Appendix to:
C.A.J. Appelo, Principles, caveats and improvements in databases for calculating hydrogeochemical reactions in saline waters from 0 - 200 ºc and 1 - 1000 atm.

This appendix has figures showing experimental solubilities and PHREEQC calculations, using the Pitzer interaction coefficients given in Table 1, and the temperature dependent log *K*'s in Table 2 of the paper. The PHREEQC input files are in the directory:
c:\phreeqc\high_P_T\appendix_AG15
The main directory contains pitzer.dat and input files that calculate the figures presented by Pabalan and Pitzer, 1987. Input files for other minerals and CO_2 gas are in sub-directories.
It is easiest to run the files with Notepad++ adapted for PHREEQC. Download from:
http://www.hydrochemistry.eu/ph3/phreeqc3.Installer.exe
and install in your computer. In Notepad++, open a file (Ctrl+O), and press Ctrl+F6 to start the PHREEQC calculations.

Table 3. List of figures with mineral solubilities as a function of *T, P* and solution composition.

Mineral solubility in water or aqueous solution	Temp ºC	Pressure / atm	Figure
halite (NaCl)	0 - 300	1 - P_{sat}	A1
sylvite (KCl)	10 - 300	1 - P_{sat}	A2
bischofite ($MgCl_2$:$6H_2O$), $MgCl_2$:$2H_2O$, $MgCl_2$:$4H_2O$	0 - 200	1 - P_{sat}	A3
mirabilite (Na_2SO_4:$10H_2O$), thenardite (Na_2SO_4)	0 - 220	1 - P_{sat}	A4
arcanite (K_2SO_4)	0 - 210	1 - P_{sat}	A5
epsomite ($MgSO_4$:$7H_2O$), hexahydrite ($MgSO_4$:$6H_2O$), kieserite ($MgSO_4$:H_2O)	0 - 200	1 - P_{sat}	A6
halite (NaCl), sylvite (KCl) in Na/K-Cl solutions	0 - 200	1 - P_{sat}	A7
carnallite ($KMgCl_3$:H_2O) in K/Mg-Cl solutions	0 - 75	1	A8
gypsum ($CaSO_4$:$2H_2O$)	0 - 95	1	A9
gypsum ($CaSO_4$:$2H_2O$) in NaCl solutions	0.5 - 95	1	A10
gypsum ($CaSO_4$:$2H_2O$), mirabilite (Na_2SO_4:$10H_2O$), glauberite ($Na_2Ca(SO_4)_2$) and thenardite (Na_2SO_4) in Na_2SO_4 solutions	25 - 100	1	A11
gypsum ($CaSO_4$:$2H_2O$) and anhydrite ($CaSO_4$)	30 - 160	1 - 1000	A12
anhydrite ($CaSO_4$) in NaCl solutions	100 - 200	1 - P_{sat}	A13
anhydrite ($CaSO_4$) in NaCl solutions	100 - 200	1 - 987	A14
anhydrite ($CaSO_4$) and glauberite ($Na_2Ca(SO_4)_2$) in Na_2SO_4 solutions	100 - 200	1 - P_{sat}	A15
anhydrite ($CaSO_4$), Goergeyite ($K_2Ca_5(SO_4)_6H_2O$) and syngenite ($K_2Ca(SO4)_2$:H_2O) in K_2SO_4 solutions	100 - 200	1 - P_{sat}	A16
amorphous silica (SiO_2(a)) in NaCl solutions	25 - 300	1 - P_{sat}	A17
amorphous silica (SiO_2(a)) in Na_2SO_4 solutions	25 - 300	1 - P_{sat}	A18
amorphous silica (SiO_2(a)) in $MgCl_2$ solutions	25 - 300	1 - P_{sat}	A19
amorphous silica (SiO_2(a)) in $MgSO_4$ solutions	25 - 250	1 - P_{sat}	A20
amorphous silica (SiO_2(a)) in Li-Cl/NO_3 solutions	25	1	A21

amorphous silica (SiO_2(a)) in K-Cl/NO_3 solutions	25	1	A22
amorphous silica (SiO_2(a)) in $CaCl_2$ solutions	25	1	A23
barite ($BaSO_4$) in NaCl solutions	1 - 250	1 - P_{sat}	A24
barite ($BaSO_4$) in NaCl solutions	150 - 250	493	A25
calcite ($CaCO_3$) in NaCl solutions	10 - 60	1	A26
calcite ($CaCO_3$) in 3 M NaCl, variable CO_2	200	580	A27
calcite ($CaCO_3$) in NaCl solutions	120 - 260	12	A28
calcite ($CaCO_3$) at 1 bar CO_2 pressure	0 - 300	1 - (P_{sat}+1)	A29
calcite ($CaCO_3$) in NaCl solutions at 1 bar CO_2 pressure	0 - 250	1 - 1450	A30
CO_2 gas	25 - 100	1 - 710	A31
CO_2 gas in 1 and 6 M NaCl solution	25 - 300	35 - 200	A32
CO_2 gas in 4 M NaCl solution	80 - 180	9 - 95	A33
CO_2 gas in Na_2SO_4 solutions	140	12 - 96	A34
CO_2 gas in 2.3 M $CaCl_2$ solution	75 - 120	22 - 655	A35
CO_2 fugacity coefficients	0 - 300	99 - 987	A36

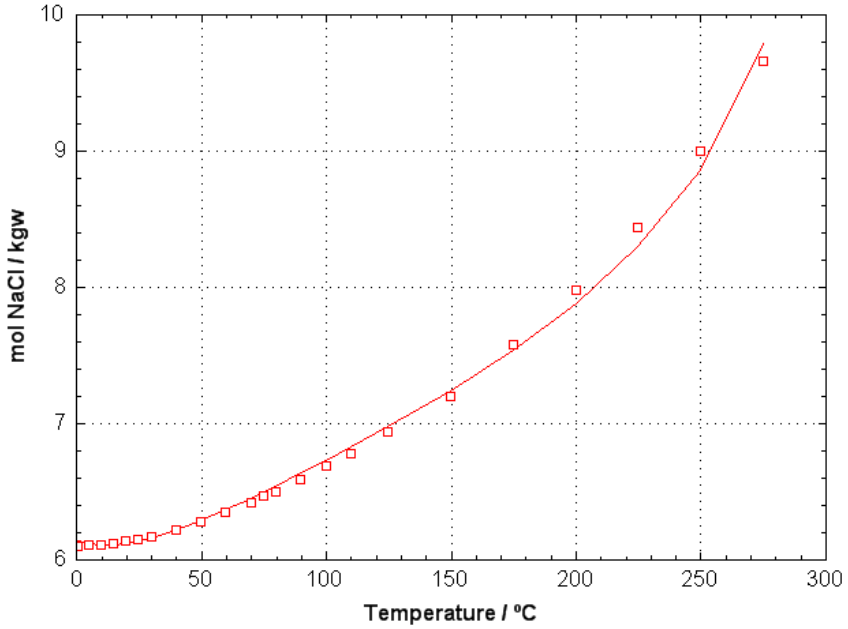

Figure A1. Halite (NaCl) solubility as a function of temperature. Data points from Pabalan and Pitzer, 1987; Clarke and Glew, 1985. File Halite.phr

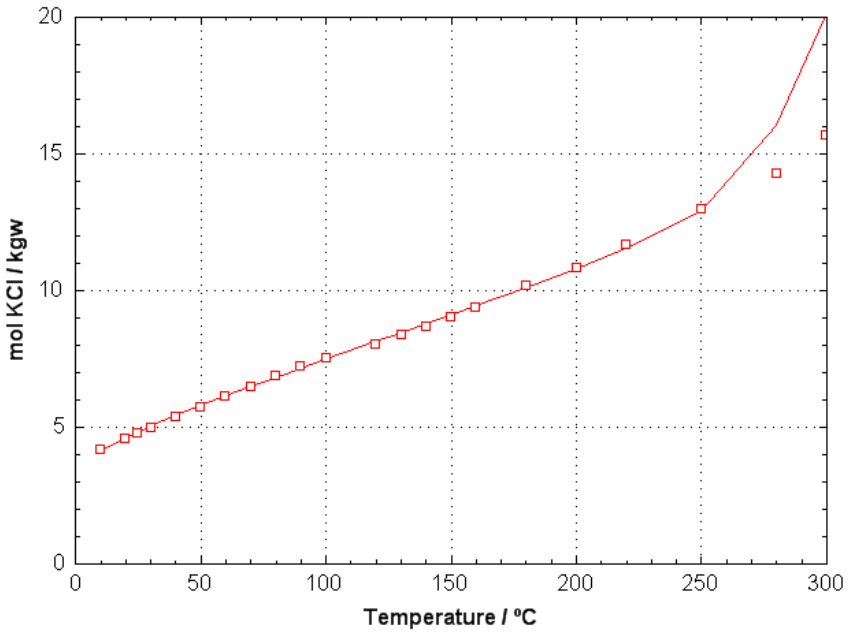

Figure A2. Sylvite (KCl) solubility as a function of temperature. Data points from Pabalan and Pitzer, 1987. File Sylvite.phr

