ELECTRONIC NOTEBOOK #679

20.06002.01.211

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The entries in this electronic scientific notebook #679 document activities conducted during the period September 1, 2004, through February 28, 2005, under the Quantity and Chemistry of Water Contacting Engineered Barriers Integrated Subissue (Project Number 20.06002.01.211).

September 27, 2004

Initial Entry for: Verification and Validation of Mixed-Solvent Electrolyte Model for the Environmental Simulation Program and Analyzer Codes Developed by OLI Systems, Inc. (Morris Plains, NJ)

Conducted by: R. Pabalan

Description:

OLI Systems, Inc. developed a new thermodynamic model, referred to as the Mixed-Solvent Electrolyte (MSE) model, and associated thermodynamic database on electrolyte solutions for use with its chemical process simulation codes, including Environmental Simulation Program, StreamAnalyzer, and CorrosionAnalyzer. A description of the new model is given in the following references:

1. P. Wang and A. Anderko, "Computation of Dielectric Constants of Solvent Mixtures and Electrolyte Solutions ", Fluid Phase Equilibria, 186 (2001) 103-122.
2. A. Anderko, P. Wang and M. Rafal, "Electrolyte Solutions: From Thermodynamic and Transport Property Models to the Simulation of Industrial Processes", Fluid Phase Equilibria, 194-197 (2002) 123-142.
3. P. Wang, A. Anderko and R.D. Young, "A Speciation-Based Model for Mixed-Solvent Electrolyte Systems", Fluid Phase Equilibria, 203 (2002) 141-176.
4. P. Wang, R.D. Springer, A. Anderko and R.D. Young, "Modeling Phase Equilibria and Speciation in Mixed-Solvent Electrolyte Systems", Fluid Phase Equilibria, 222-223 (2004) 11-17.

Objective and Approach:

The objective of this task is to verify and validate the MSE model by comparing calculated values with experimental data. Verification and validation by comparison of calculated solubilities with experimental data were done by OLI Systems, Inc. for numerous binary and ternary aqueous systems. This comparison is documented by OLI Systems, Inc. in the Excel files "Prediction-September.xls", "PredSolid2.xls", "PredSolid3ClNO3.xls", "PredSolid3CO3.xls", "PredSolid3Misc.xls", and "PredSolid3SO4.xls", with references used as data sources listed in the file "References.xls". These Excel files are included in a CD (labeled ESN679-CD-1) that accompanies this scientific notebook.

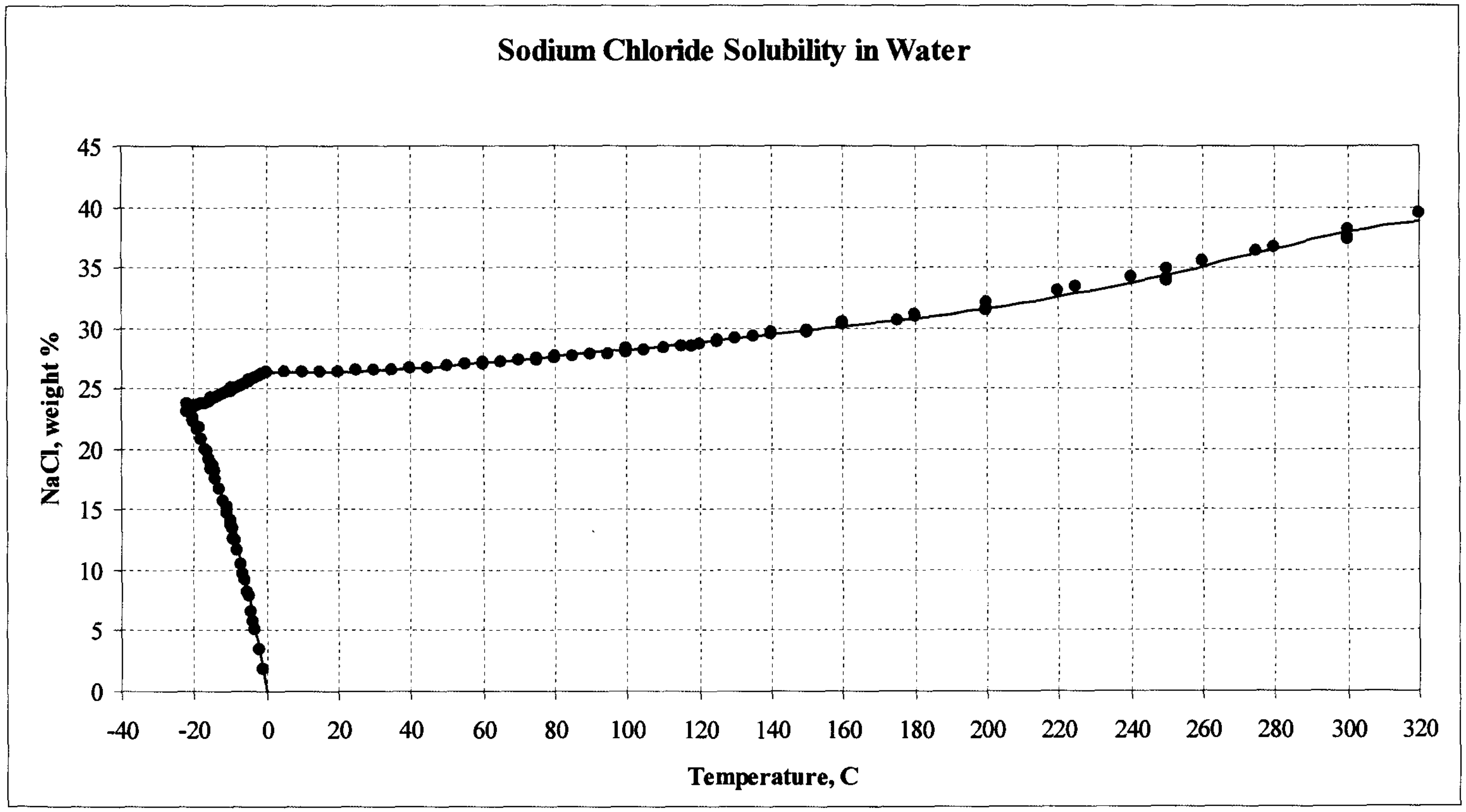
Additional verification and validation of the MSE model are documented in this notebook. The approach is to calculate solubilities, vapor pressures, deliquescence relative humidities, or other thermodynamic properties of electrolyte solutions using one of the OLI codes, and compare the results with published experimental data or other model results published in peer-reviewed literature. All the OLI codes use the same set of thermodynamic models and databases.

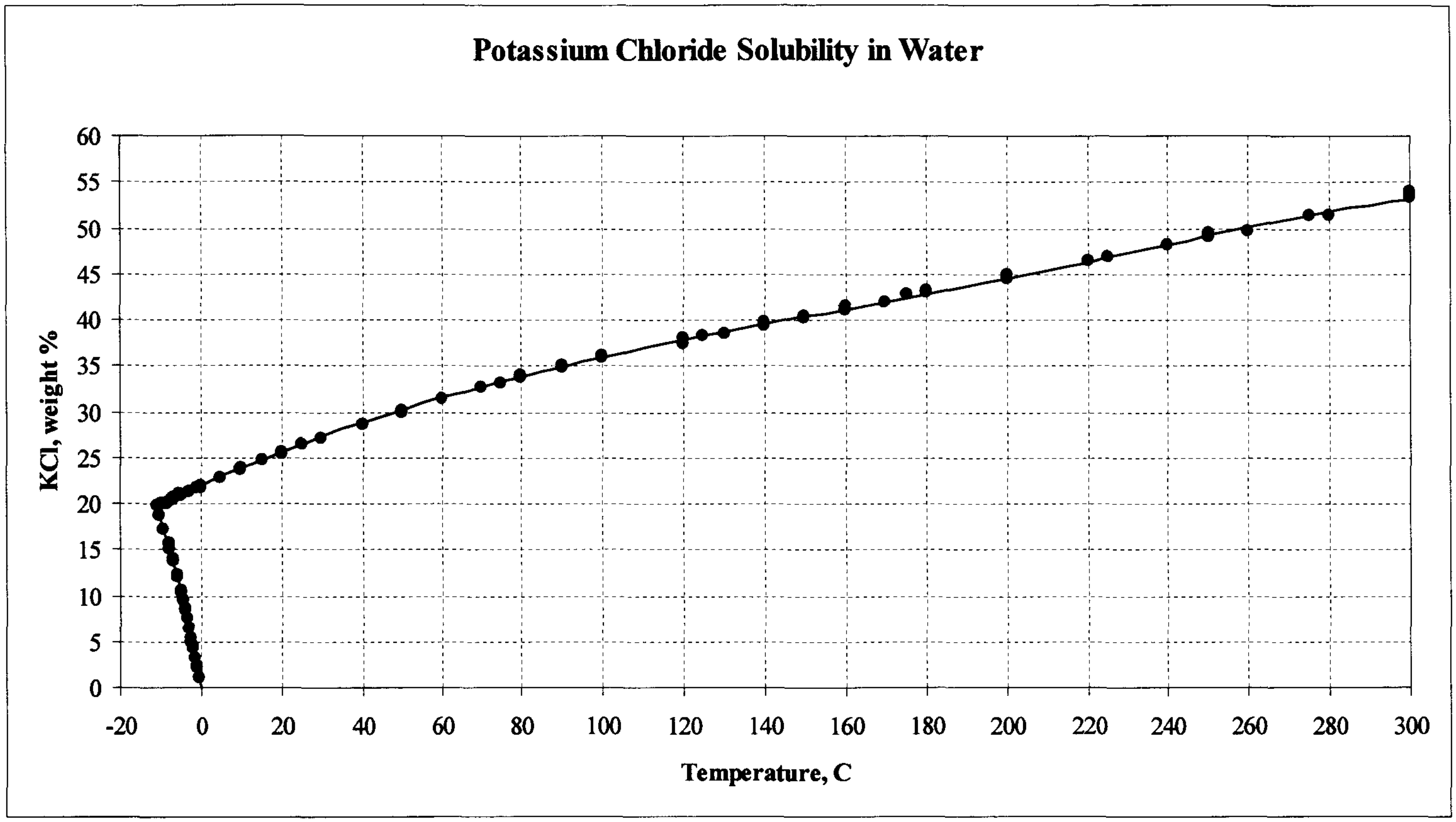
The following OLI codes have been validated and are under CNWRA configuration control: Environmental Simulation Program (ESP) Version 6.6, Corrosion Simulation Program (CSP) Version 2.3, Environmental Simulation Program for Concentrated Brines (ESPCB) Version 7.0-alpha, and StreamAnalyzer 1.2 (Yang, 2003, CNWRA software validation report). The intent of this task is to verify and validate the more recent versions of the OLI codes, including ESP Version 7.0 (equivalent to ESPCB) and StreamAnalyzer 2.0.

