$ (OLI - Harvie)/Harvie (%)
0.0000	0.0208	0.014	0.02118	0.00087	0.009	0.017	0.0027	1.9	-58.5
0.2373	0.0179	0.010	0.01341	0.00032	0.006	0.014	0.0014	-24.9	-67.5
0.4097	0.0207	0.010	0.01237	0.00034	0.006	0.016	0.0015	-40.3	-72.5
0.6644	0.0179	0.010	0.01132	0.00035	0.006	0.018	0.0017	-36.9	-68.3
1.4779	0.0112	0.010	0.01003	0.00045	0.006	0.032	0.0024	-10.6	-42.2
2.1207	0.0075	0.010	0.01037	0.00061	0.008	0.052	0.0029	37.7	9.9
2.6498	0.0076	0.011	0.01119	0.00082	0.011	0.081	0.0033	47.9	42.3
3.2198	0.0097	0.012	0.01238	0.00116	0.015	0.133	0.0037	28.2	54.2
3.8088	0.0070	0.014	0.01400	0.00174	0.021	0.224	0.0039	100.2	205.8
4.0924	0.0048	0.015	0.01495	0.00213	0.026	0.289	0.0040	214.5	438.7
Mean	0.0125	0.0116	0.0131	0.0009	0.0113	0.0878	0.0028	na	na
Std. Dev.	0.0062	0.0020	0.0032	0.0006	0.0071	0.0979	0.0010	na	na
Mean of absolute values of residuals								54.3	106.0
Std. Dev. of absolute values of residuals								62.2	127.8
Minimum of absolute values of residuals								1.9	9.9
Maximum of absolute values of residuals								214.5	438.7
Pearson Correlation Coefficient (Precision)								0.348	-0.713
Bias (Location)								0.00945	0.01590
Scale Differential								0.21632	0.00942
Imprecision (1 - r)								0.65224	1.71263
Deviance (Bias + Scale Diff. + Imprecision)								0.87800	1.73795
Accuracy = 1/(1 + Bias + Scale Diff.)								0.816	0.975
Concordance (Accuracy * Precision)								0.284	-0.695

* Nesquehonite is included in OLI's AQ databank but not the MSE databank. Magnesite solubility is simulated instead in the MSE model case. $Mg(OH)_2$ (Brucite) is also allowed to form where indicated.