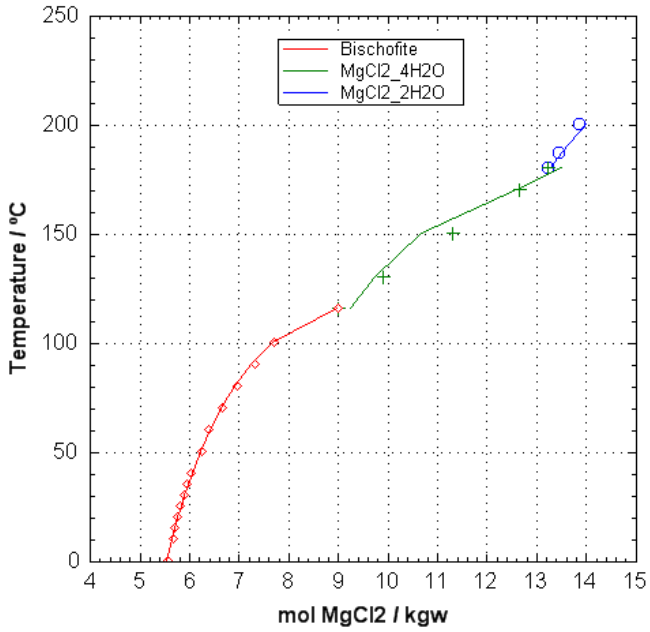

Figure A3. Solubility of $MgCl_2$-hydrates. Data points from Pabalan and Pitzer, 1987. File $MgCl_2$.phr

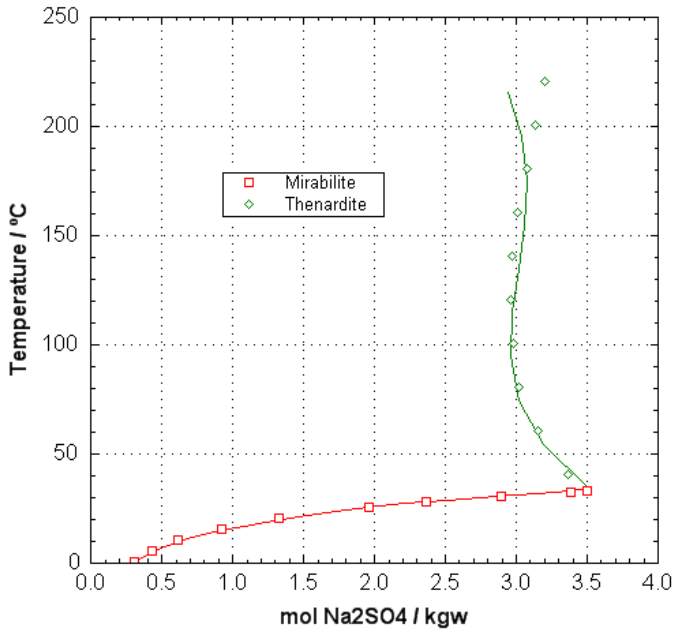

Figure A4. Solubility of Na_2SO_4-(an)hydrate. Data points from Pabalan and Pitzer, 1987. File Na2SO4.phr

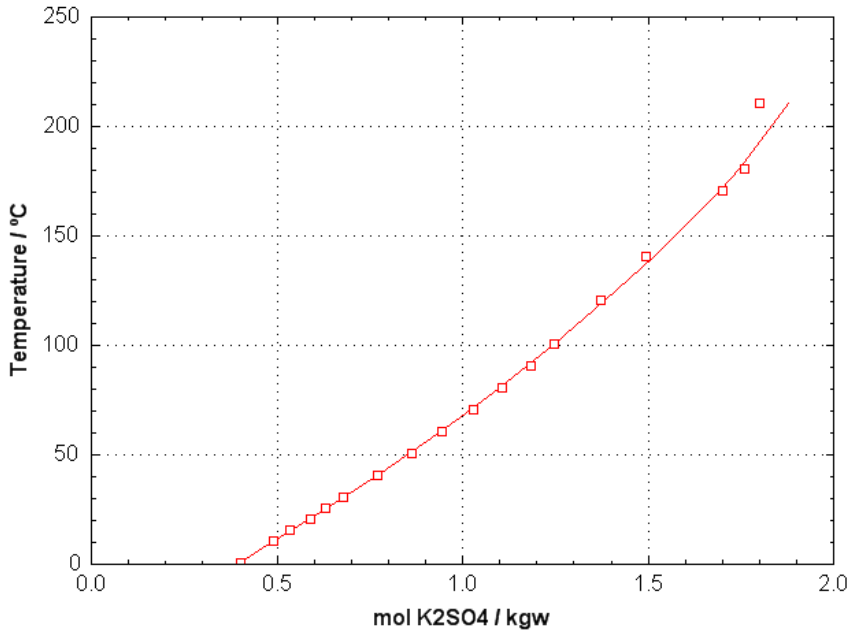

Figure A5. Solubility of arcanite (K_2SO_4). Data points from Pabalan and Pitzer, 1987. File K2SO4.phr

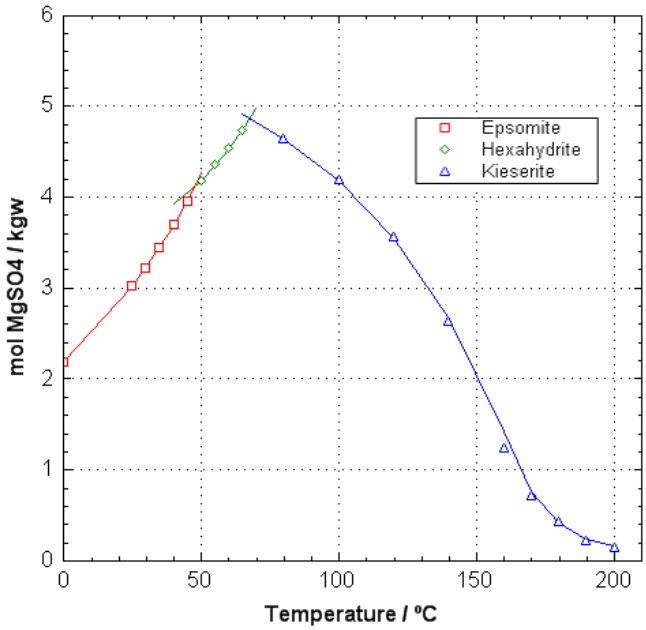

Figure A6. Solubility of $MgSO_4$-hydrates. Data points from Pabalan and Pitzer, 1987. File MgSO4.phr

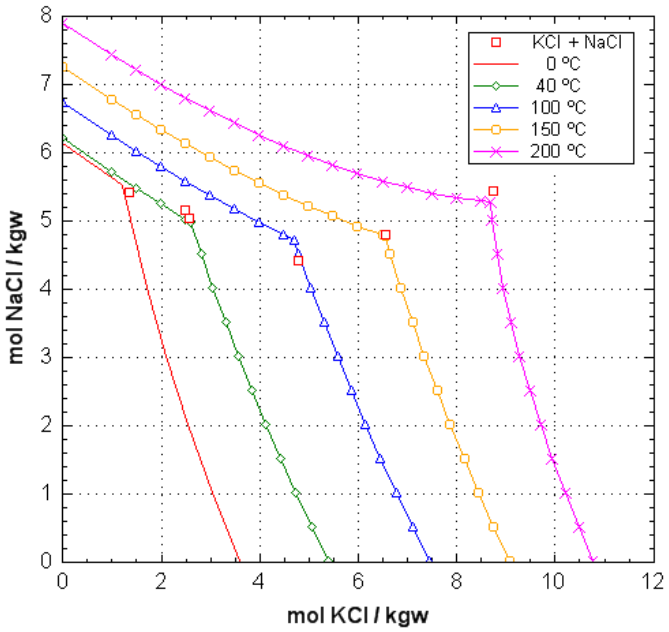

Figure A7. Mutual influence of NaCl and KCl solutions on halite and sylvite solubilities, with triple points KCl + NaCl + H_2O from Pabalan and Pitzer, 1987. File NaKCl.phr