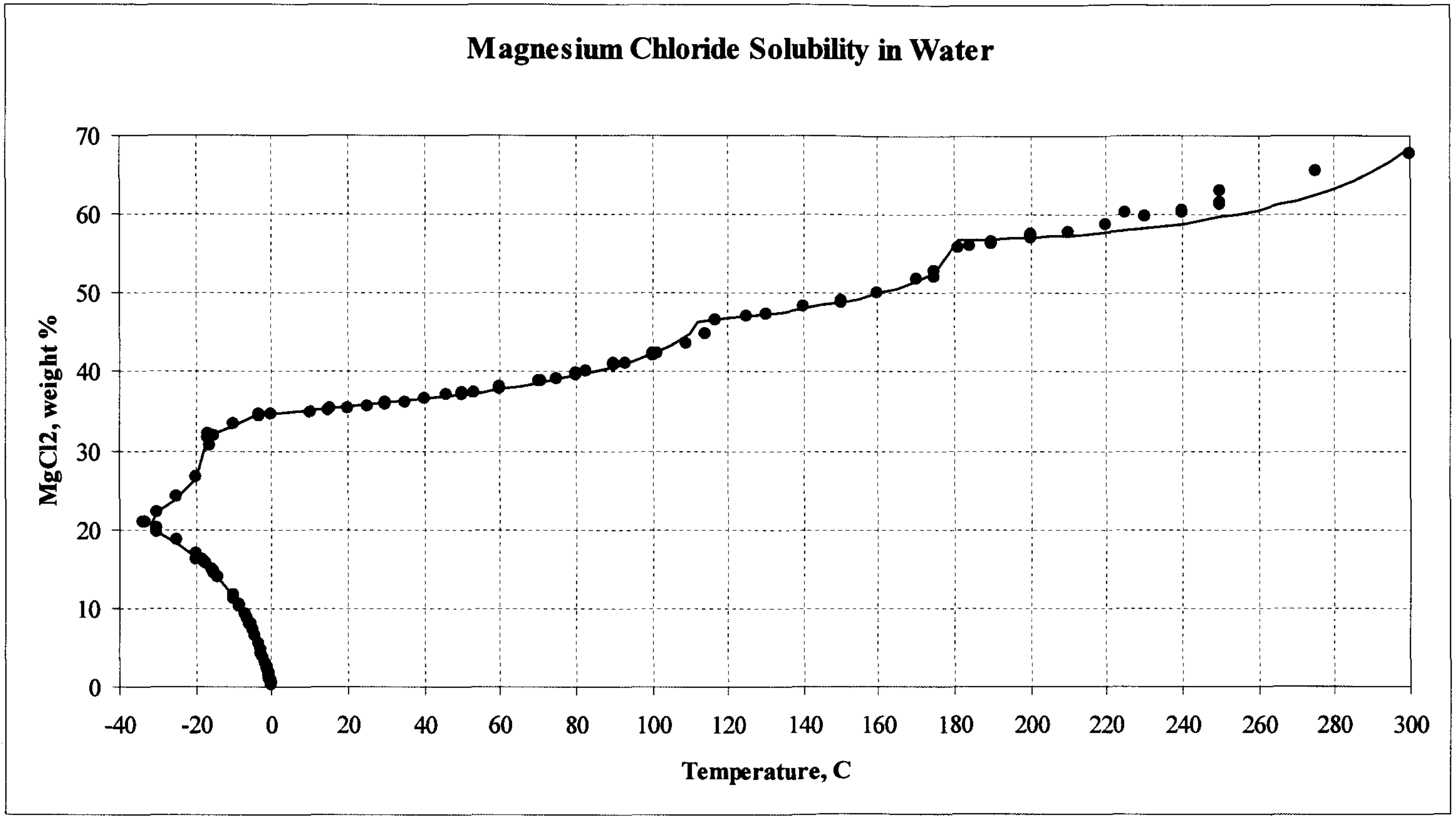
October 7, 2004

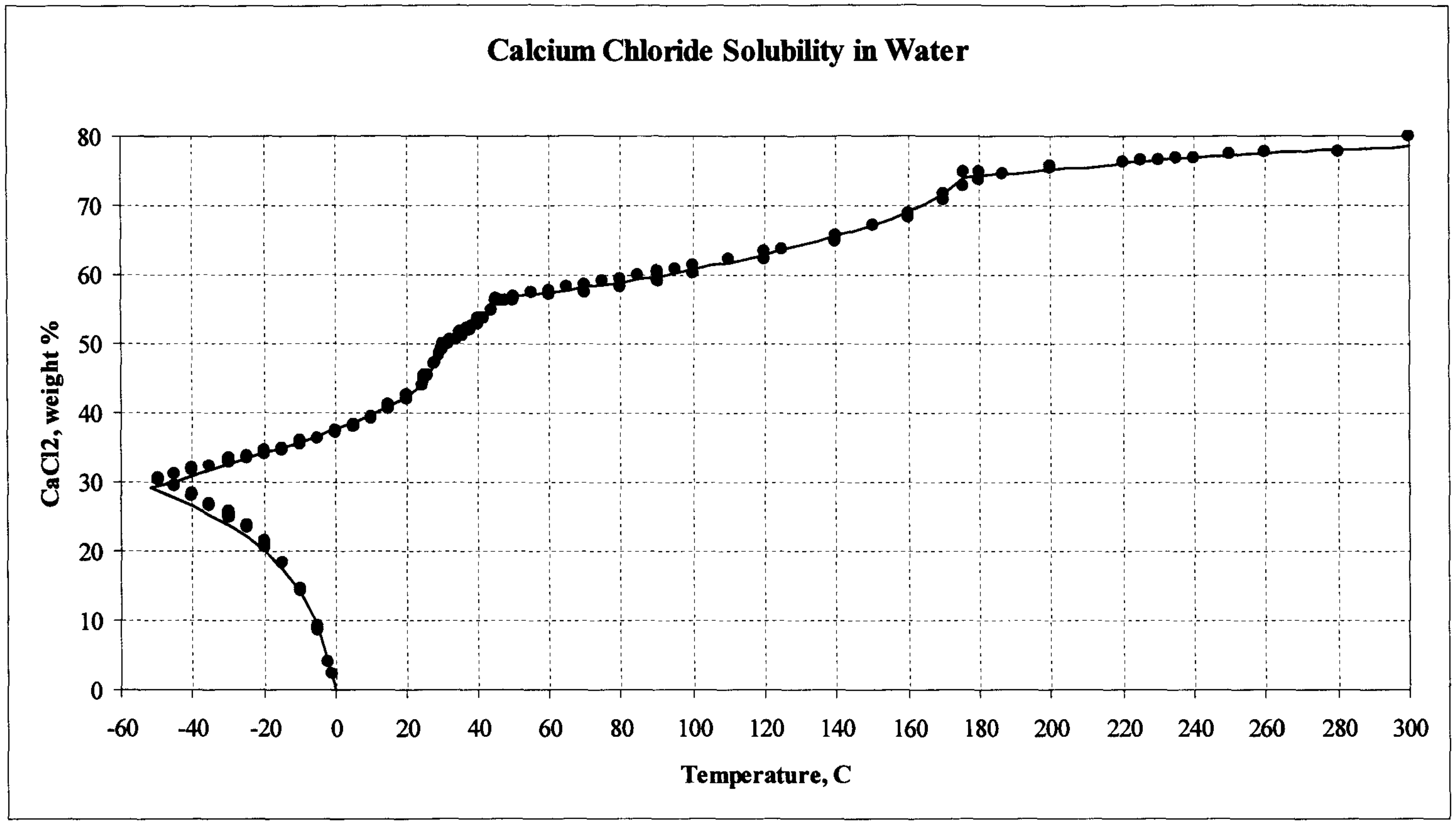
In the following pages (p. 3 to 113) are plots comparing solubilities calculated by OLI Systems, Inc. using ESP Version 7.0, build 20. The figures, provided by OLI Systems, Inc. in Excel spreadsheets that give the experimental and calculated values, were extracted and copied into this notebook. The following table lists the systems for which comparisons of experimental and calculated values are provided by OLI System, Inc., as well as the page numbers in this notebook corresponding to the different systems.

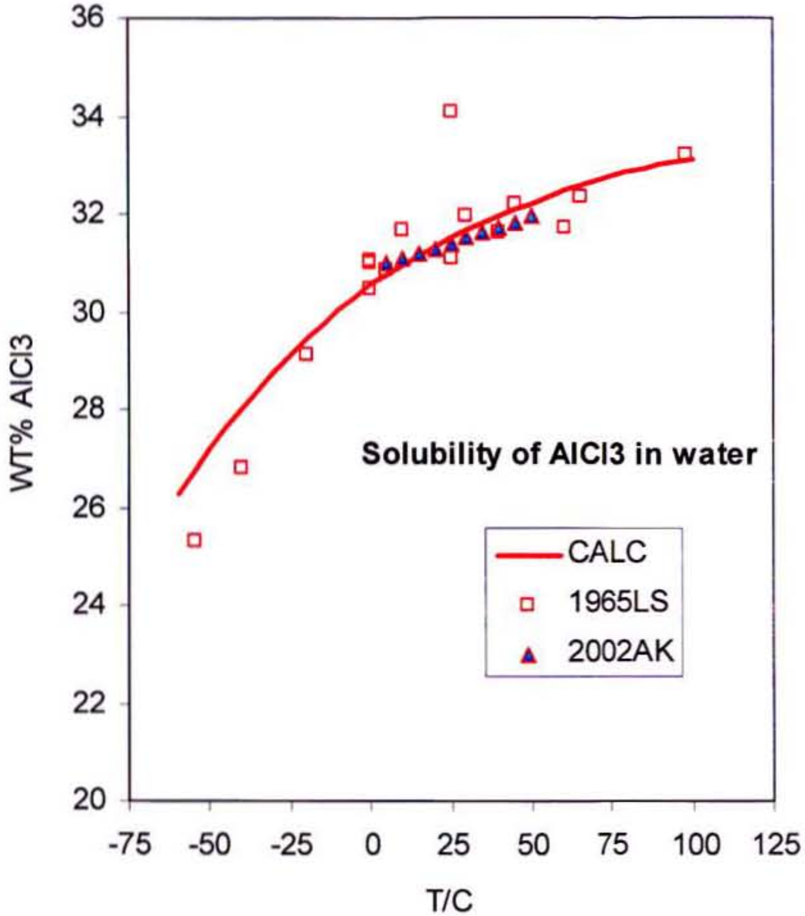
Binary Systems	Page #	Ternary Systems	Page #	Ternary Systems (Cont'd)	Page #	Ternary Systems (Cont'd)	Page #
NaCl	3	NaH2PO4	32	MgCl2-KNO3	65	NaH2PO4-KH2PO4	91
KCl	4	Na2HPO4	33	CaCl2-KNO3	66	H2SO4-(NH4)2SO4	92
MgCl2	5	KH2PO4	34	MgCl2-Mg(NO3)2	67	H2SO4(saltfree)-(NH4)2SO4	93
CaCl2	6	K2HPO4	35	CaCl2-Ca(NO3)2	68		
AlCl3	7						
		NaF	36	Na2SO4-NaCl	69	NaF-NaCl	94
NaNO3	8	KF	37	CaSO4-NaCl	70	KF-NaCl	95
KNO3	9	MgF2	38	Al2(SO4)3-NaCl	71	MgF2-NaCl	96
Mg(NO3)2	10	CaF2	39	CaSO4-CaCl2	72	CaF2-NaCl	97
Ca(NO3)2	11	AlF3	40			AlF3-NaCl	98
Al(NO3)3	12			Na2SO4-NaNO3	73	KF-KCl	99
		KOHvp	41			NaF-KCl	100
Na2SO4	13	KOHphi	42	Na2SO4-K2SO4	74		
K2SO4	14	KOHhdil	43	Na2SO4-CaSO4	75	Al(OH)3-NaOH	101
(NH4)2SO4	15	KOHcp	44	Na2SO4-Al2(SO4)3	76	Al(OH)3-NaCl	102
MgSO4	16			K2SO4-CaSO4	77	AlOOH-NaCl-constNaCl	103
CaSO4	17	NaCl-KCl	45			AlOOH-NaCl-ConstT	104
Al2(SO4)3	18	NaCl-MgCl2	46	NaCl-CaCO3	78		
		NaCl-CaCl2	47	CaCl2-CaCO3	79	Al(OH)3,AlOOH vs pH	105
Na2CO3	19	NaCl-AlCl3	48				
K2CO3	20	KCl-MgCl2	49	Na2CO3-K2CO3	80	**Acids**	
MgCO3	21	KCl-CaCl2	50	Na2CO3-MgCO3	81		
CaCO3	22	MgCl2-CaCl2	51	Na2CO3-CaCO3	82	TPA	106
		AlCl3-HCl	52			Na2TPT	107
NaHCO3	23			Na2CO3-NaHCO3	83	IPA	108
KHCO3	24	NaNO3-KNO3	53	K2CO3-KHCO3	84	TMA	109
		NaNO3-Mg(NO3)2	54			NA	110
NaOH	25	NaNO3-Ca(NO3)2	55	Na2CO3-Na2SO4	85,86	Na2NT	111
KOH	26	KNO3-Mg(NO3)2	56				
CaOH2	27	KNO3-Ca(NO3)2	57	MgCO3 vs pCO2	87	H2SO4-SO3vp300h	112
Al(OH)3	28	Mg(NO3)2-Ca(NO3)2	58	CaCO3 vs pCO2	88	H3PO4vp	113
H3PO4	29	NaCl-NaNO3	59	NaOH-NaCl	89		
Na3PO4	30	NaCl-KNO3	60	NaOH-Na2SO4	90		
K3PO4	31	NaCl-Ca(NO3)2	61				
		NaCl-Al(NO3)2	62				
		KCl-KNO3	63				
		KCl-Ca(NO3)2	64				

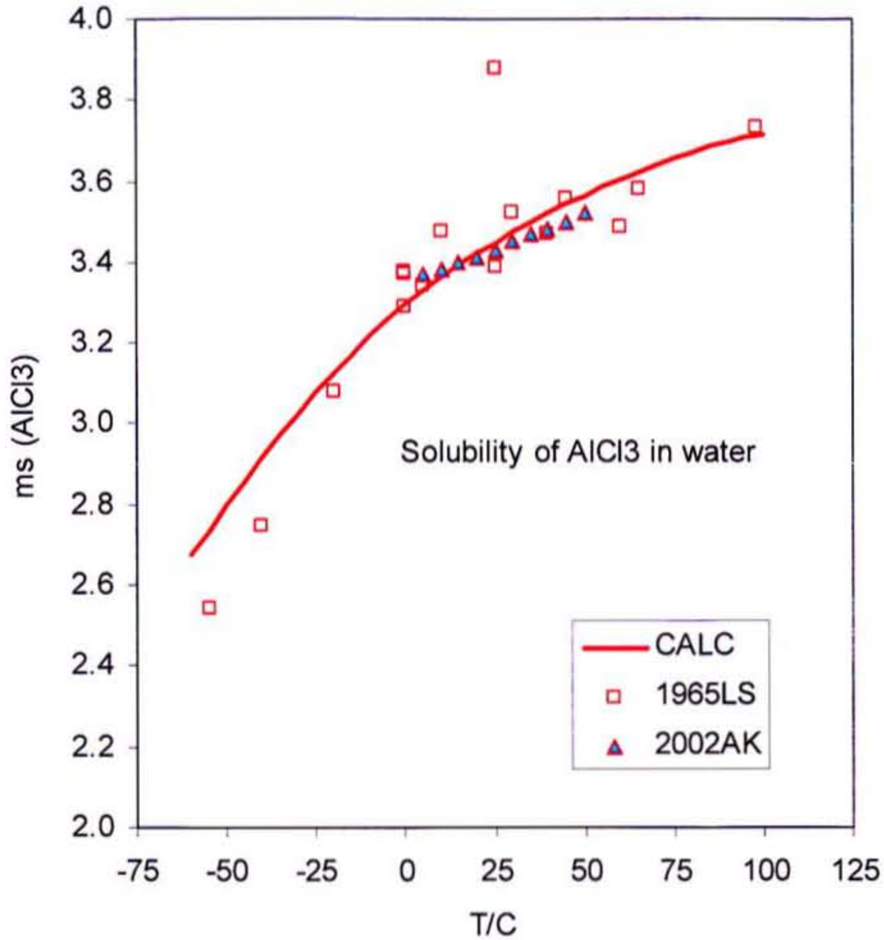

Sodium Chloride Solubility in Water
NaCl, weight %
45
40
35
30
25
20
15
10
5
0
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
Temperature, C

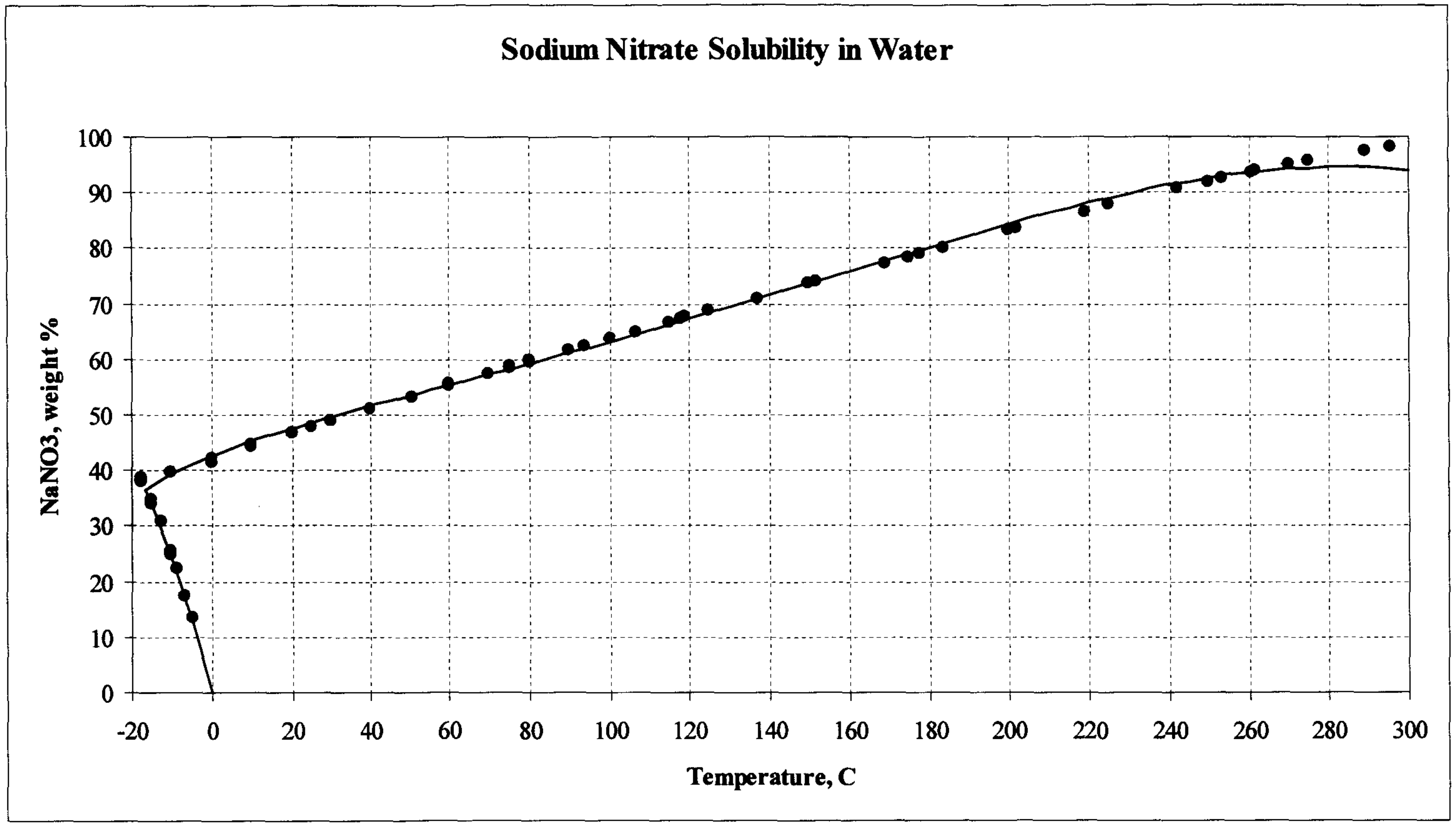

Potassium Chloride Solubility in Water
KCl, weight %
Temperature, C
60
55
50
45
40
35
30
25
20
15
10
5
0
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300