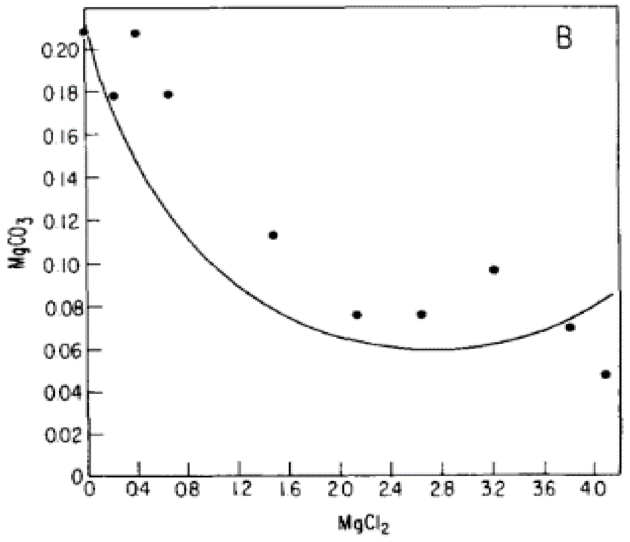
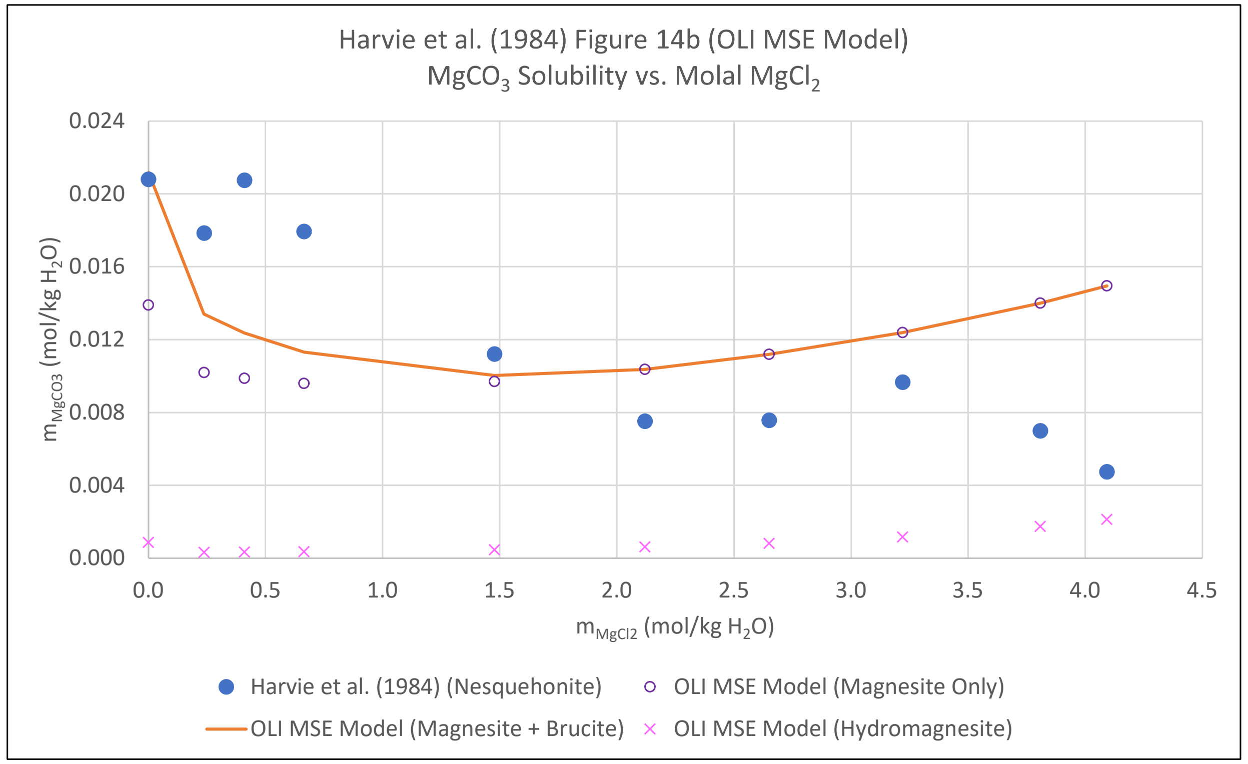
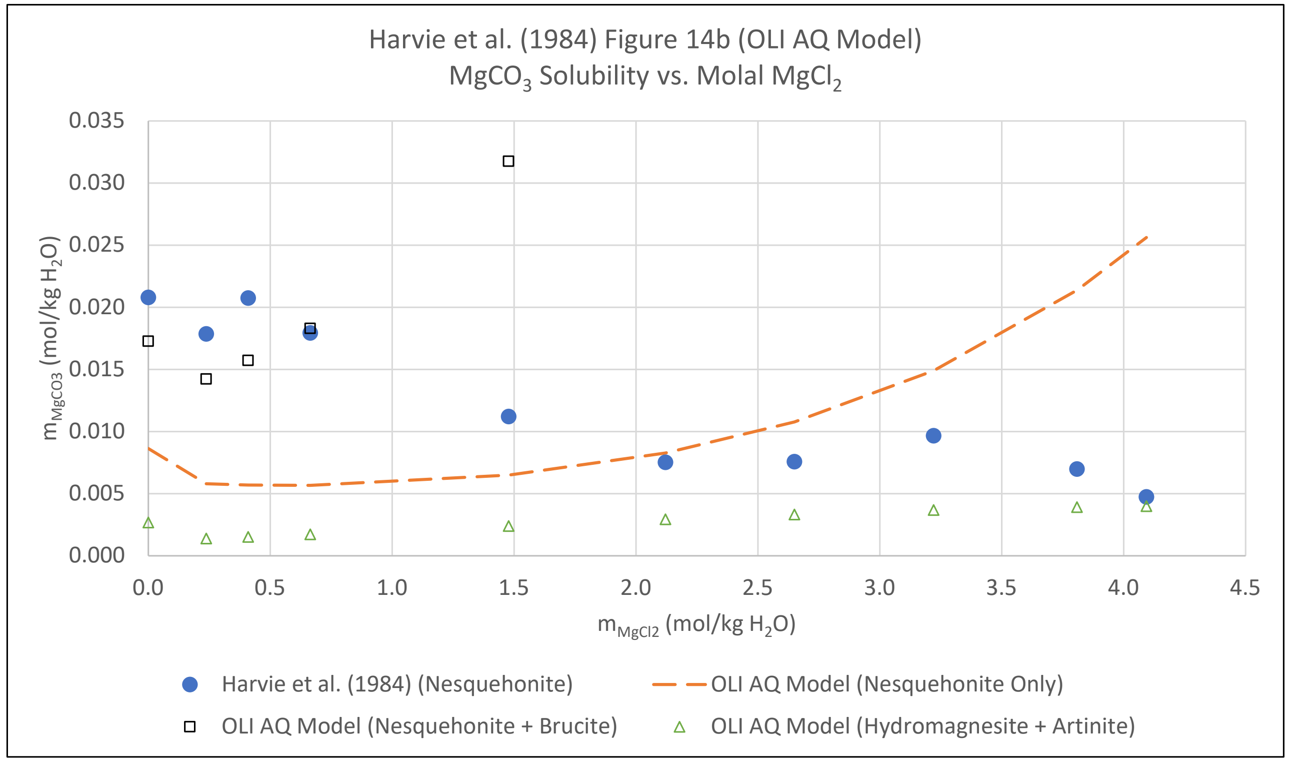