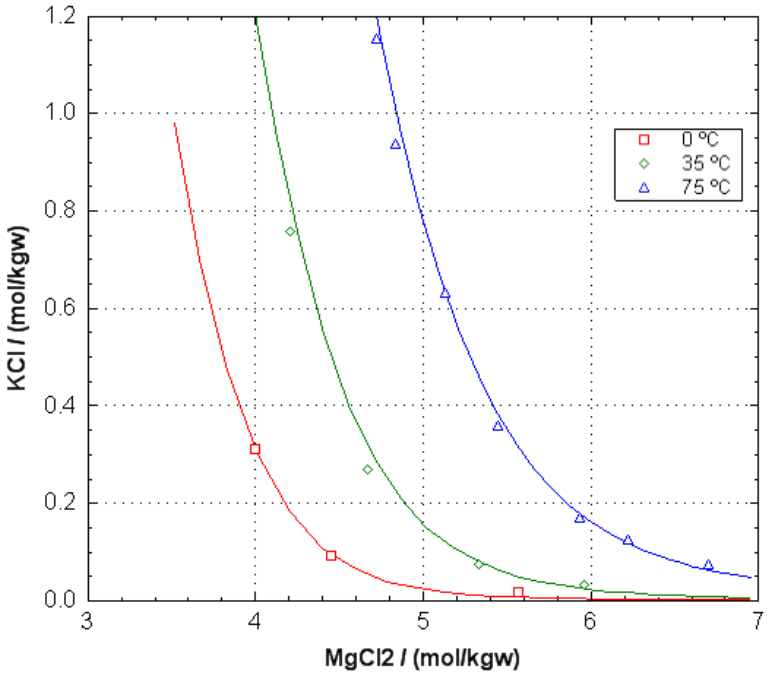

Figure A8. Solubility of carnallite ($KMgCl_3$:H_2O). Data points from Pabalan and Pitzer, 1987. File Carnallite.phr

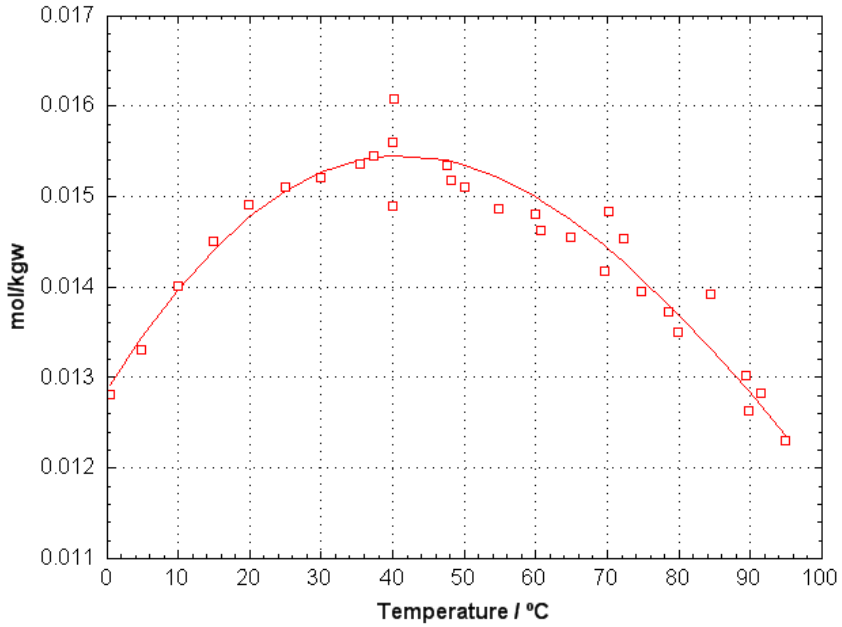

Figure A9. Solubility of gypsum ($CaSO_4:2H_2O$). Data points from Marshall and Slusher, 1966; Blount and Dickson, 1969. File gypsum.phr

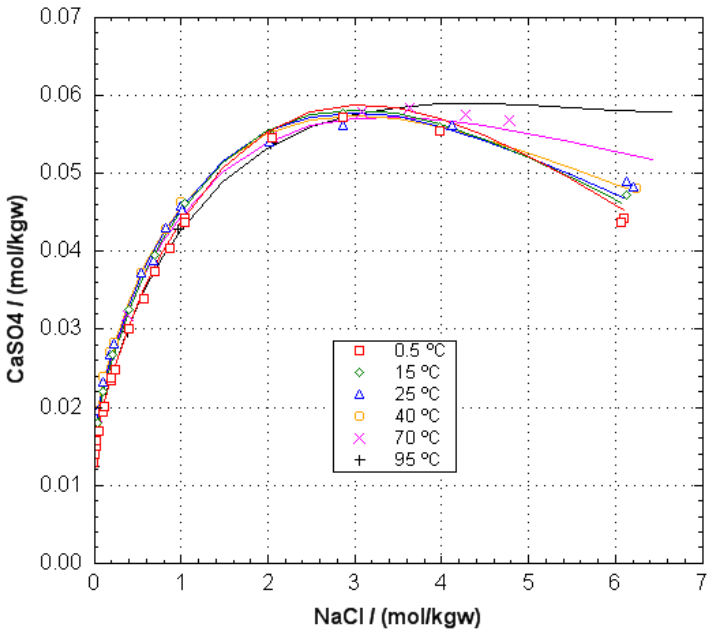

Figure A10. Solubility of gypsum ($CaSO_4:2H_2O$) in NaCl solutions. Data points from Marshall and Slusher, 1966. File gyps_NaCl.phr

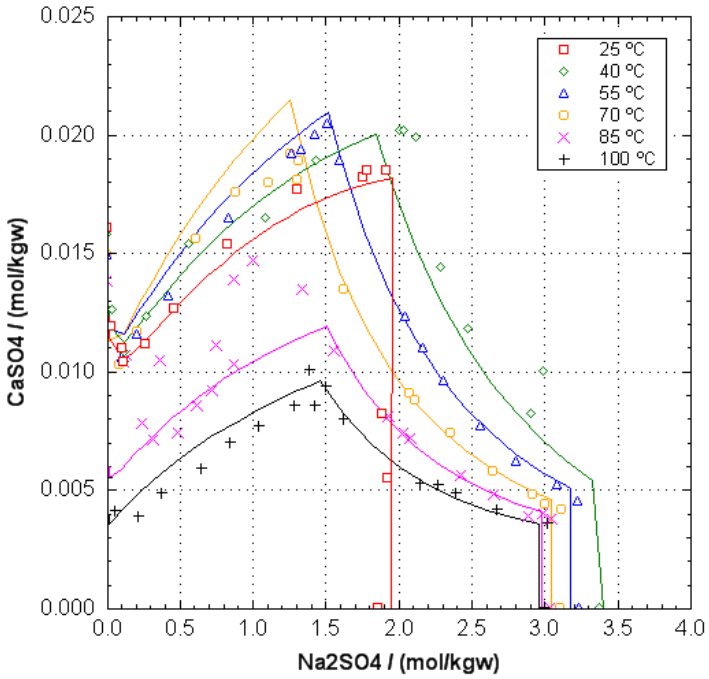

Figure A11. Solubility of gypsum ($CaSO_4 \cdot 2H_2O$) in Na_2SO_4 solutions. Data points from Block and Waters, 1968. File gyps_Na2SO4.phr. The concentration decrease of $CaSO_4$ at Na_2SO_4 concentrations above 1 M is due to mirabilite precipitation (25ºC), or glauberite and thenardite precipitation at higher temperatures. At 85 and 100ºC, and possibly at 70ºC, gypsum transforms into anhydrite.

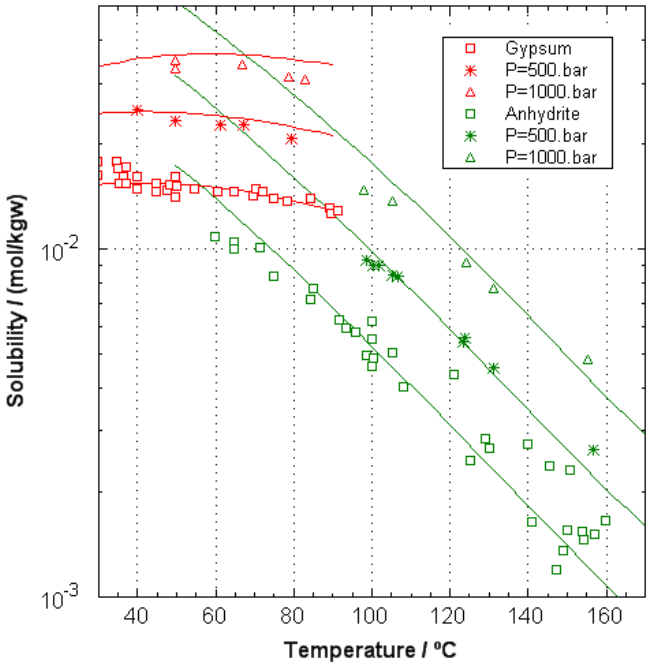

Figure A12. Solubility of gypsum ($CaSO_4 \cdot 2H_2O$) and anhydrite ($CaSO_4$) as a function of temperature and pressure. Data points from Blount and Dickson, 1973. File gypsum_P.phr.