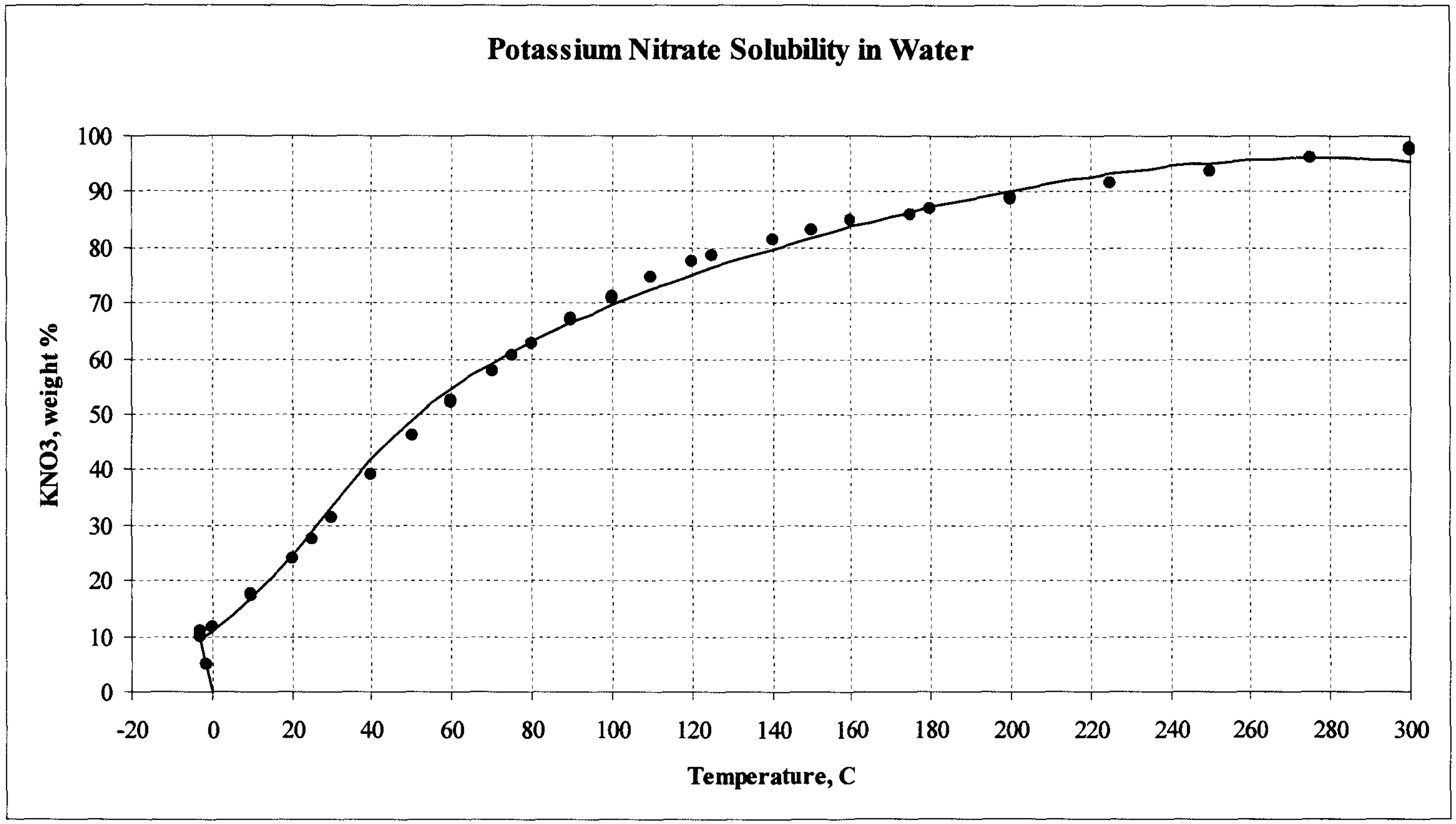

Magnesium Chloride Solubility in Water
MgCl2, weight %
Temperature, C
0
10
20
30
40
50
60
70
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300

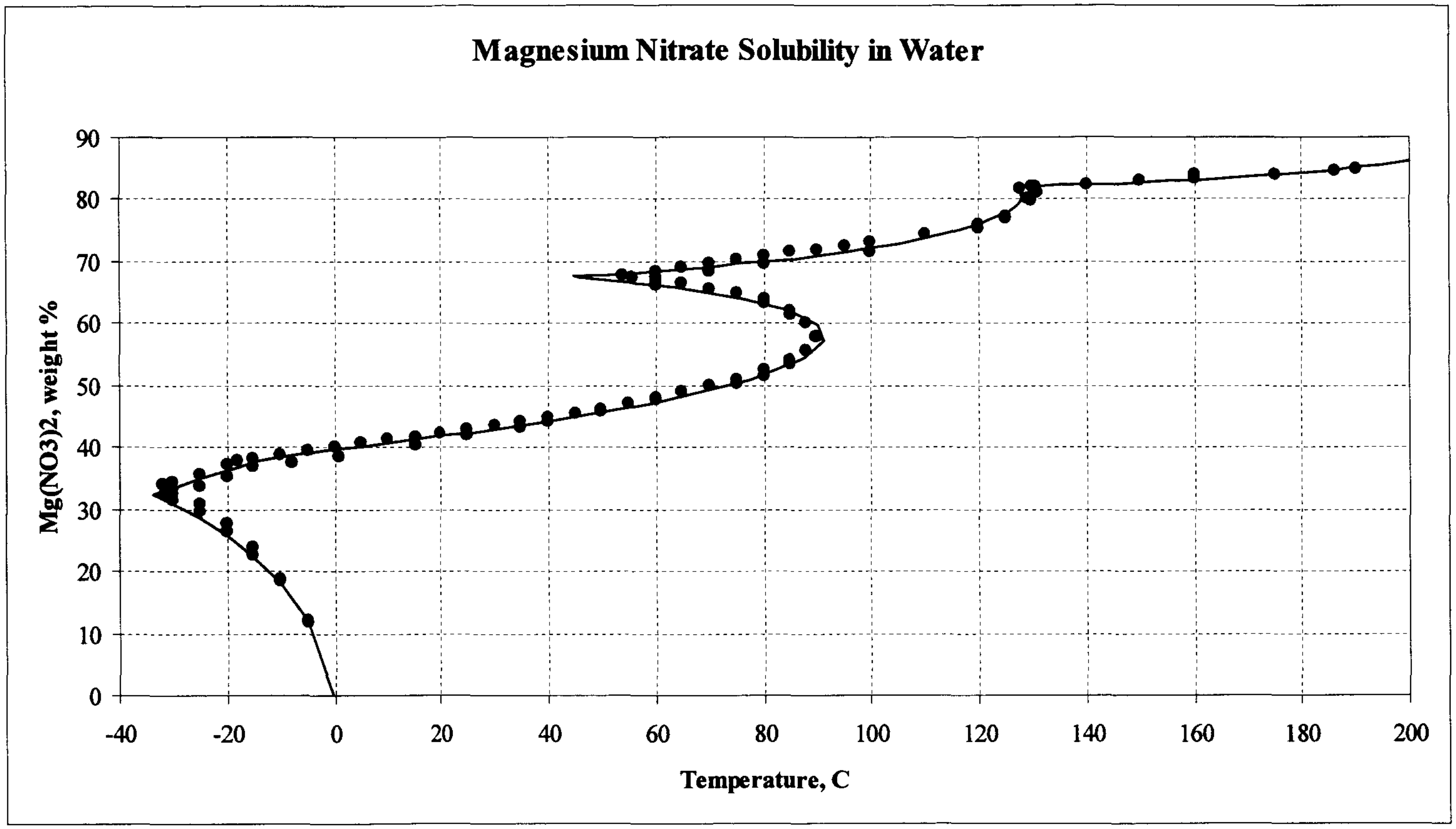

Calcium Chloride Solubility in Water
CaCl2, weight %
80
70
60
50
40
30
20
10
0
-60
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C

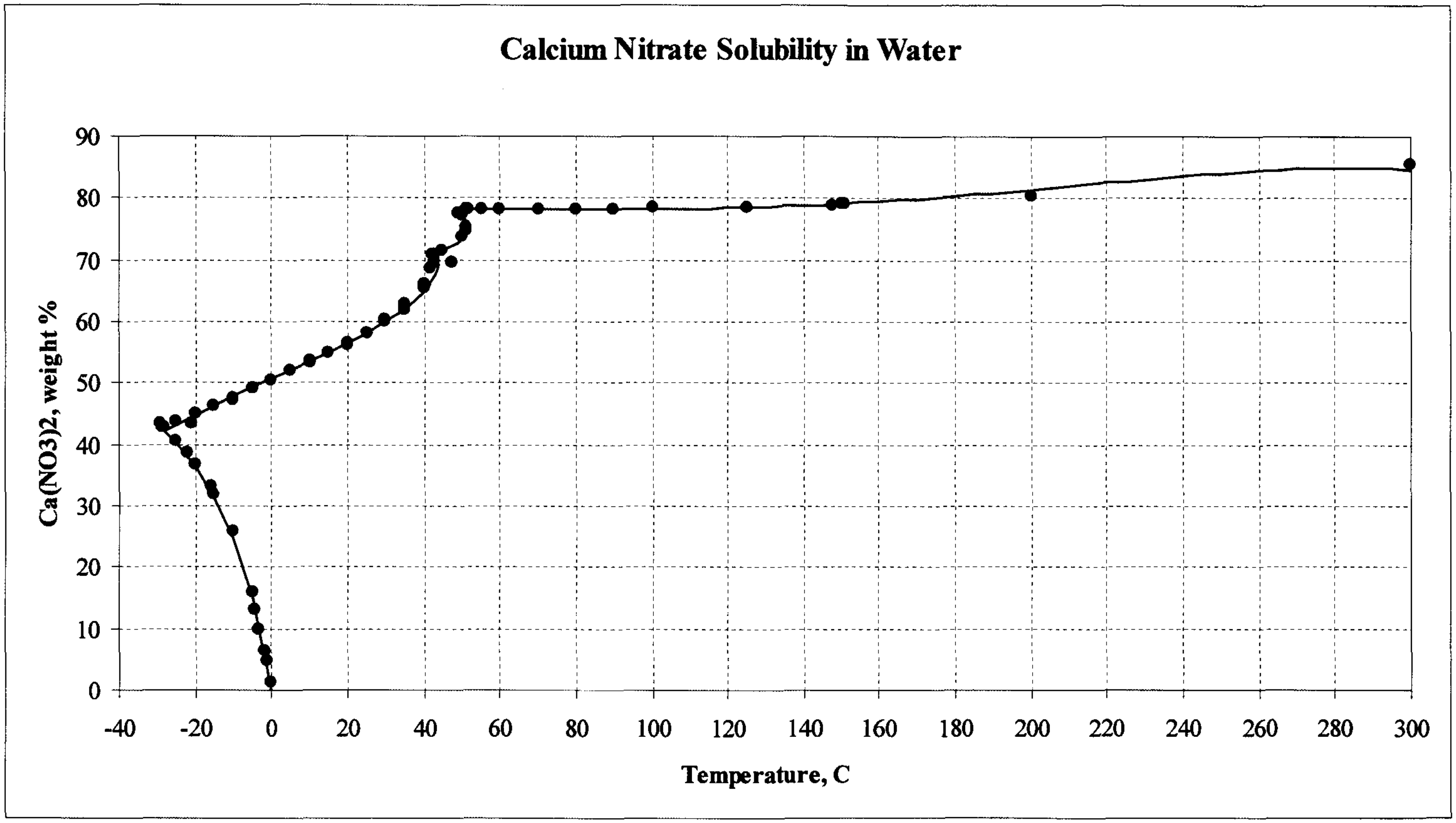

36
34
32
30
28
26
24
22
20
WT% AlCl3
-75
-50
-25
0
25
50
75
100
125
T/C
Solubility of AlCl3 in water
CALC
1965LS
2002AK


4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
ms (AlCl3)
-75
-50
-25
0
25
50
75
100
125
T/C
Solubility of AlCl3 in water
CALC
1965LS
2002AK

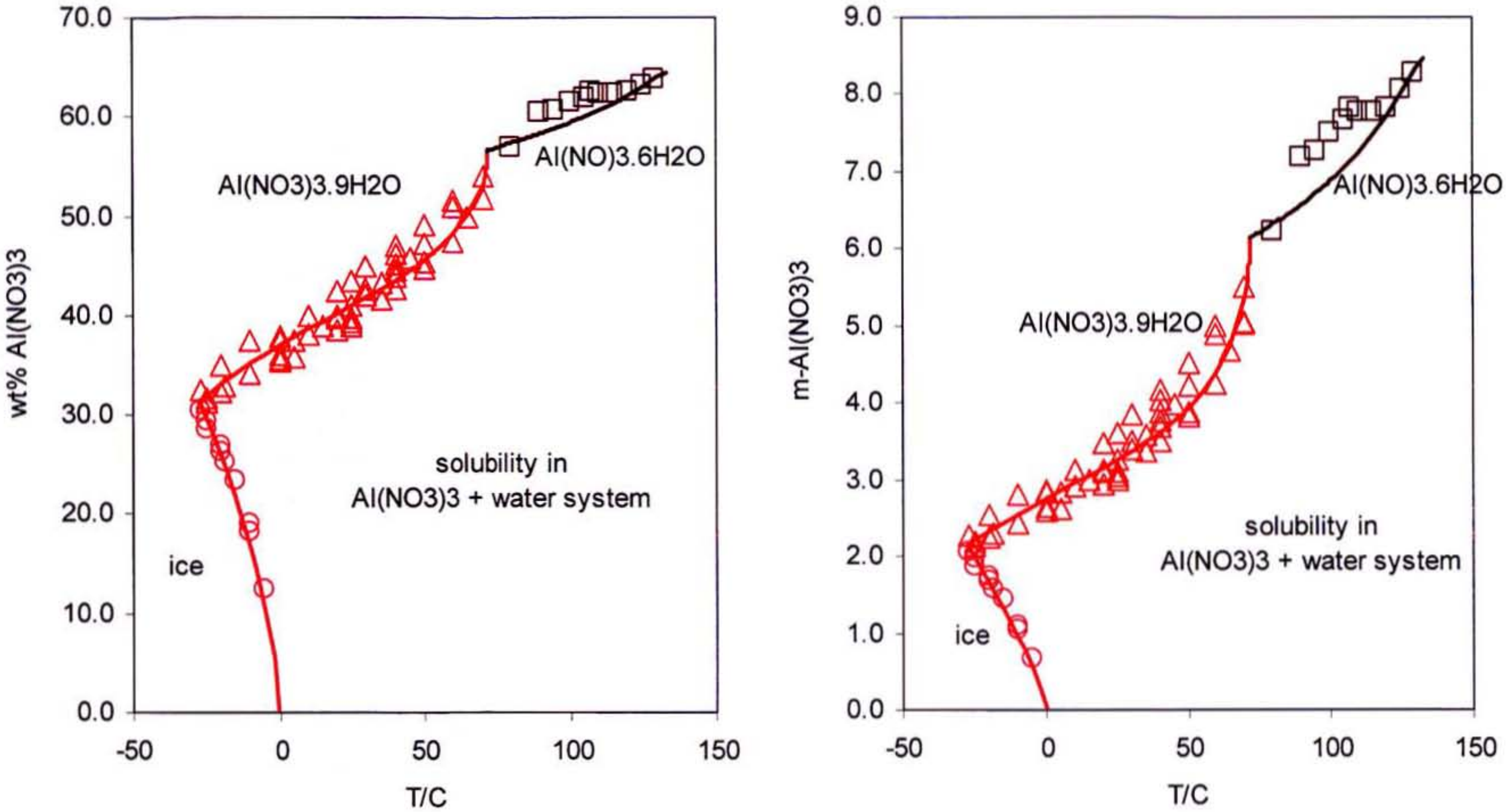

Sodium Nitrate Solubility in Water
NaNO3, weight %
100
90
80
70
60
50
40
30
20
10
0
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C