FIG. 14. Predicted solubility of nesquehonite in $MgSO_4$ (a) and $MgCl_2$ (b) solutions.

Harvie, C. E., Møller, N., & Weare, J. H. (1984). The prediction of mineral solubilities in natural waters: The Na-K-Mg-Ca-H-Cl-SO4-OH-HCO3-CO3-CO2-H2O system to high ionic strengths at 25 C. Geochimica et Cosmochimica Acta, 48(4), 723-751.





Appendix B. Summary Statistics

The summary statistics reported in Appendix A are calculated using the following equations (van Belle, 2008):

Residual

$$\% \, Residual = \frac{\left(Model - Data\right)}{Data} \times 100\% \tag{B.1}$$

Pearson Correlation Coefficient (Precision)

$$r = \frac{\sum\left(x_i - \bar{x}\right)\left(y_i - \bar{y}\right)}{\sqrt{\sum\left(x_i - \bar{x}\right)^2 \sum\left(y_i - \bar{y}\right)^2}} \tag{B.2}$$

where:

$r =$ Pearson correlation coefficient (precision)
$x_i =$ Harvie et al. data points
$\bar{x} =$ mean of Harvie et al. data points
$y_i =$ corresponding OLI MSE model points
$\bar{y} =$ mean of corresponding OLI MSE model points

Bias (Location)

$$Bias = \frac{n(\bar{x} - \bar{y})^2}{2\left(n-1\right) s_x s_y} \tag{B.3}$$

where:

$n =$ number of data points (samples)
$\bar{x} =$ mean of Harvie et al. data points
$\bar{y} =$ mean of corresponding OLI MSE model points
$s_x =$ sample standard deviation of Harvie et al. data points
$s_y =$ sample standard deviation of OLI MSE model points

Scale Differential

$$Scale \, Differential = \frac{\left(s_x - s_y\right)^2}{2 s_x s_y} \tag{B.4}$$

where:

$s_x =$ sample standard deviation of Harvie et al. data points
$s_y =$ sample standard deviation of OLI MSE model points

Imprecision

$$Imprecision = 1 - r \tag{B.5}$$

where:

$r =$ Pearson correlation coefficient

Deviance

$$Deviance = Bias + Scale\,Differential + Imprecision \tag{B.6}$$

Accuracy

$$Accuracy = \frac{1}{\left(1 + Bias + Scale\,Differential\right)} \tag{B.7}$$

Concordance

$$Concordance = Accuracy \times Precision \tag{B.8}$$

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