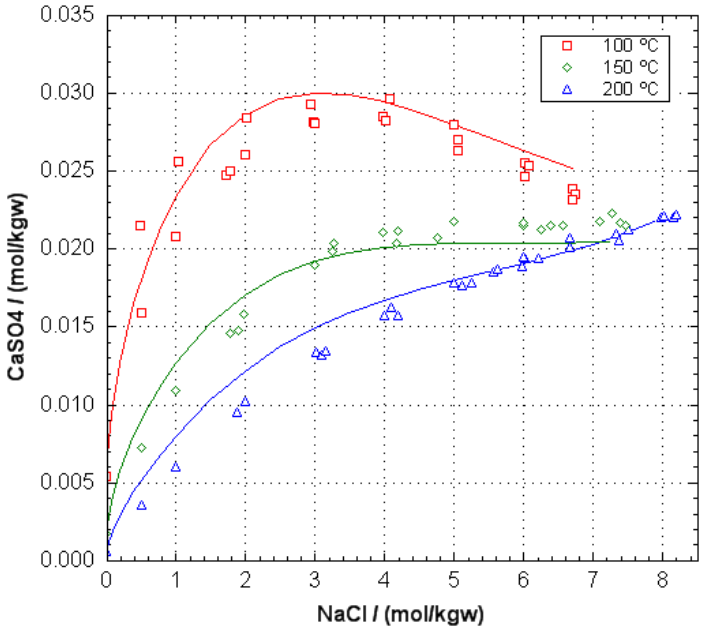

Figure A13. Solubility of anhydrite ($CaSO_4$) in NaCl solutions. Data points from Block and Waters, 1968; Blount and Dickson, 1969; Freyer and Voigt, 2004. File anhy_NaCl.phr.

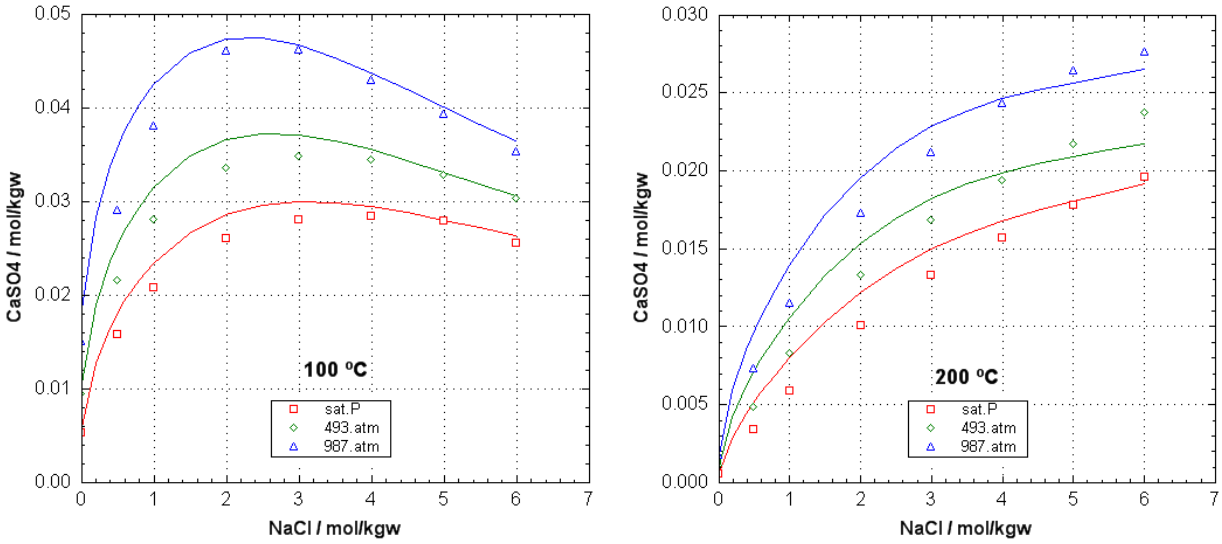

Figure A14. Solubility of anhydrite ($CaSO_4$) in NaCl solutions as a function of pressure at 100ºC and 200ºC. Data points from the summary table in Blount and Dickson, 1969. File anhy_P_NaCl.phr.

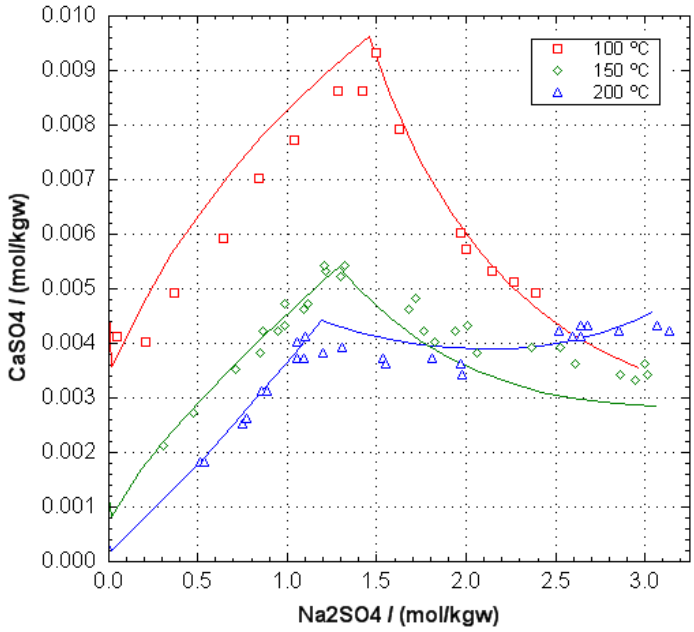

Figure A15. Solubility of anhydrite ($CaSO_4$) in Na_2SO_4 solutions. Data points from Freyer and Voigt, 2004. The decrease of the $CaSO_4$ concentration at Na_2SO_4 concentrations above 1 M is due to glauberite precipitation. File anhy_Na2SO4.phr.

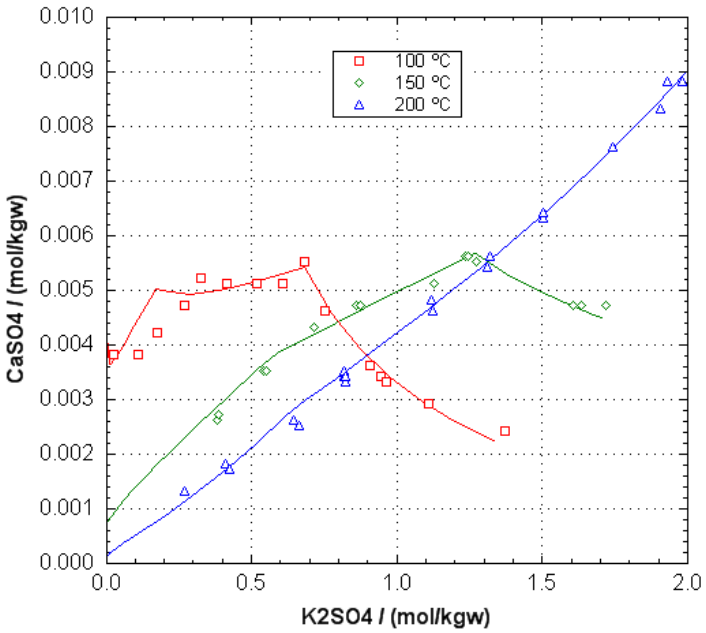

Figure A16. Solubility of anhydrite ($CaSO_4$) in K_2SO_4 solutions. Data points from Freyer and Voigt, 2004. The breaks in the concentration lines result from precipitation of Goergeyite ($K_2Ca_5(SO_4)_6H_2O$) and, at 100 and 150ºC, Syngenite ($K_2Ca(SO4)_2{:}H_2O$). File anhy_K2SO4.phr.