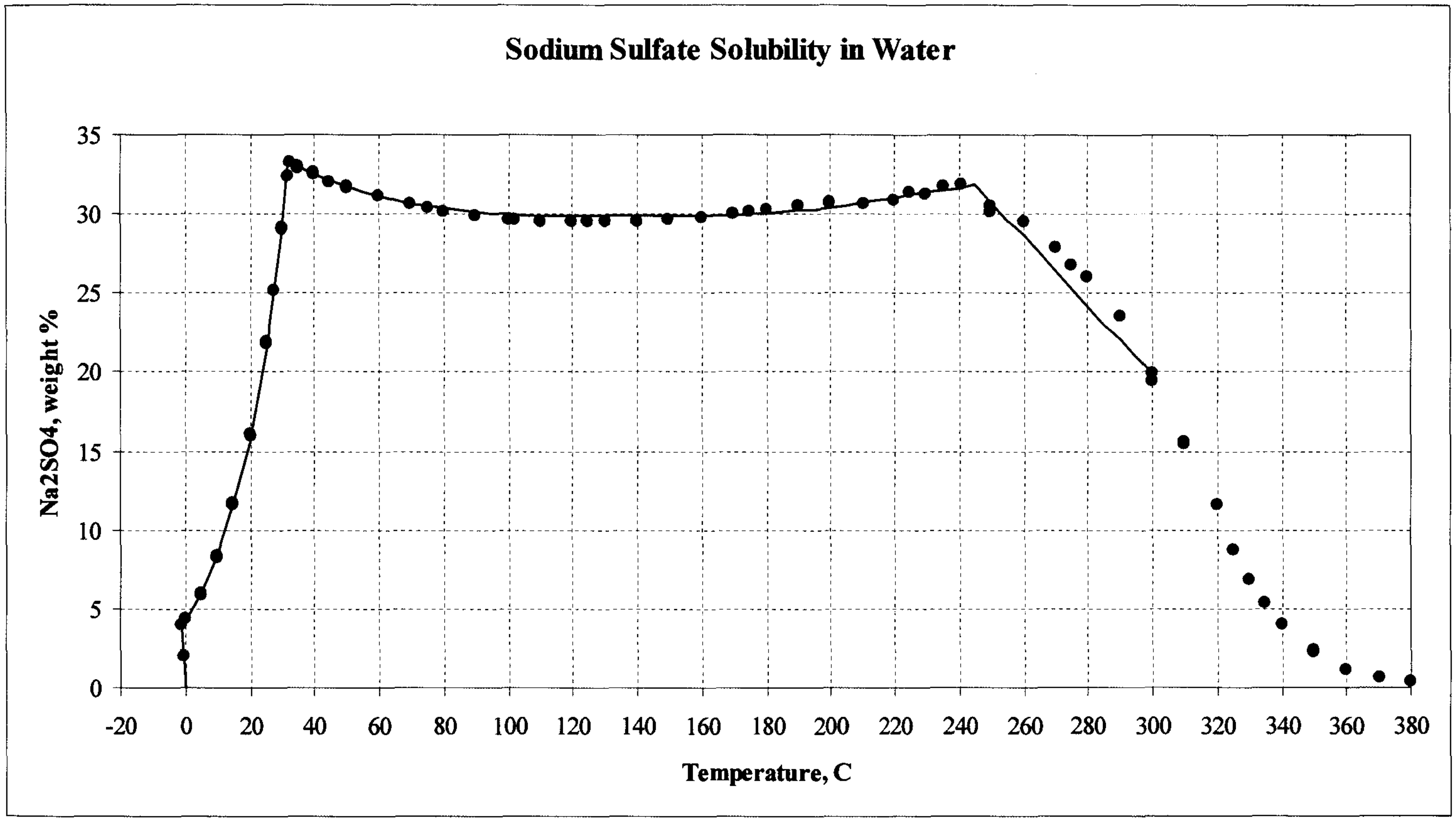

Potassium Nitrate Solubility in Water
KNO3, weight %
100
90
80
70
60
50
40
30
20
10
0
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C

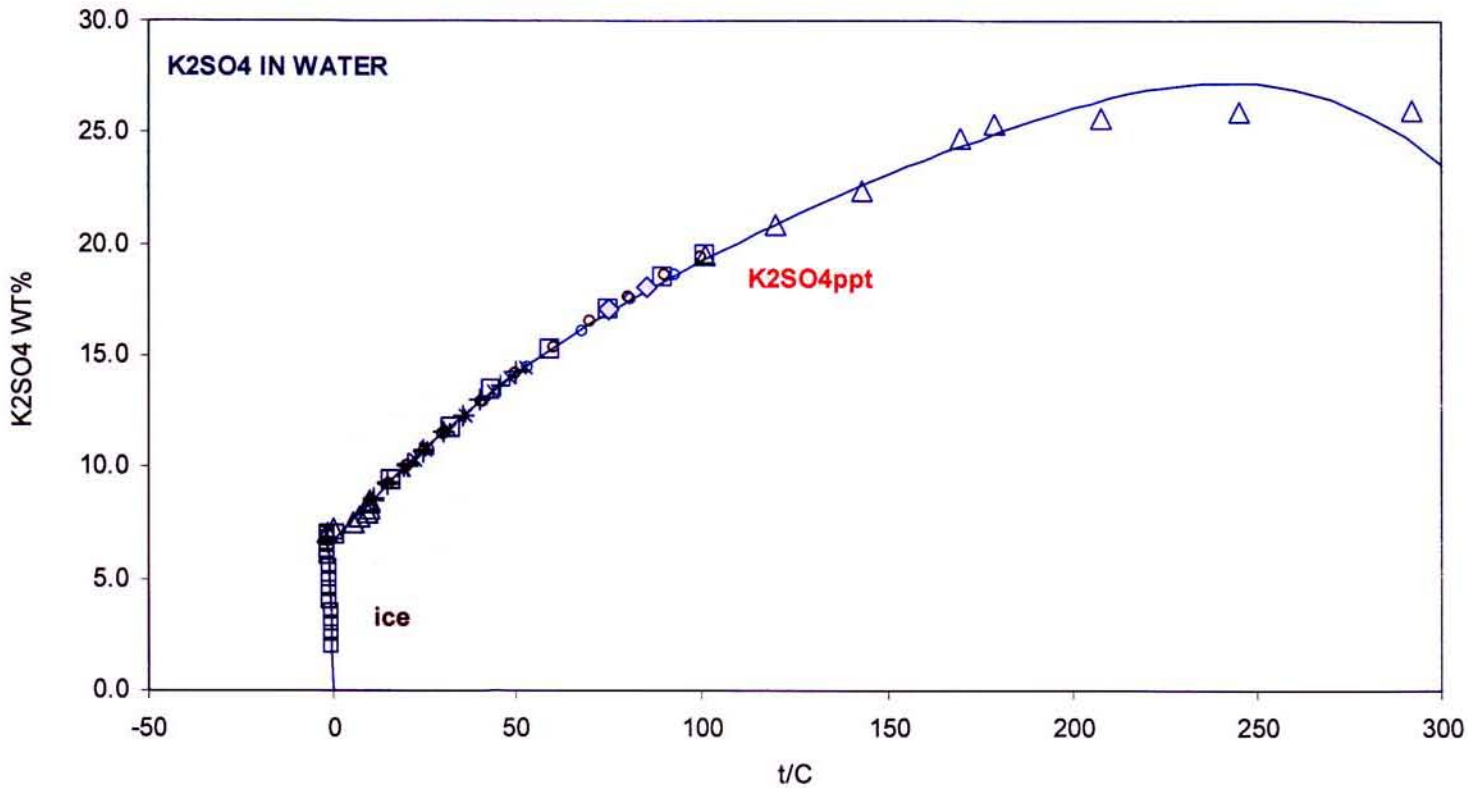

Magnesium Nitrate Solubility in Water
Mg(NO3)2, weight %
90
80
70
60
50
40
30
20
10
0
-40
-20
0
20
40
60
80
100
120
140
160
180
200
Temperature, C

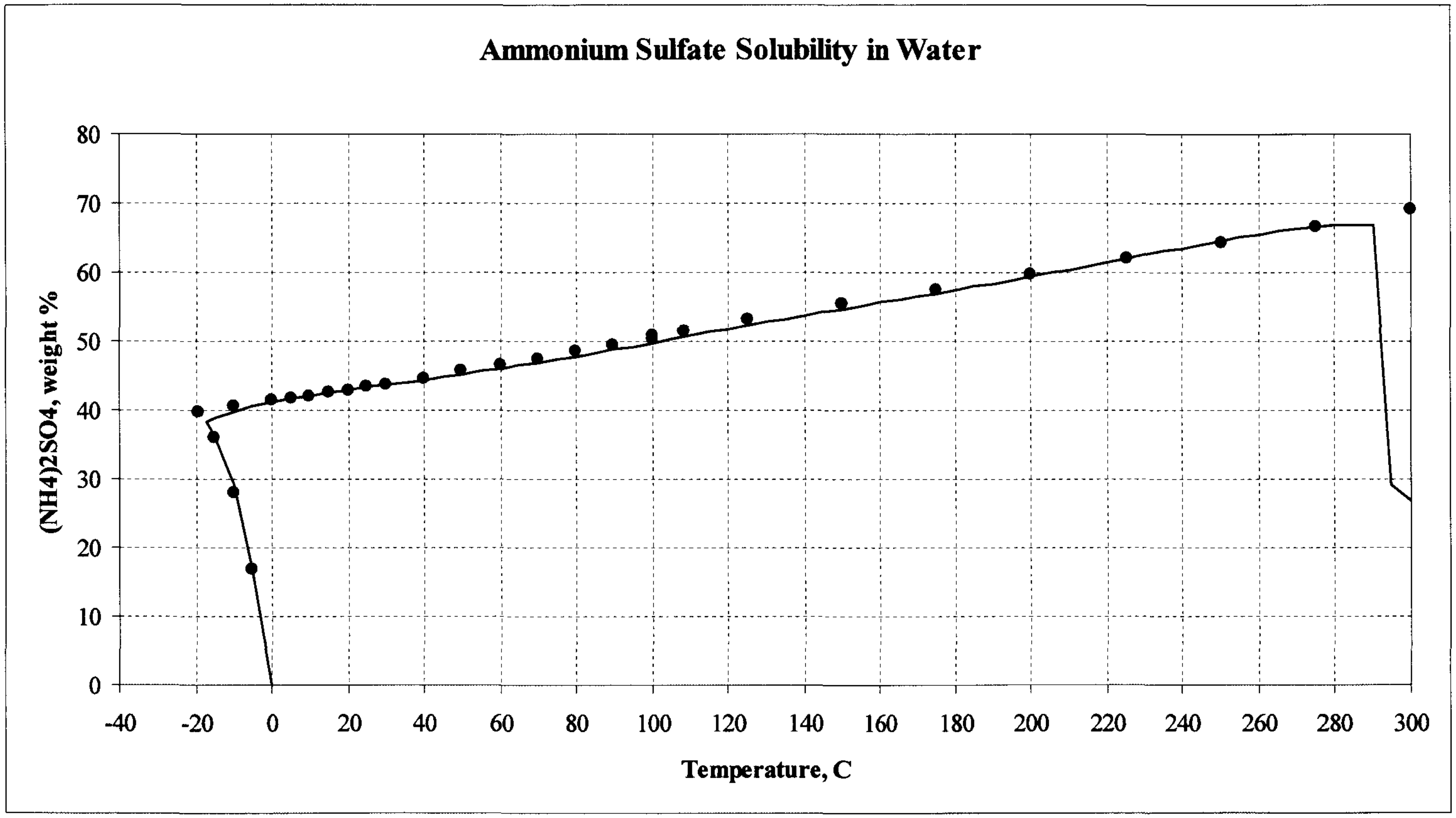


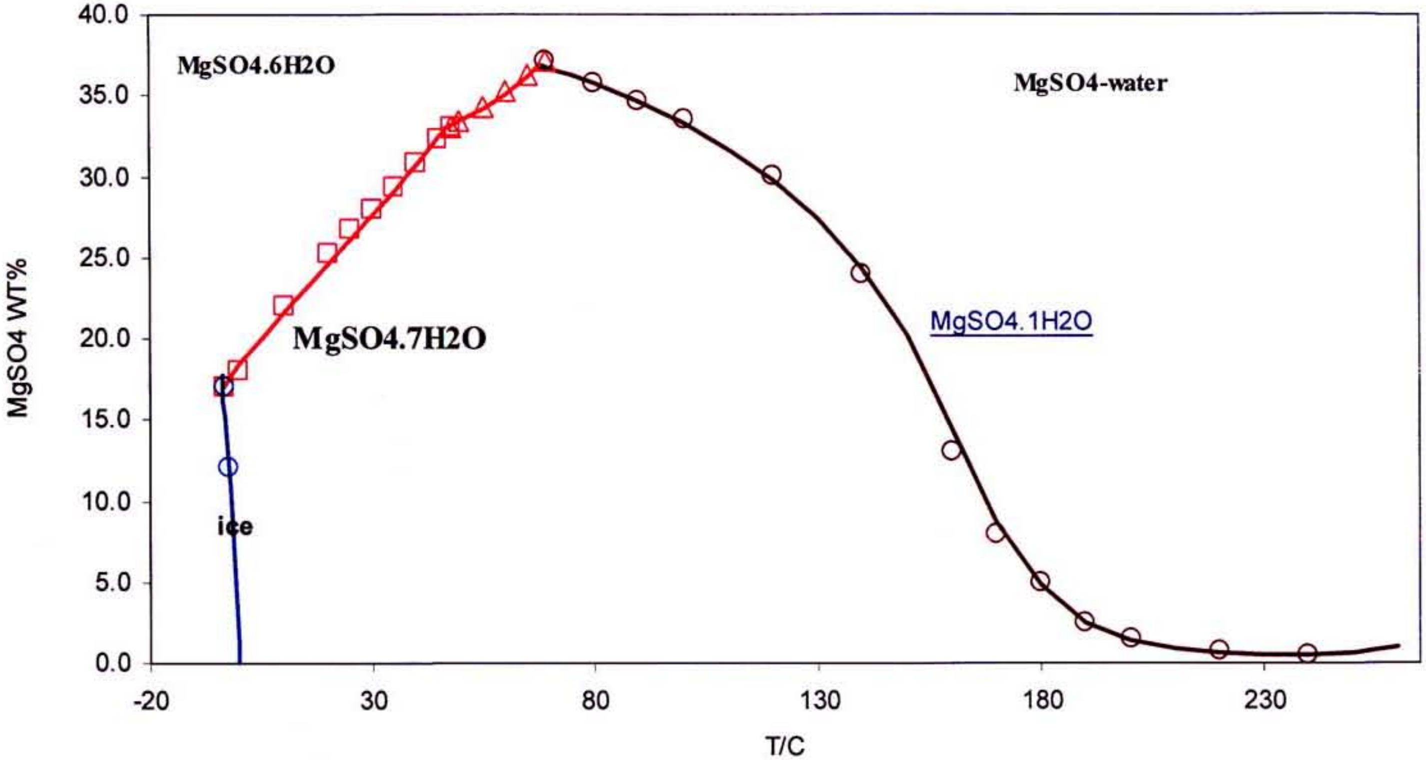
Calcium Nitrate Solubility in Water
Ca(NO3)2, weight %
90
80
70
60
50
40
30
20
10
0
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C