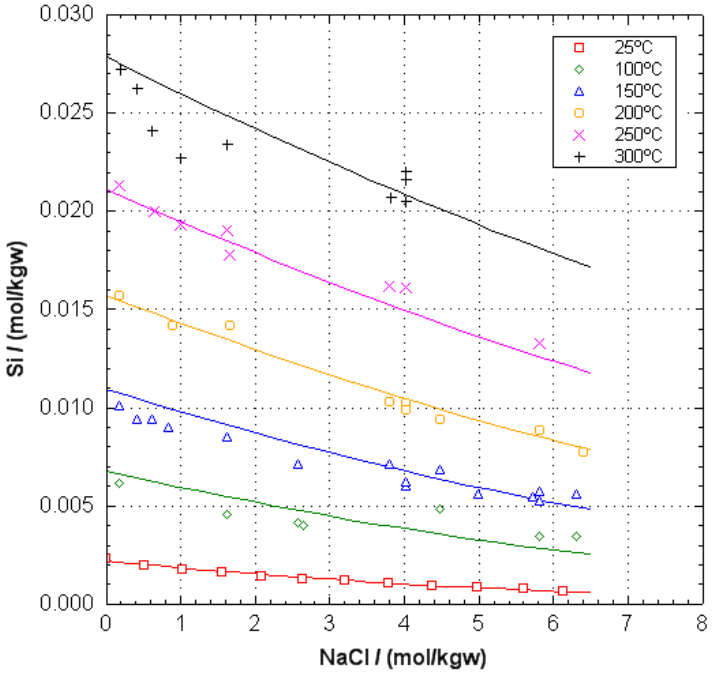

Figure A17. Solubility of amorphous silica (SiO_2(a)) in NaCl solutions. Data points from Marshall and Warakomski, 1980, and Chen and Marshall, 1982. File SiO2_NaCl.phr.

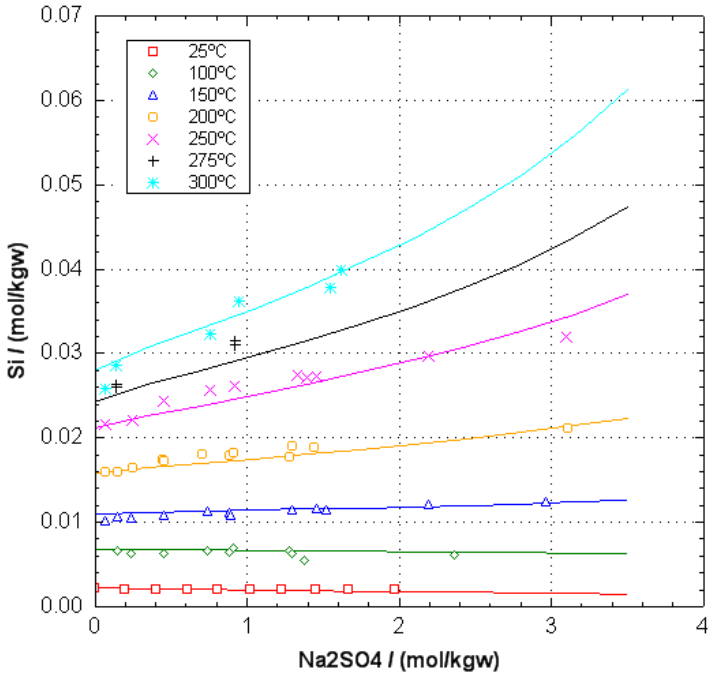

Figure A18. Solubility of amorphous silica (SiO_2(a)) in Na_2SO_4 solutions. Data points from Marshall and Warakomski, 1980, and Chen and Marshall, 1982. File SiO2_Na2SO4.phr.

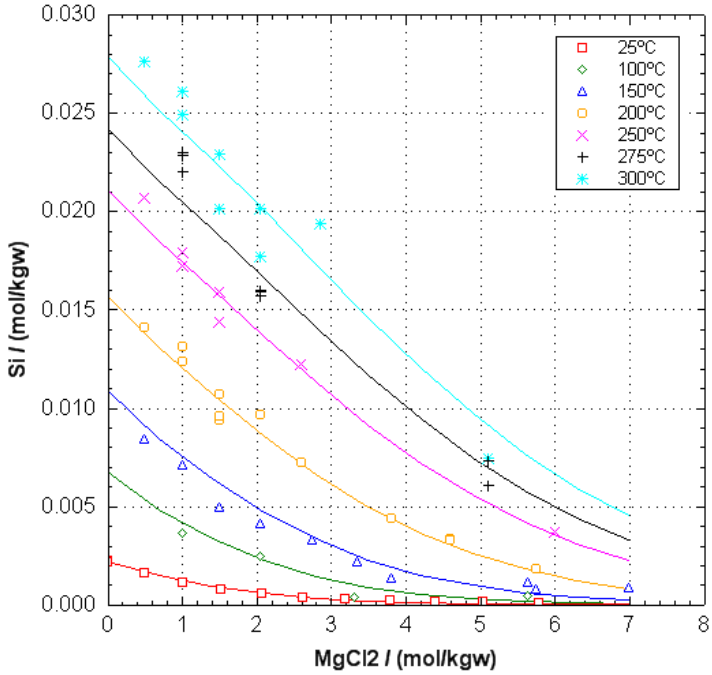

Figure A19. Solubility of amorphous silica (SiO_2(a)) in $MgCl_2$ solutions. Data points from Marshall and Warakomski, 1980, and Chen and Marshall, 1982. File SiO2_ MgCl2.phr.

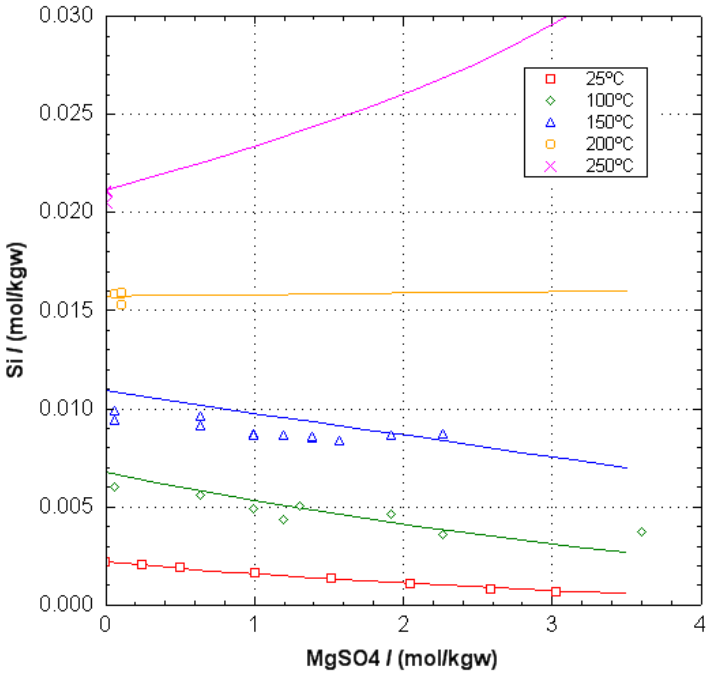

Figure A20. Solubility of amorphous silica (SiO_2(a)) in $MgSO_4$ solutions. Data points from Marshall and Warakomski, 1980, and Chen and Marshall, 1982. File SiO2_MgSO4.phr.

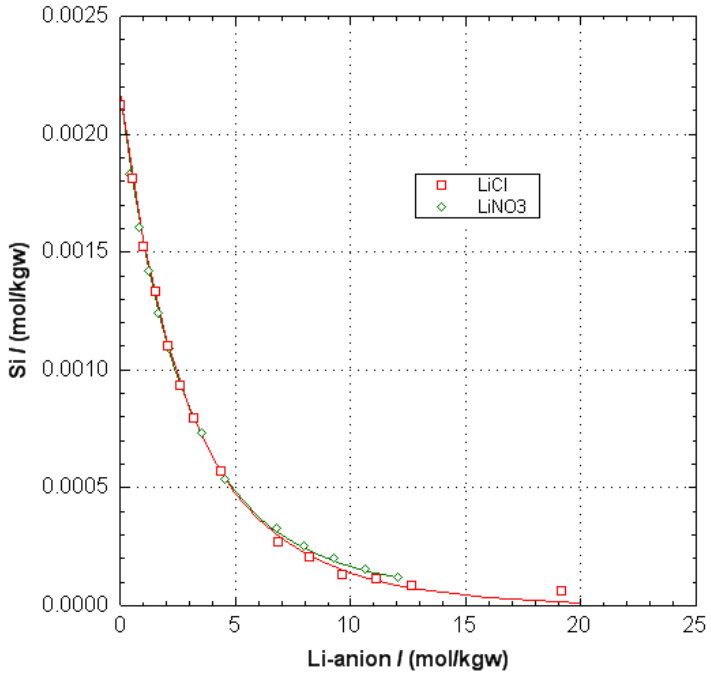

Figure A21. Solubility of amorphous silica (SiO_2(a)) in LiCl and $LiNO_3$ solutions at 25ºC. Data points from Marshall and Warakomski, 1980. File SiO2_Li.phr.