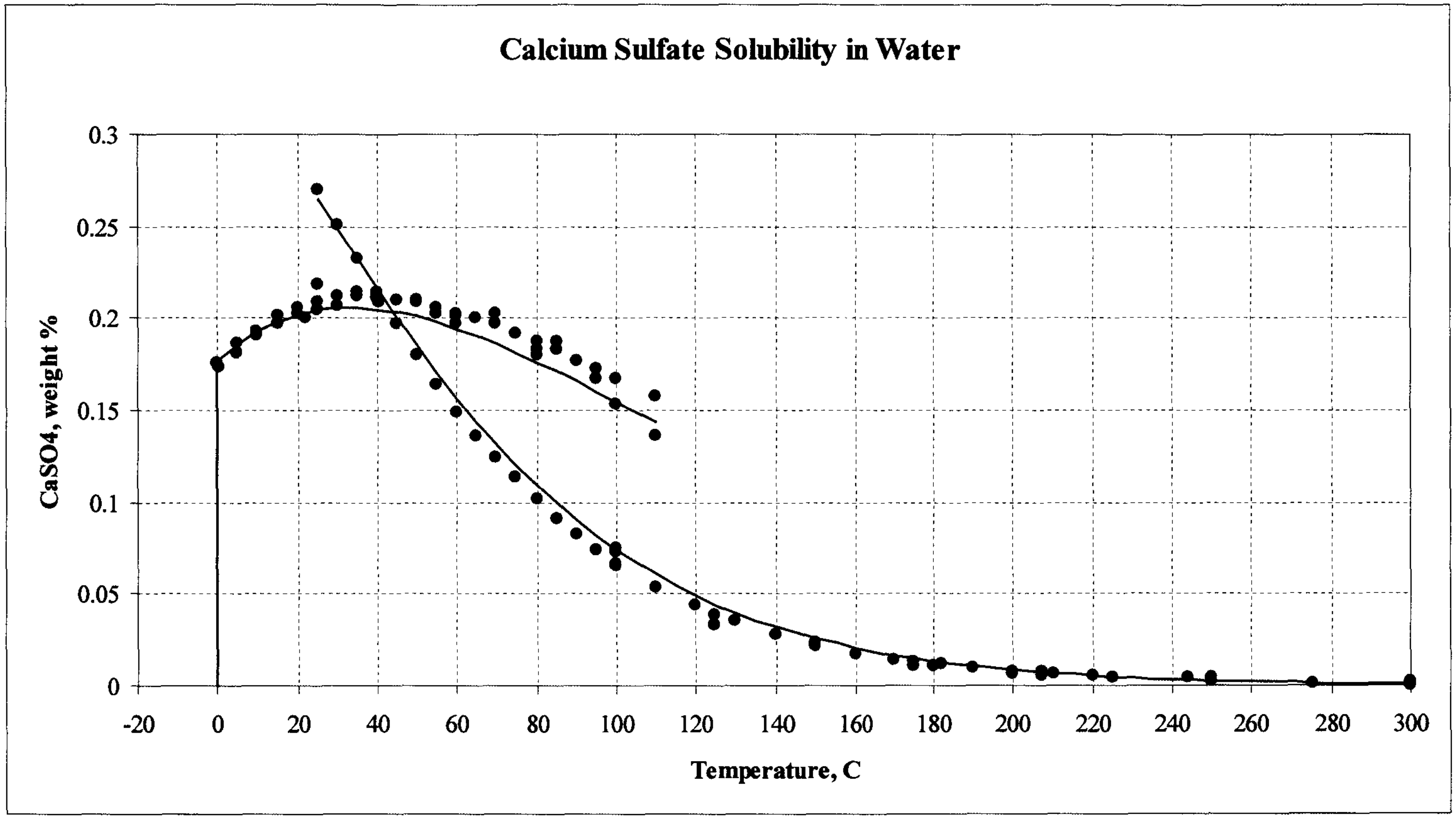

70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
wt% Al(NO3)3
Al(NO3)3.9H2O
Al(NO)3.6H2O
solubility in
Al(NO3)3 + water system
ice
-50
0
50
100
150
T/C
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
m-Al(NO3)3
Al(NO)3.6H2O
Al(NO3)3.9H2O
solubility in
Al(NO3)3 + water system
ice
-50
0
50
100
150
T/C

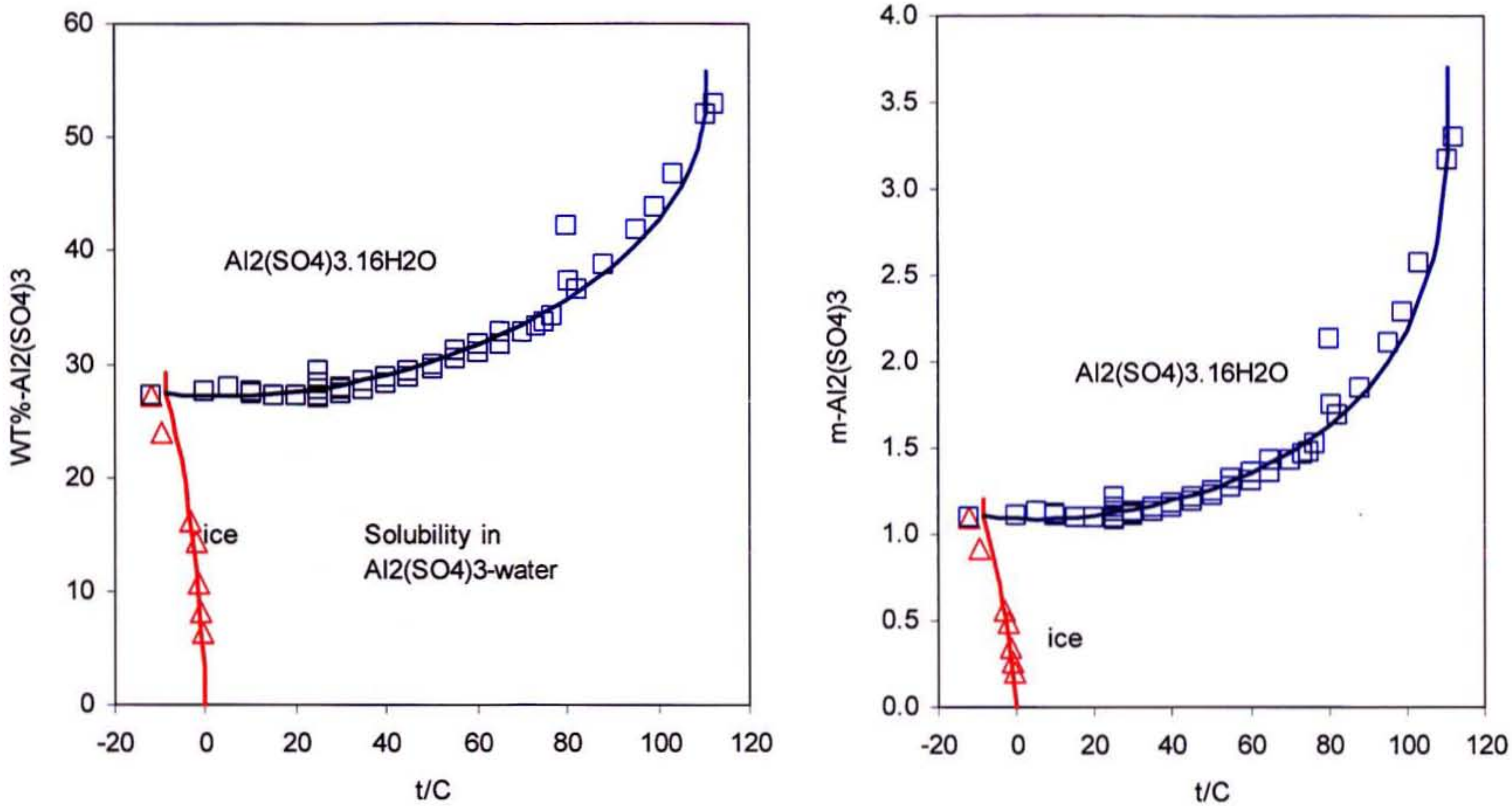

Sodium Sulfate Solubility in Water
Na2SO4, weight %
35
30
25
20
15
10
5
0
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
Temperature, C


K2SO4 IN WATER
K2SO4 WT%
t/C
K2SO4ppt
ice
30.0
25.0
20.0
15.0
10.0
5.0
0.0
-50
0
50
100
150
200
250
300

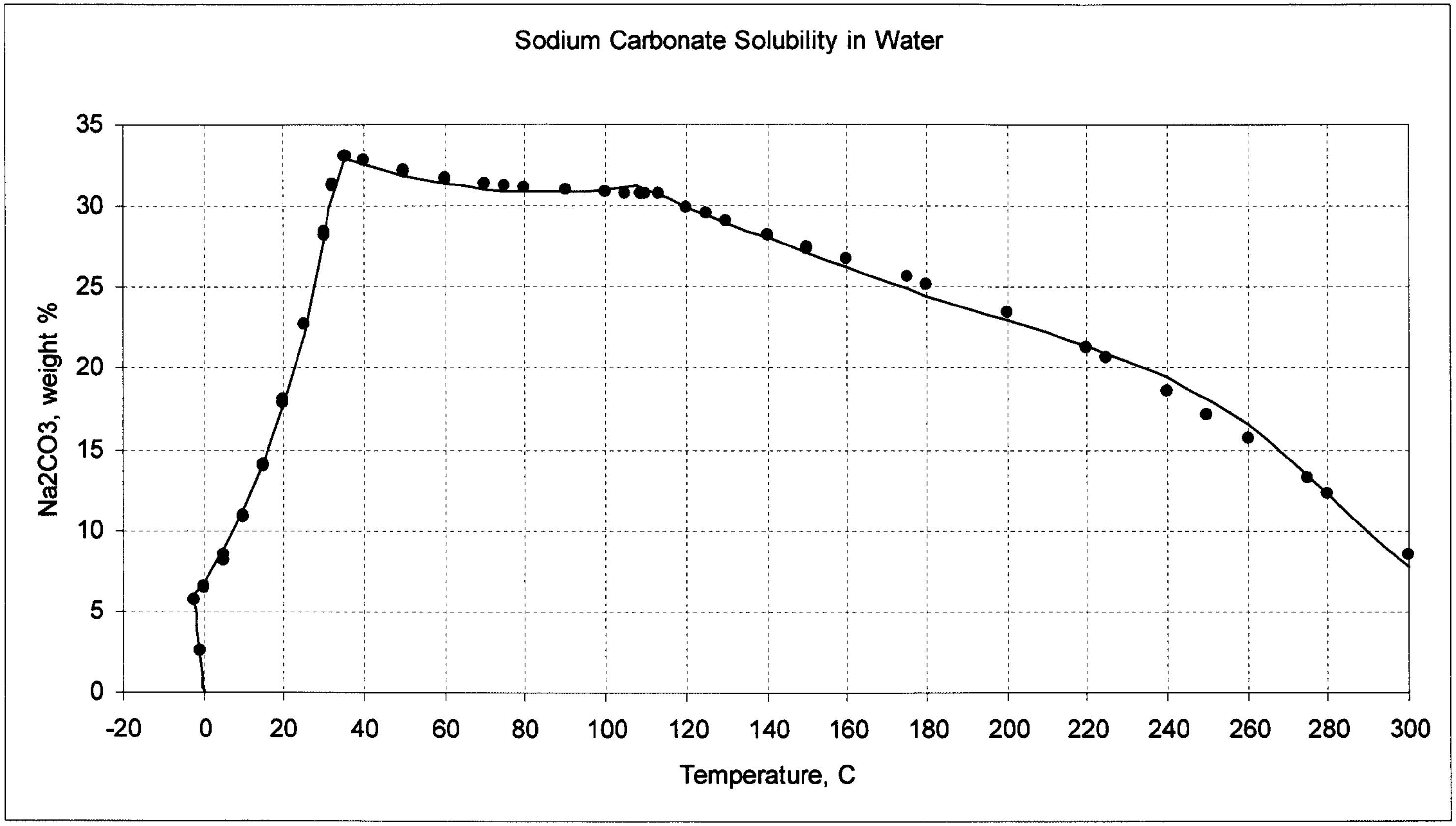

Ammonium Sulfate Solubility in Water
(NH4)2SO4, weight %
80
70
60
50
40
30
20
10
0
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C

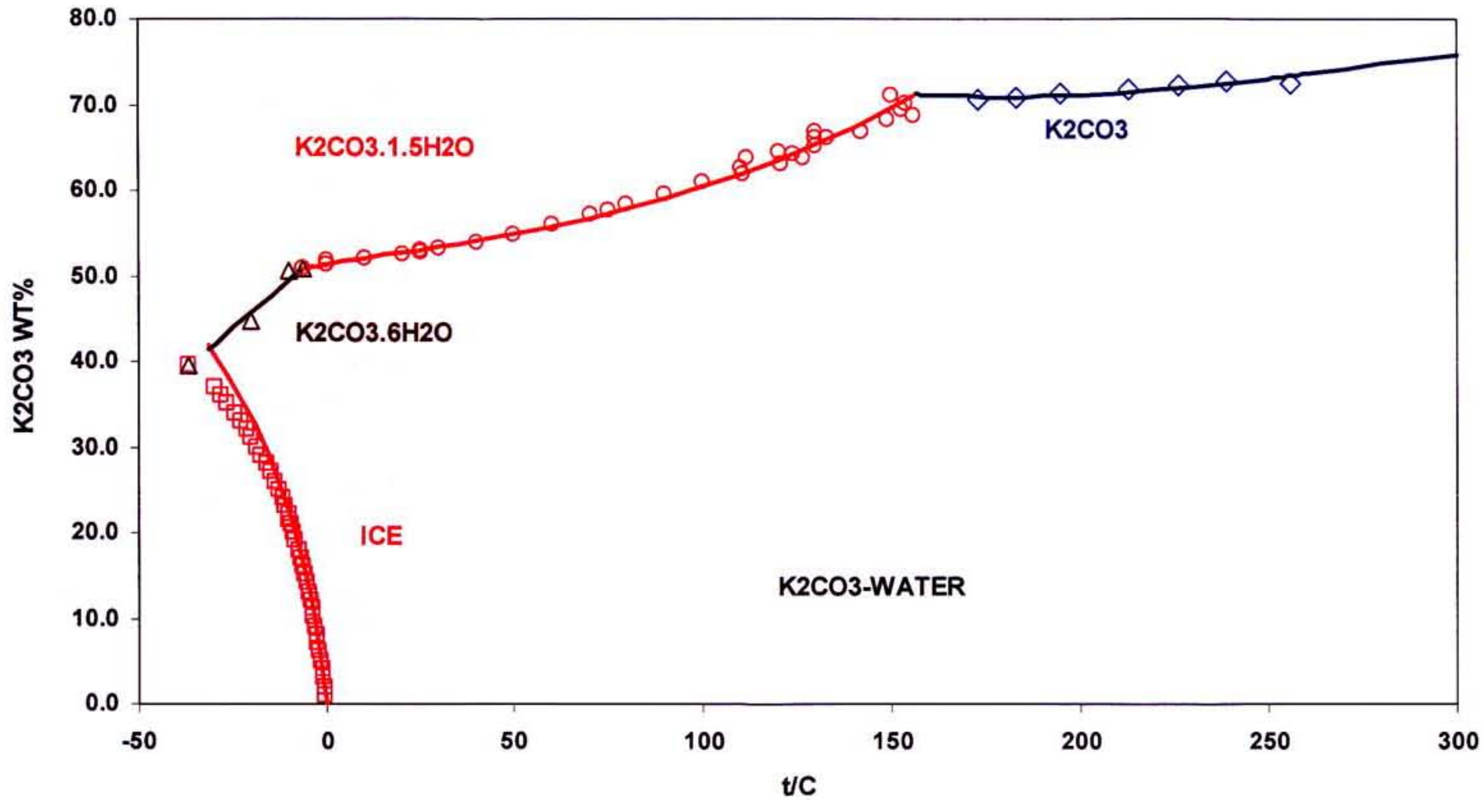

MgSO4.6H2O
MgSO4-water
MgSO4.7H2O
MgSO4.1H2O
ice
MgSO4 WT%
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
-20
30
80
130
180
230
T/C

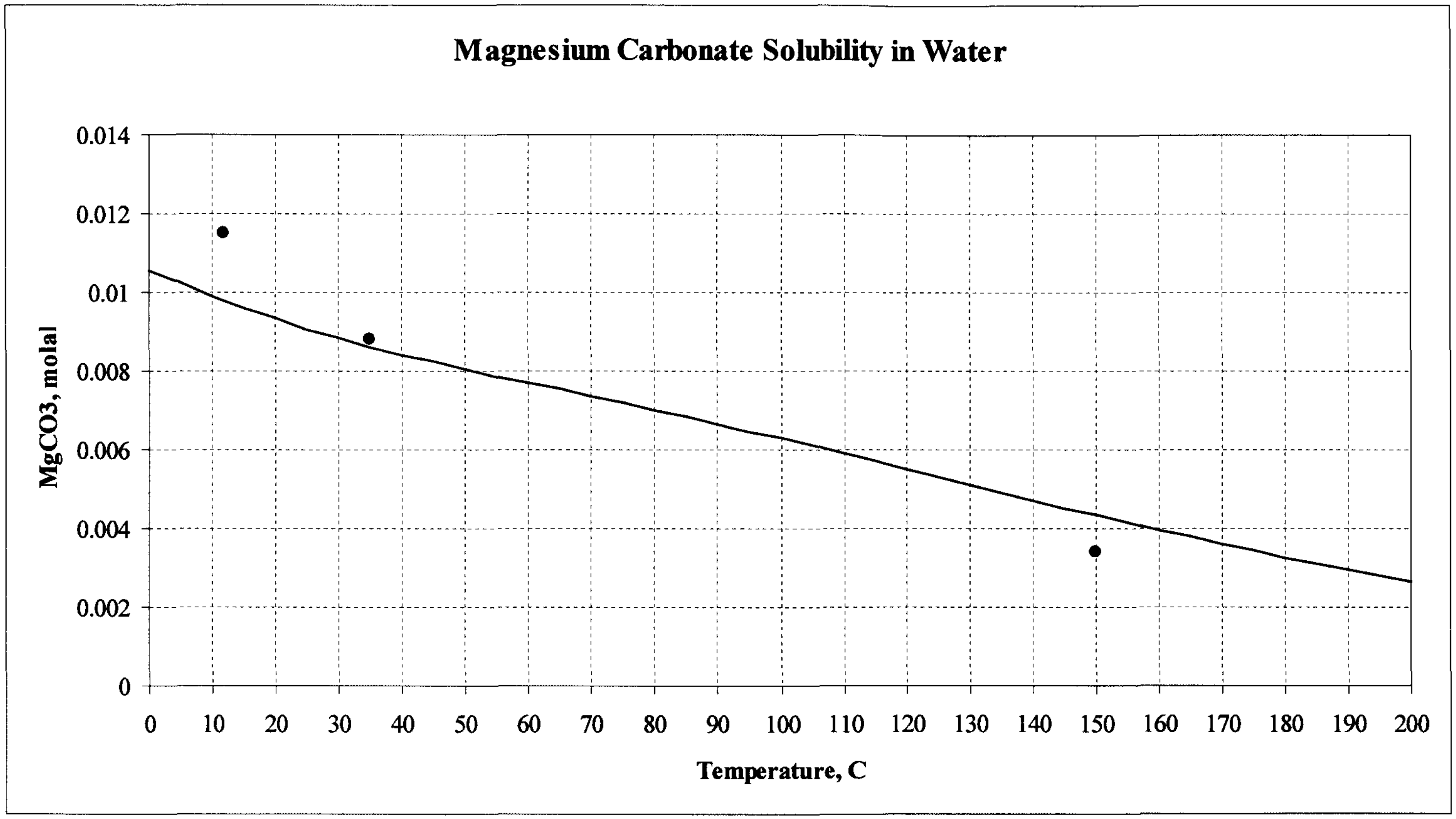

Calcium Sulfate Solubility in Water
0.3
0.25
0.2
0.15
0.1
0.05
0
CaSO4, weight %
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C



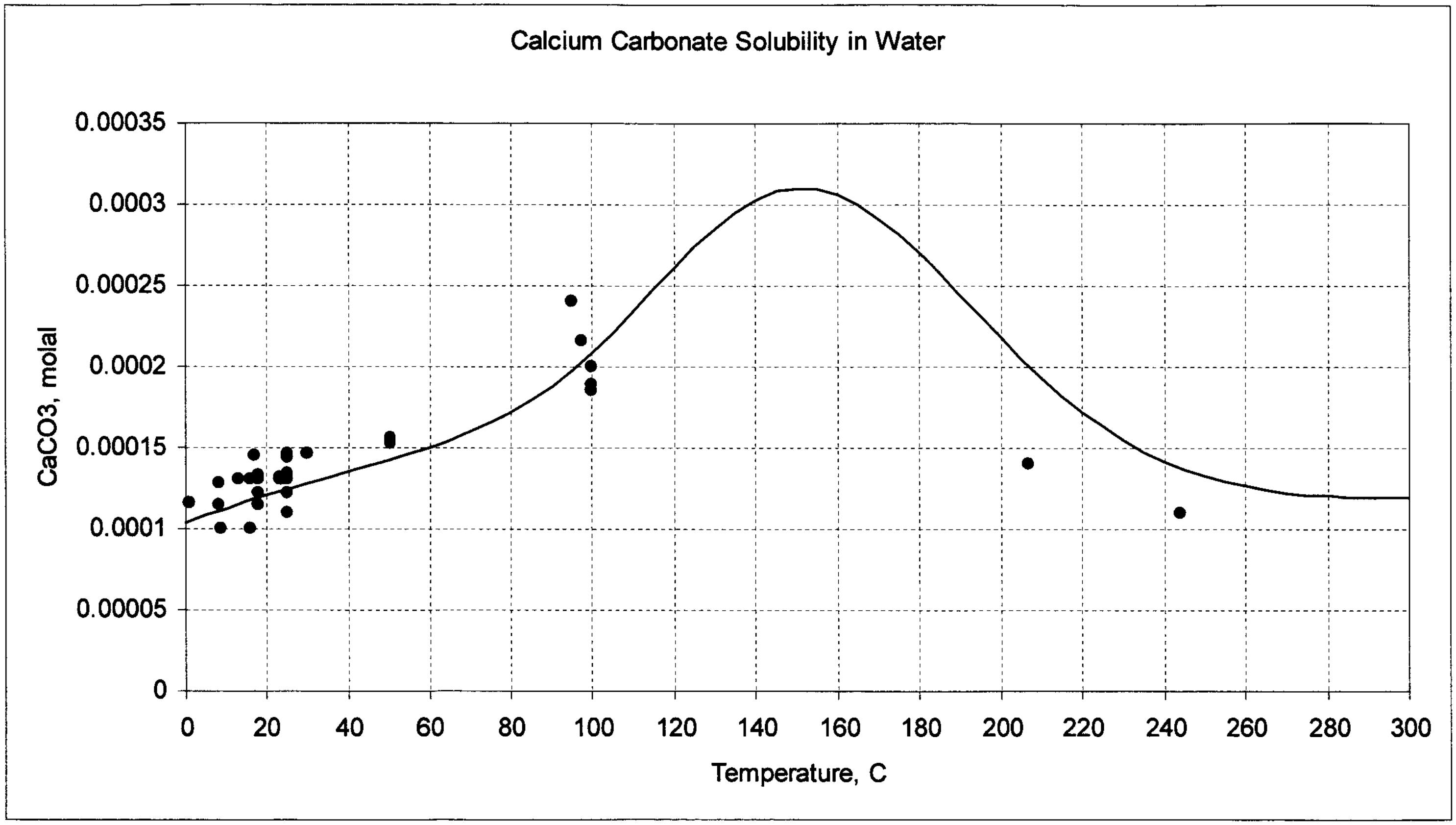
Al2(SO4)3.16H2O
ice
Solubility in
Al2(SO4)3-water
WT%-Al2(SO4)3
t/C
Al2(SO4)3.16H2O
ice
m-Al2(SO4)3
t/C

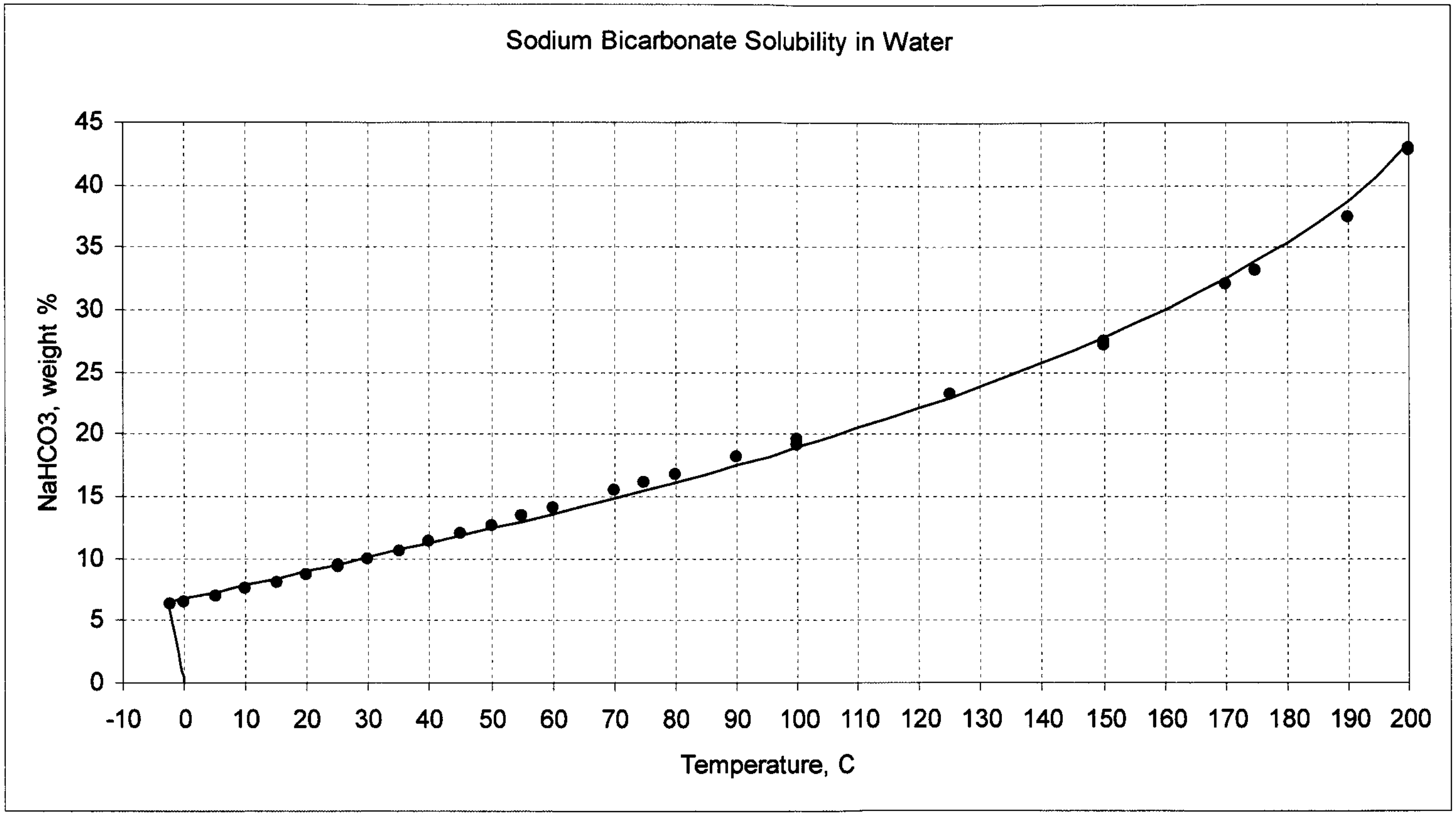

Sodium Carbonate Solubility in Water
Na2CO3, weight %
35
30
25
20
15
10
5
0
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C