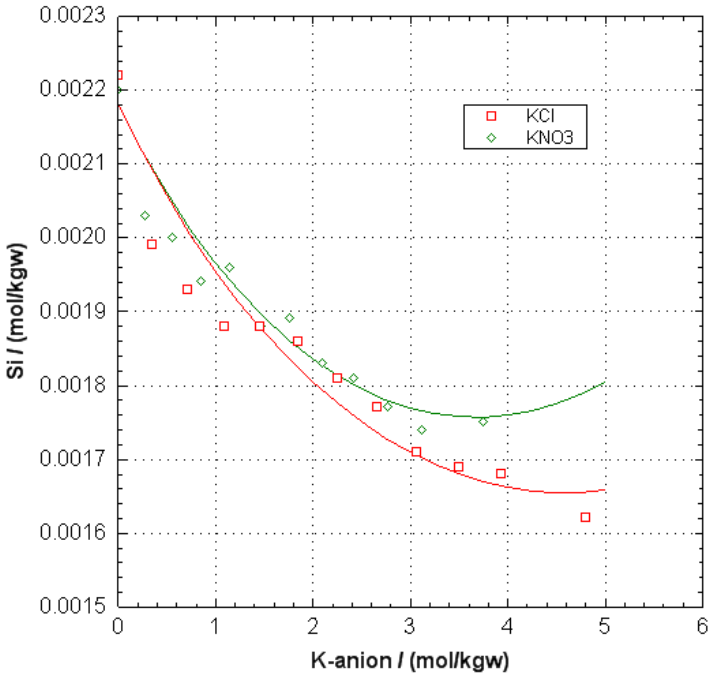

Figure A22. Solubility of amorphous silica (SiO_2(a)) in KCl and KNO_3 solutions at 25ºC. Data points from Marshall and Warakomski, 1980. File SiO2_K.phr.

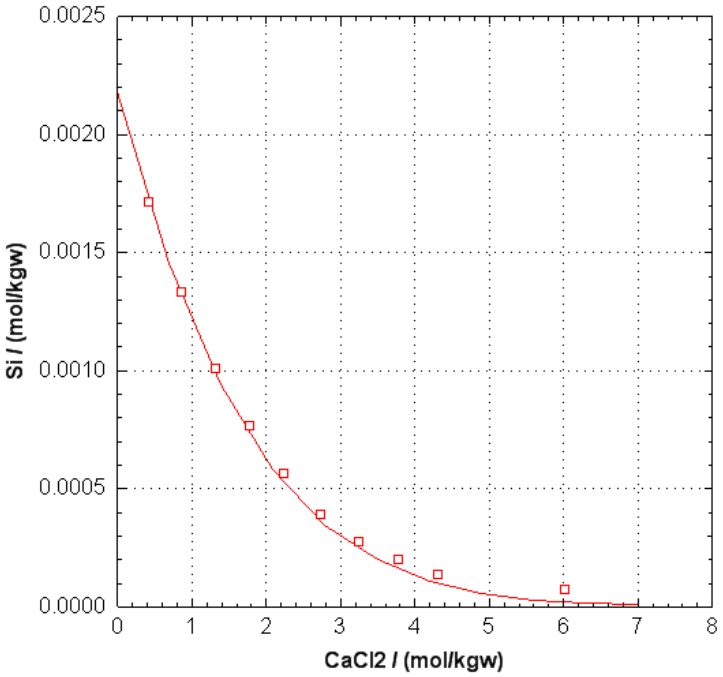

Figure A23. Solubility of amorphous silica (SiO_2(a)) in $CaCl_2$ solutions at 25ºC. Data points from Marshall and Warakomski, 1980. File SiO2_CaCl2.phr.

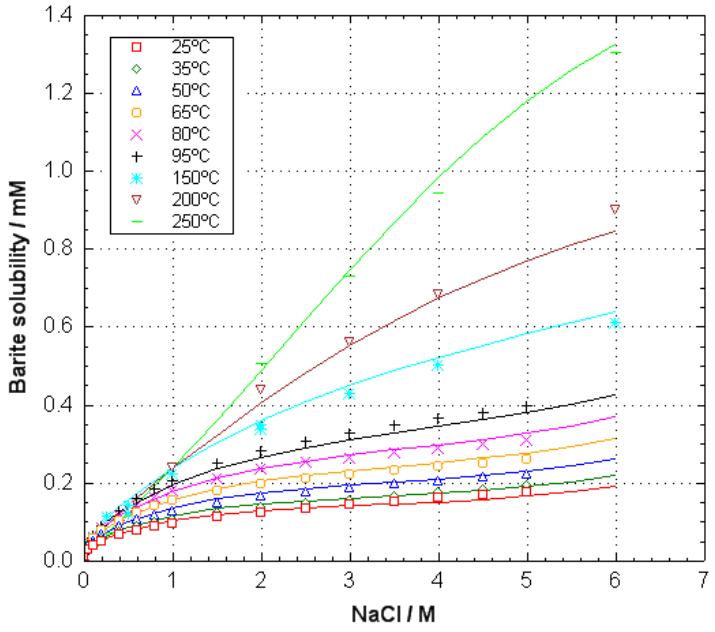

Figure A24. Solubility of barite ($BaSO_4$) in NaCl solutions. Data points < 95ºC from Templeton, 1960, > 100ºC from Uchameyshvili et al., 1966, and the summary table in Blount, 1977. File Barite_NaCl.phr.

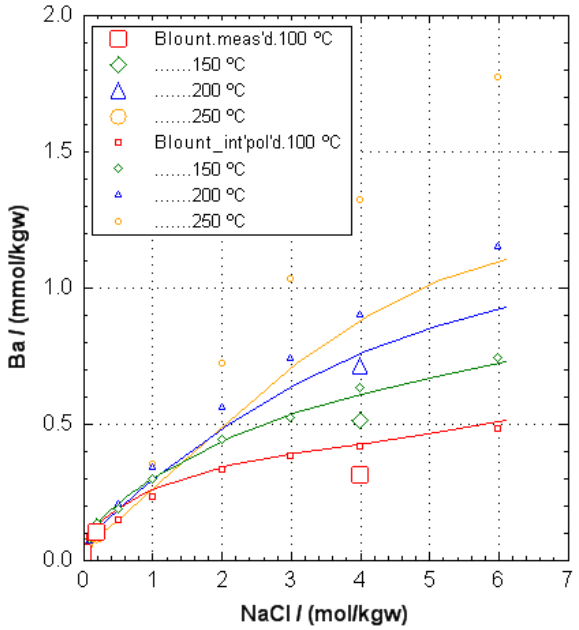

Figure A25. Solubility of barite ($BaSO_4$) in NaCl solutions at 500 bar. Measured (large symbols) and interpolated (small symbols) data from Blount, 1977. File Barite_500.phr.

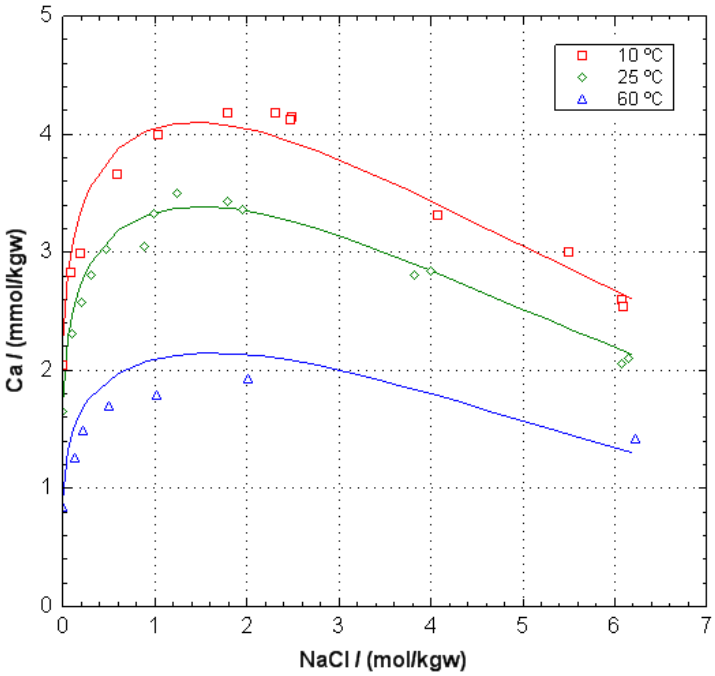

Figure A26. Solubility of calcite ($CaCO_3$) in NaCl solutions at about 0.01 atm CO_2 pressure. Measured data from Wolf et al., 1989. File cc_Wolf.phr.

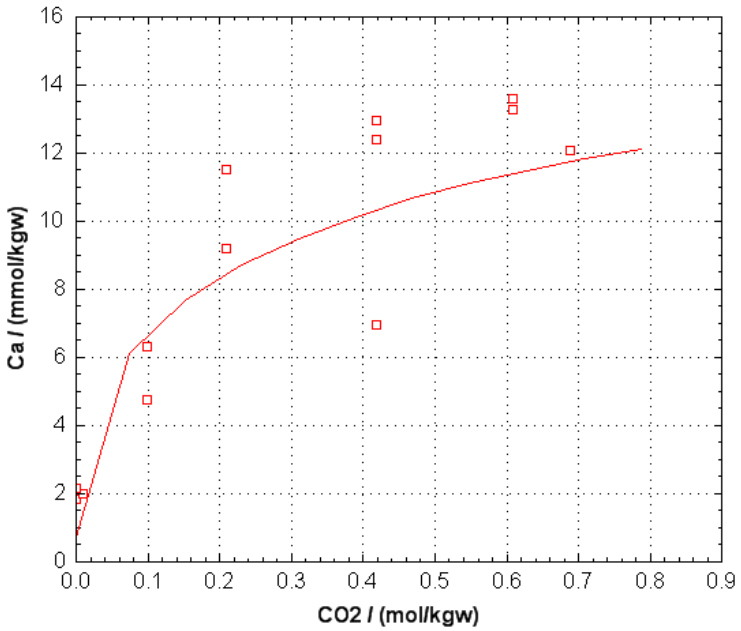

Figure A27. Solubility of calcite ($CaCO_3$) at 200 °C, 580 atm pressure in 3 M NaCl as a function of the CO_2 concentration. Measured data from Malinin and Kanukov, 1971. File cc_Malin.phr.

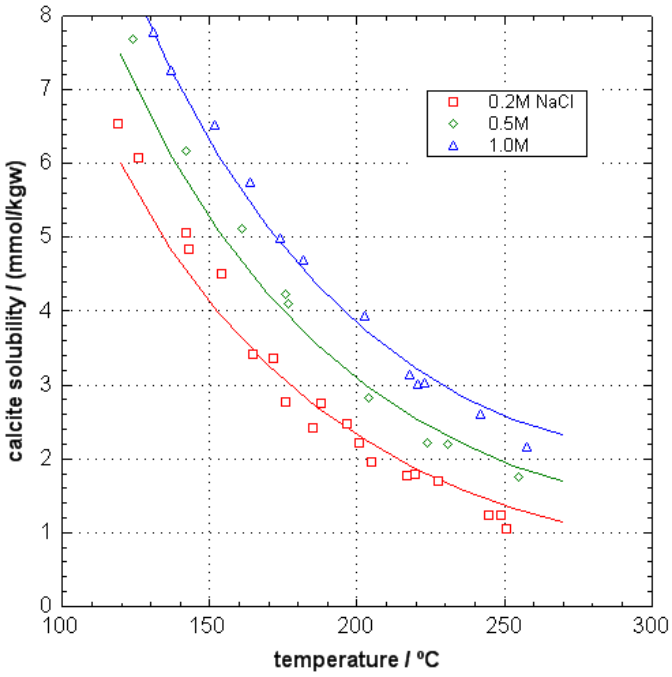

Figure A28. Solubility of calcite ($CaCO_3$) in NaCl solutions at 12 bar CO_2 pressure. Measured data from Ellis, 1963. File cc_Ellis.phr.

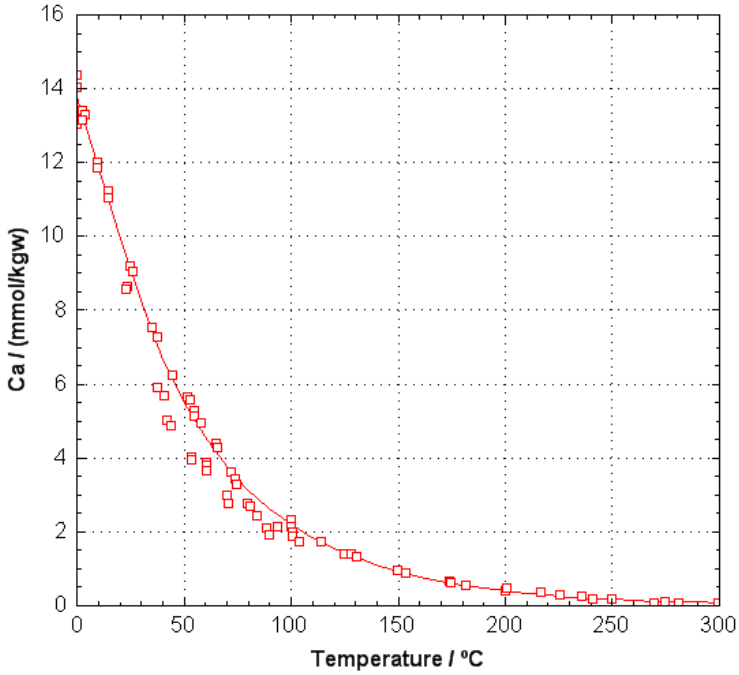

Figure A29. Solubility of calcite ($CaCO_3$) as a function of temperature at 1 bar CO_2 pressure. Measured data from Miller, 1952; Ellis, 1959; Plummer and Busenberg, 1982. File cc_1barCO2.phr.

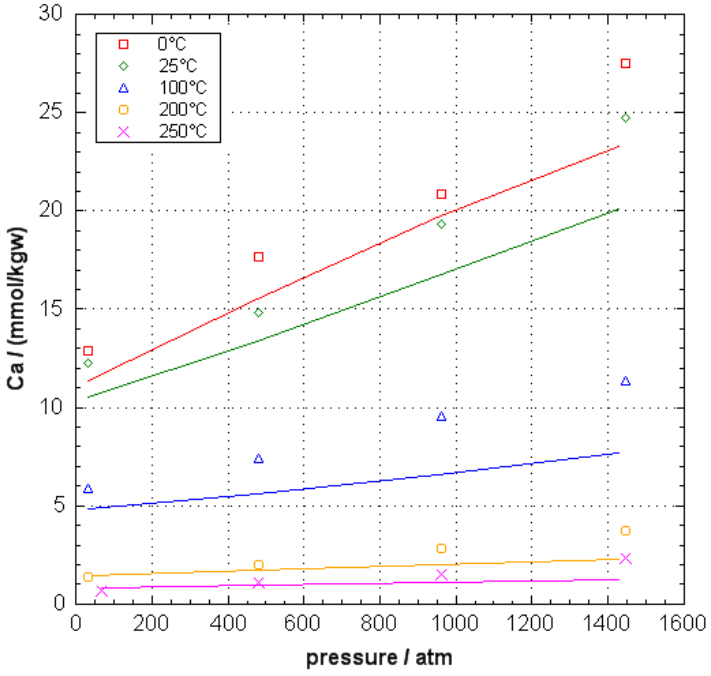

Figure A30. Solubility of calcite ($CaCO_3$) in 0.1 M NaCl as a function of temperature and pressure at 1 bar CO_2 pressure. Measured data from Shi et al., 2013. File cc_Shi.phr. Solubilities at 4 M NaCl and in a brine are also calculated when the file is run.

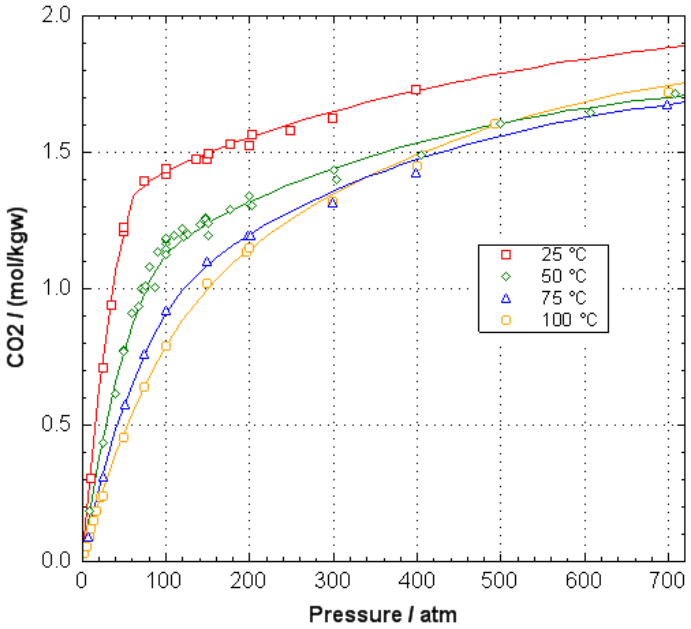

Figure A31. Solubility of CO_2 gas in water. Measured data from Wiebe and Gaddy, 1939, 1940; King et al., 1992; Takenouchi and Kennedy, 1964. File CO2_conc_PR_IS.phr.