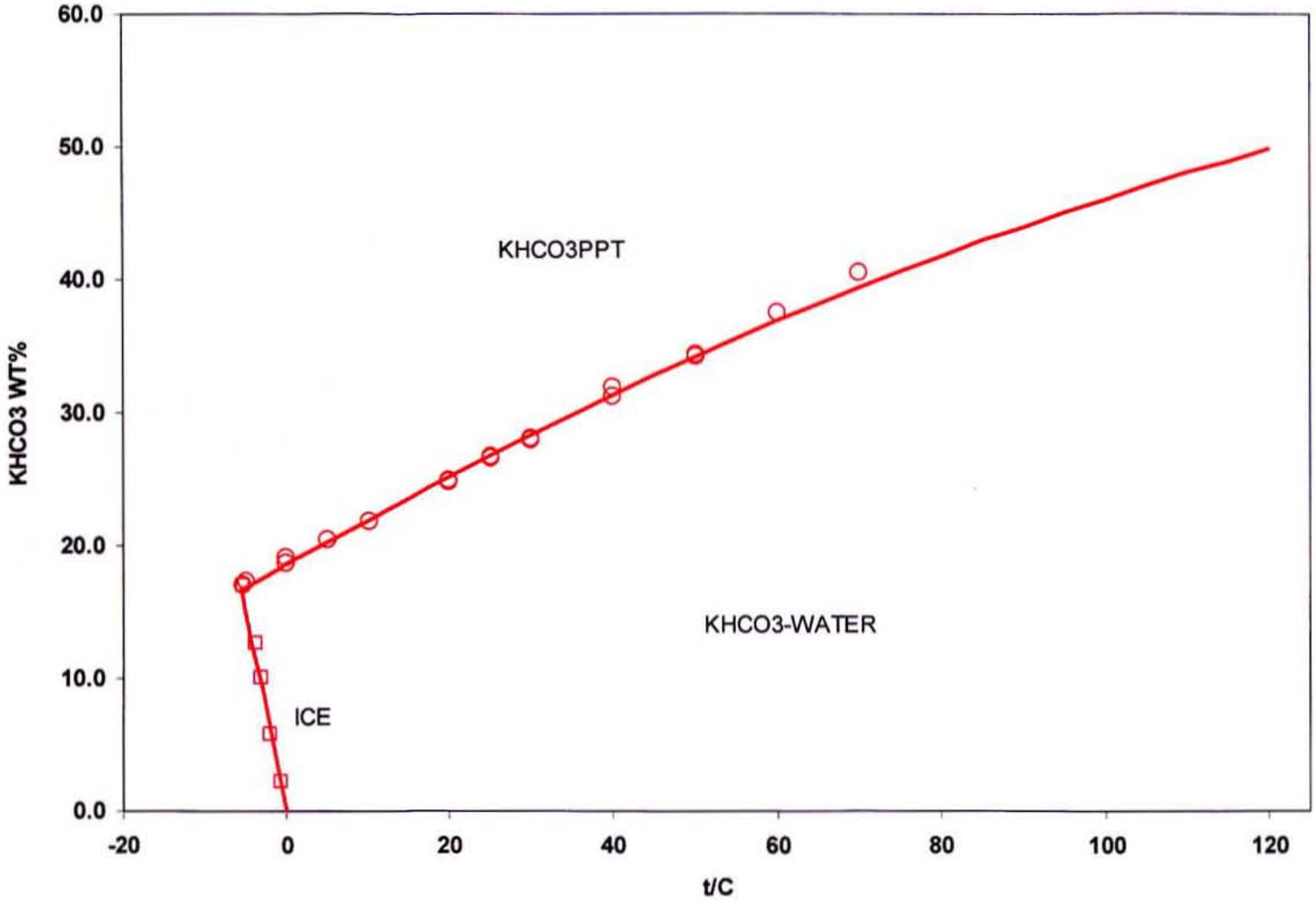

80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0.0
K2CO3 WT%
-50
0
50
100
150
200
250
300
t/C
K2CO3.1.5H2O
K2CO3
K2CO3.6H2O
ICE
K2CO3-WATER

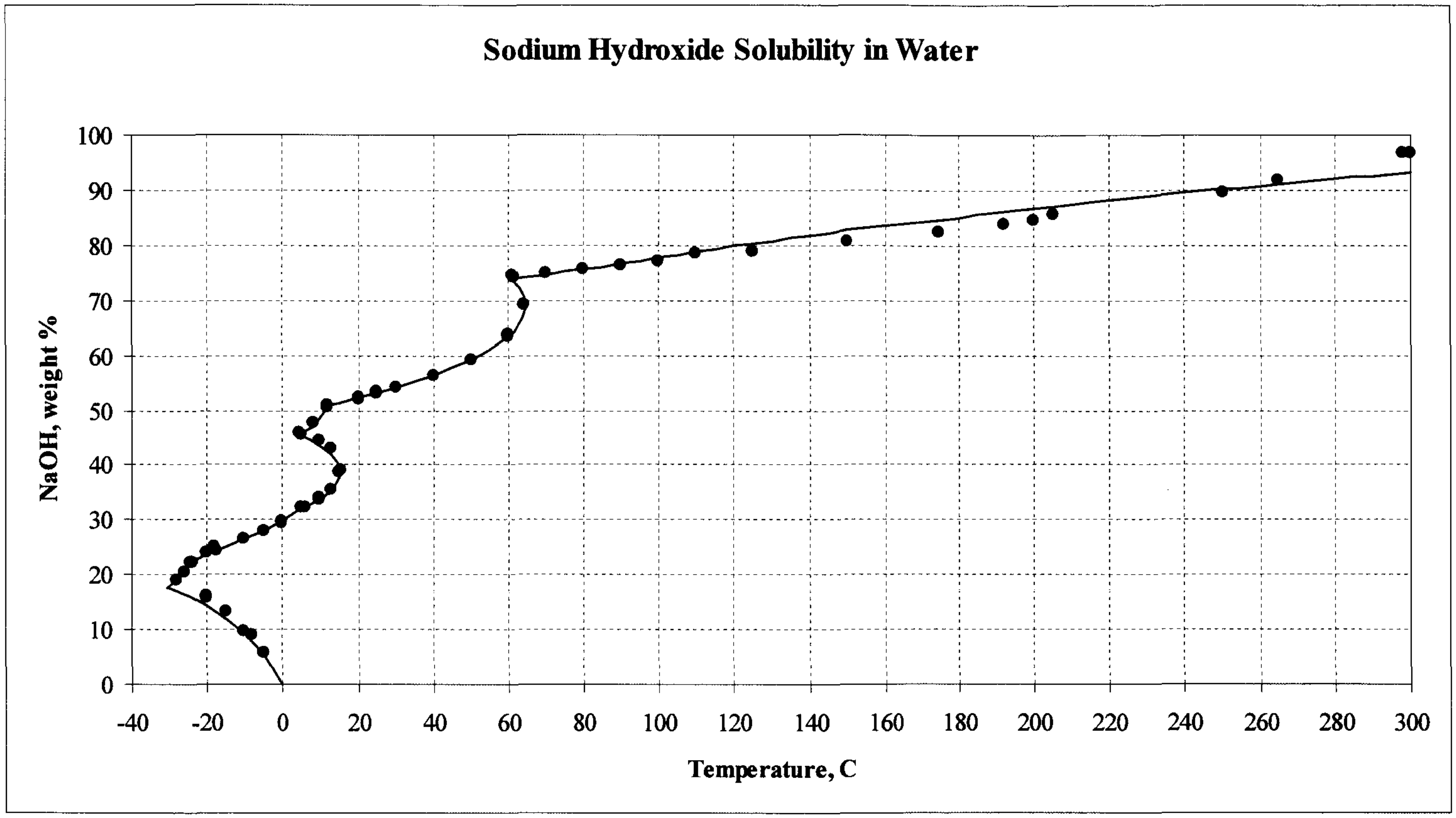


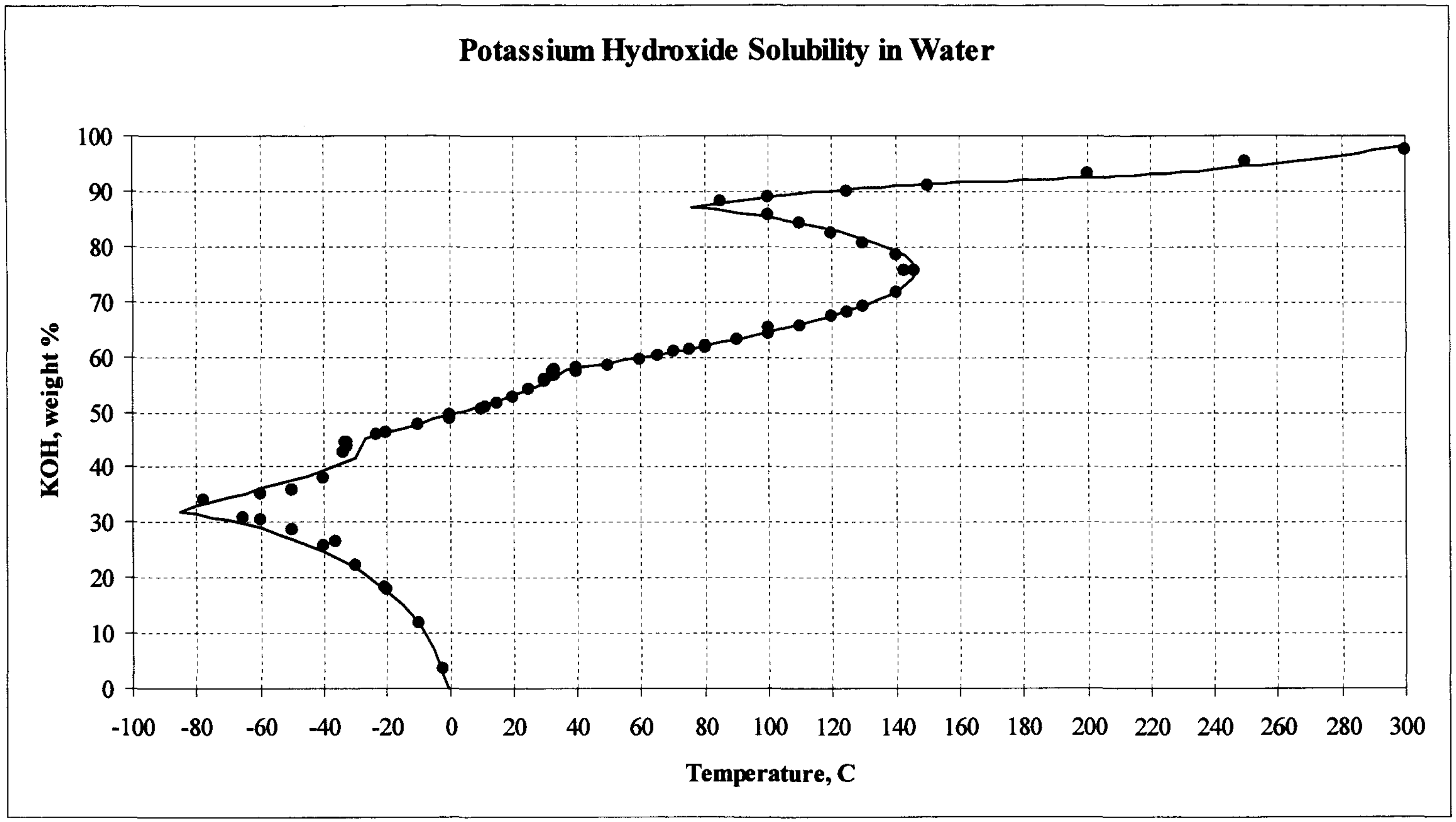
Magnesium Carbonate Solubility in Water
MgCO3, molal
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
0 10 20 30 40 50 60 70 80 90 100 110 120 130 140 150 160 170 180 190 200
Temperature, C


Calcium Carbonate Solubility in Water
0.00035
0.0003
0.00025
0.0002
0.00015
0.0001
0.00005
0
CaCO3, molal
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C

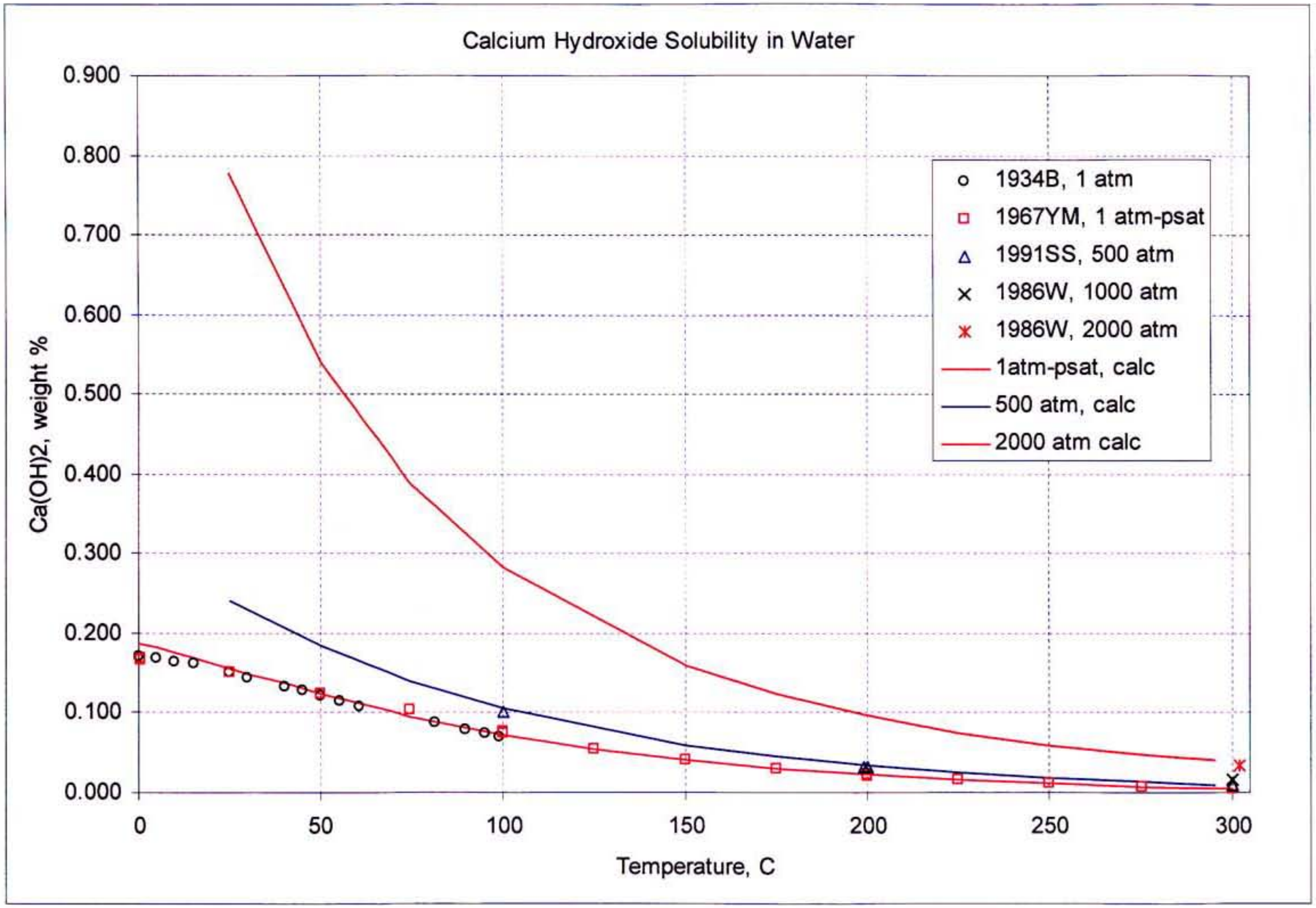

Sodium Bicarbonate Solubility in Water
NaHCO3, weight %
45
40
35
30
25
20
15
10
5
0
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
Temperature, C