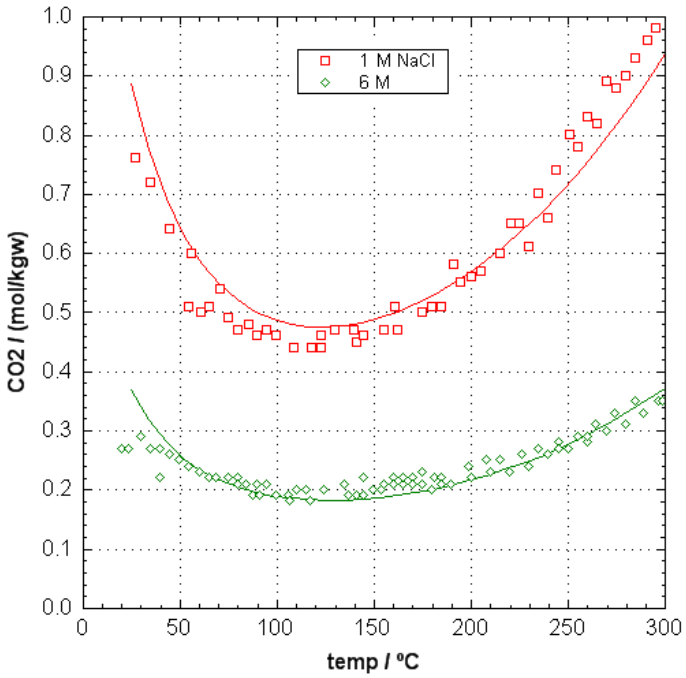

Figure A32. Solubility of CO_2 gas in 1 and 6 M NaCl solutions at about 40 atm CO_2. Measured data from Drummond, 1981. File Drummond.phr.

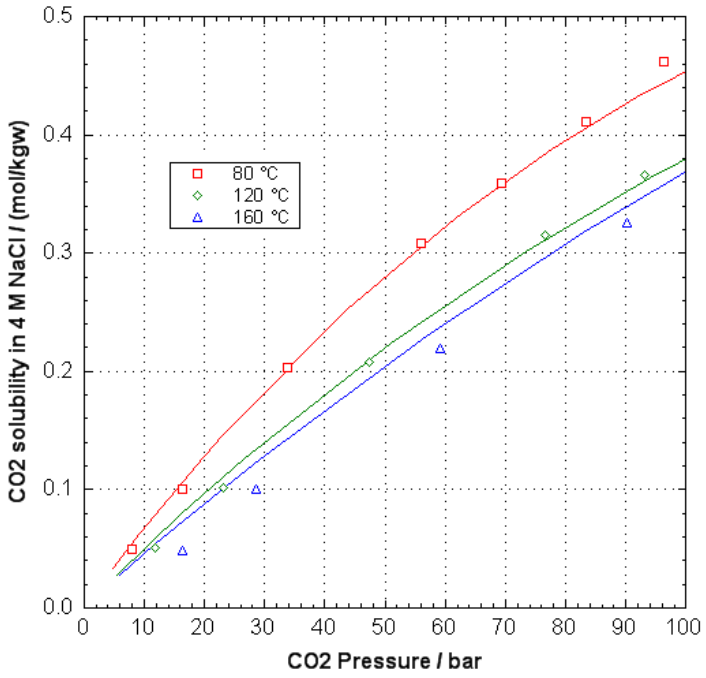

Figure A33. Solubility of CO_2 gas in 4 M NaCl solution. Measured data from Rumpf et al. 1994. File CO2_4M_NaCl.phr.

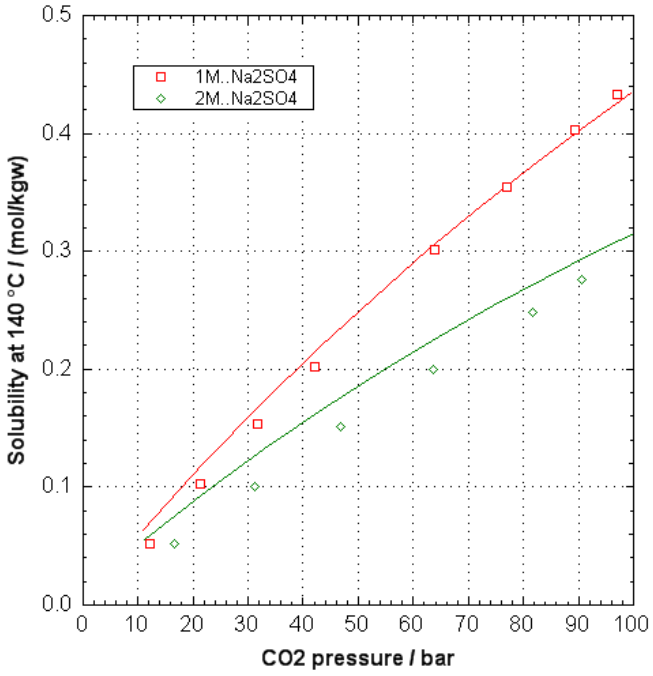

Figure A34. Solubility of CO_2 gas in Na_2SO_4 solutions at 140ºC. Measured data from Rumpf and Maurer, 1993. File P_CO2_Na2SO4.phr.

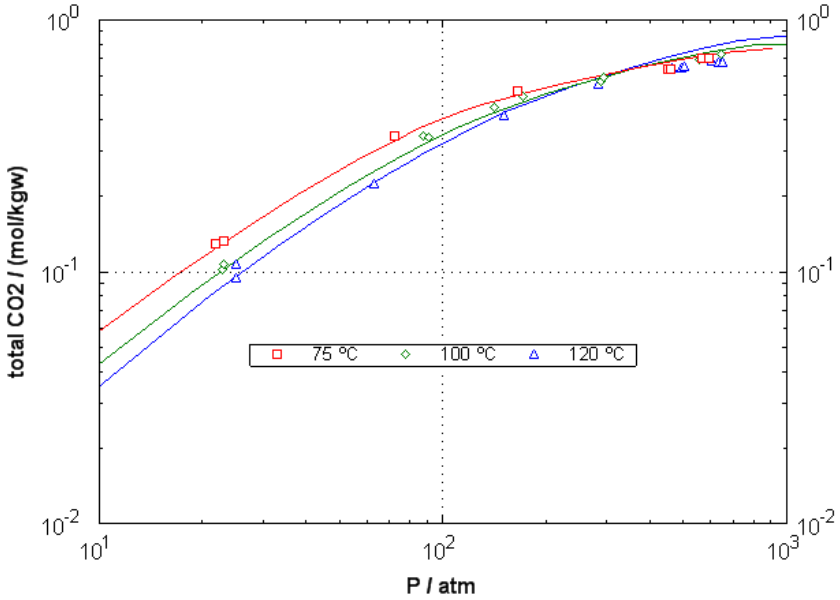

Figure A35. Solubility of CO_2 gas in 2.3 M $CaCl_2$ solution. Data from Springer et al., 2012. File CO2_CaCl2.phr.

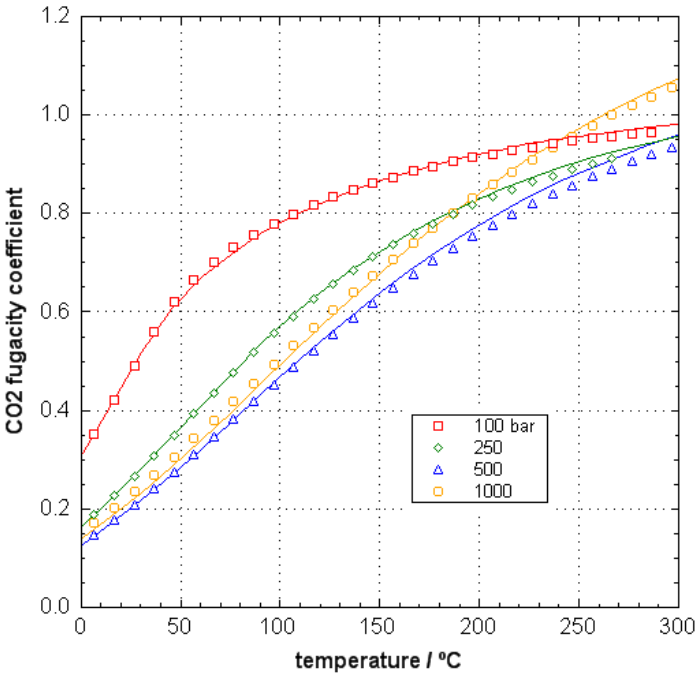

Figure A36. CO_2 fugacity coefficient as a function of temperature for CO_2 gas pressures from 100 - 1000 bar. Data from Angus et al., 1976. File phi_Angus_bar.phr.