60.0
50.0
40.0
30.0
20.0
10.0
0.0
KHCO3 WT%
KHCO3PPT
KHCO3-WATER
ICE
-20
0
20
40
60
80
100
120
t/C

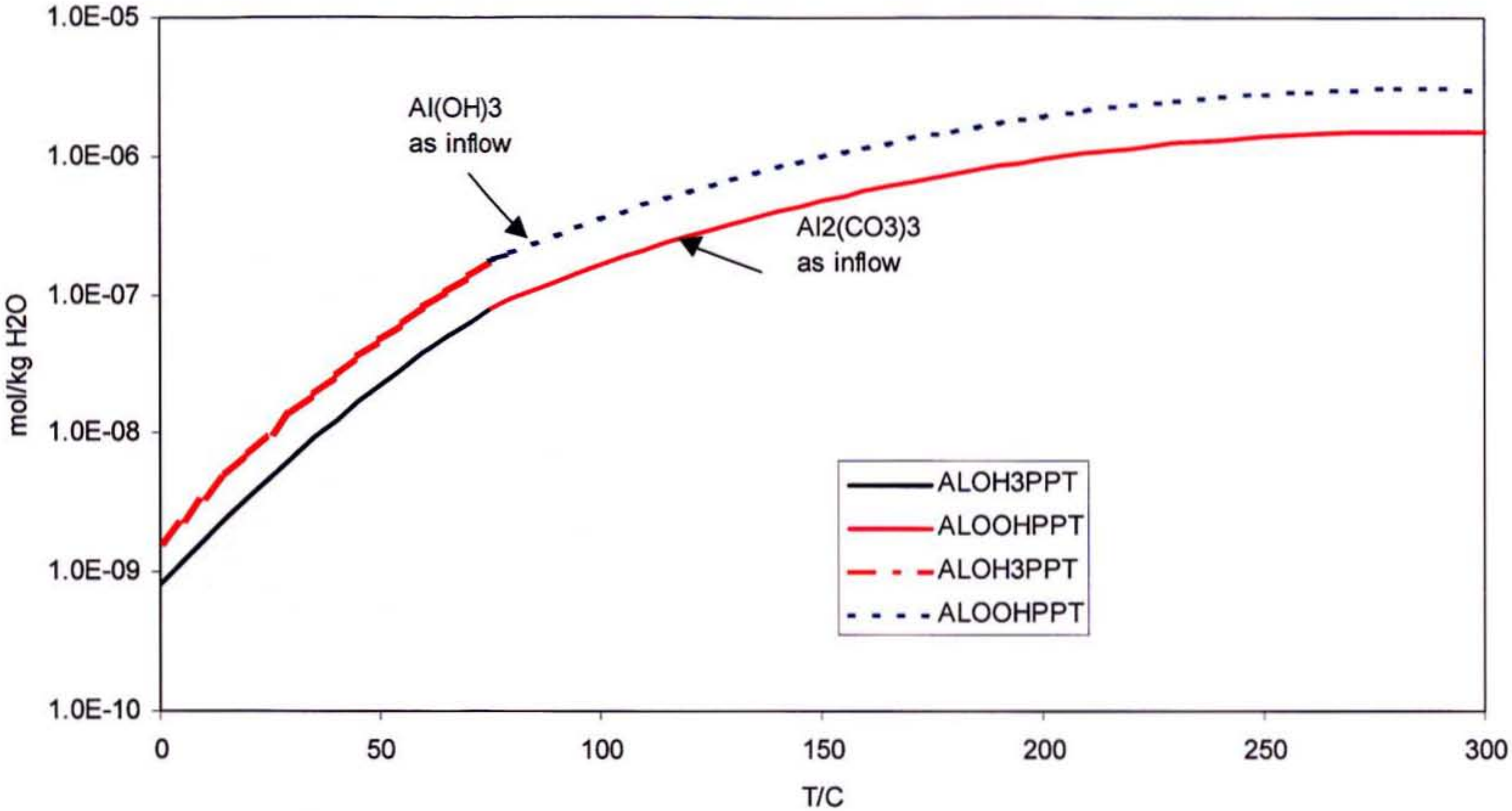

Sodium Hydroxide Solubility in Water
100
90
80
70
60
50
40
30
20
10
0
NaOH, weight %
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C



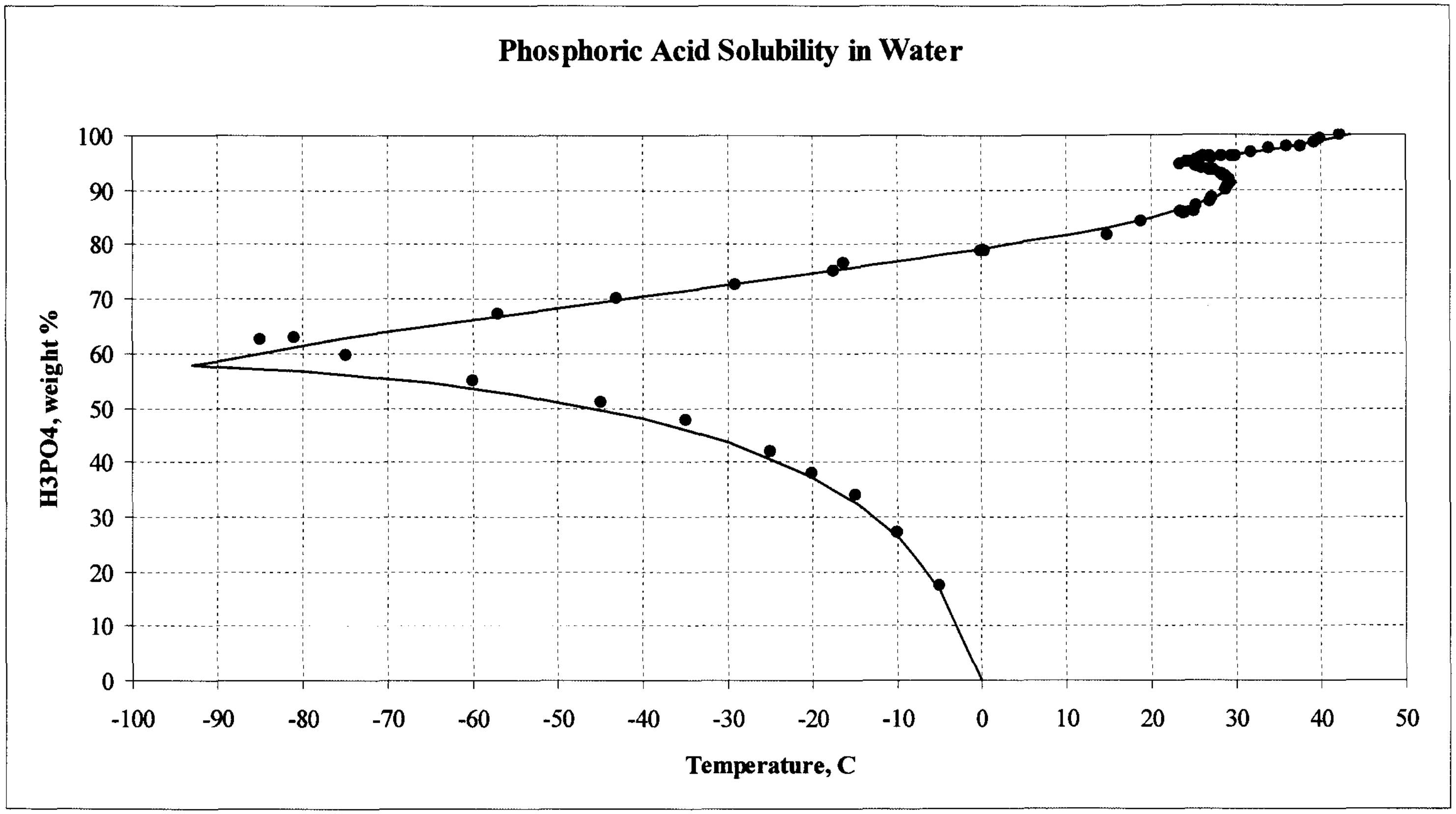
Potassium Hydroxide Solubility in Water
100
90
80
70
60
50
40
30
20
10
0
KOH, weight %
-100
-80
-60
-40
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C



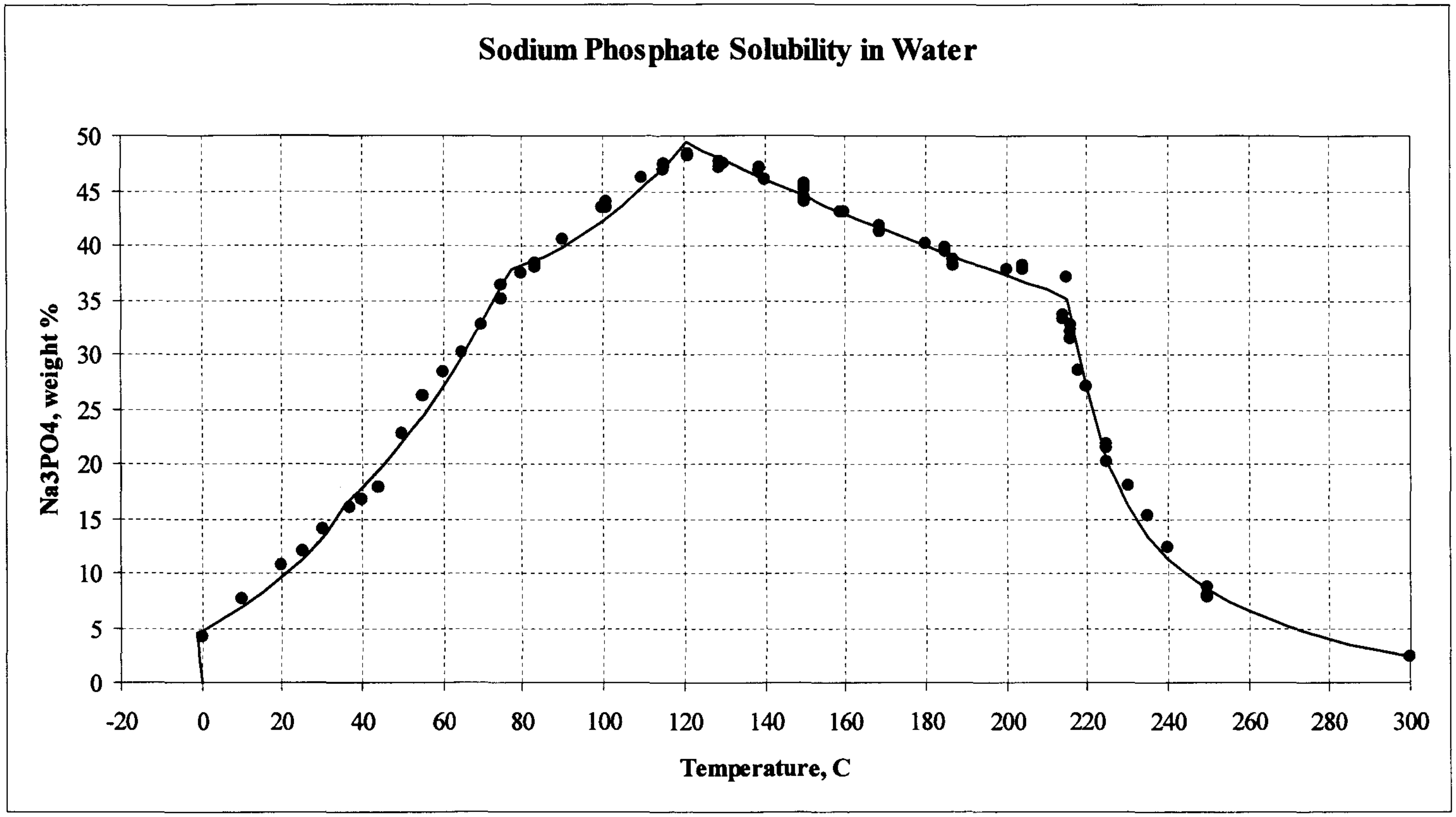
Calcium Hydroxide Solubility in Water
0.900
0.800
0.700
0.600
0.500
0.400
0.300
0.200
0.100
0.000
Ca(OH)2, weight %
0
50
100
150
200
250
300
Temperature, C
1934B, 1 atm
1967YM, 1 atm-psat
1991SS, 500 atm
1986W, 1000 atm
1986W, 2000 atm
1atm-psat, calc
500 atm, calc
2000 atm calc

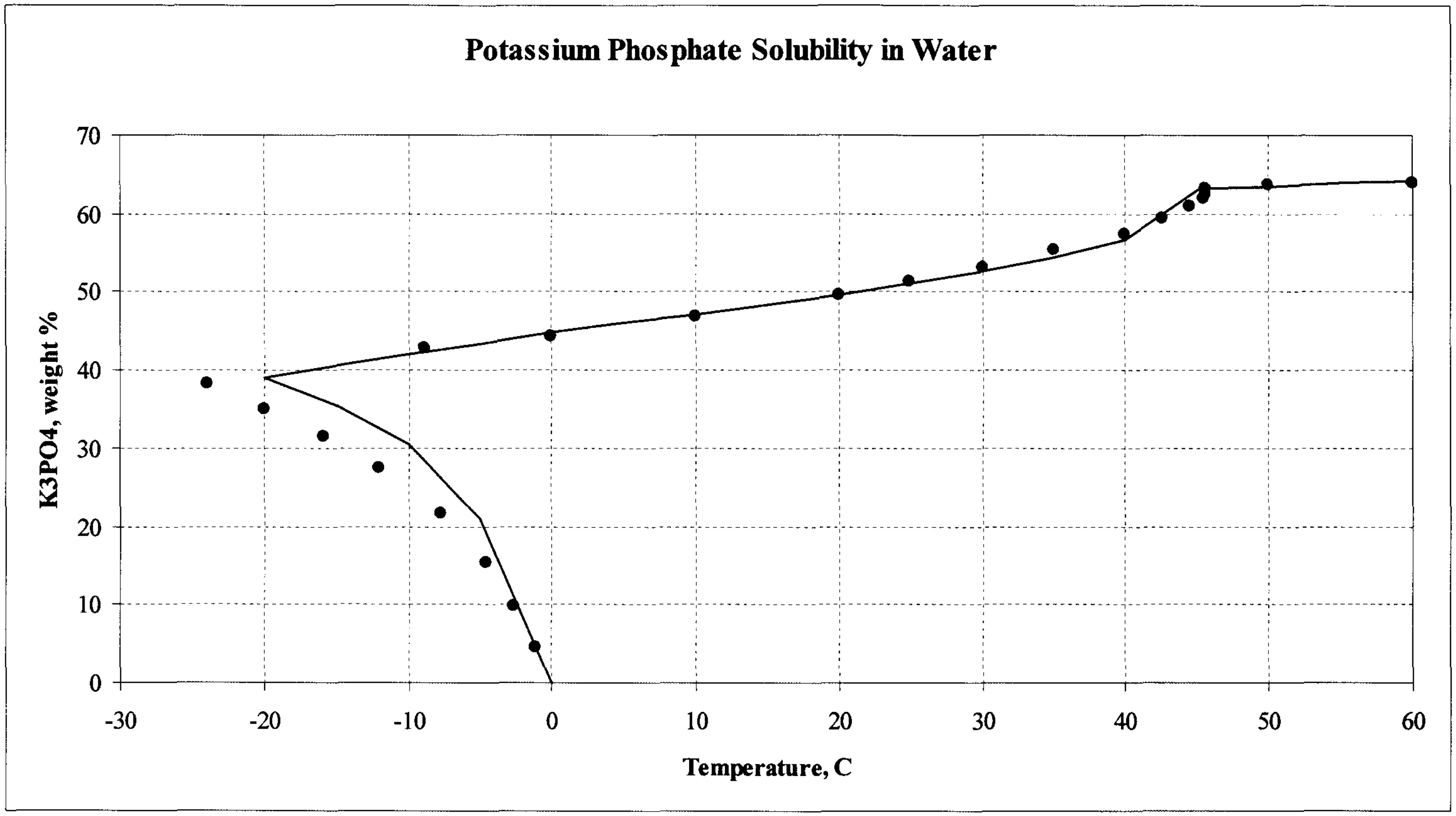


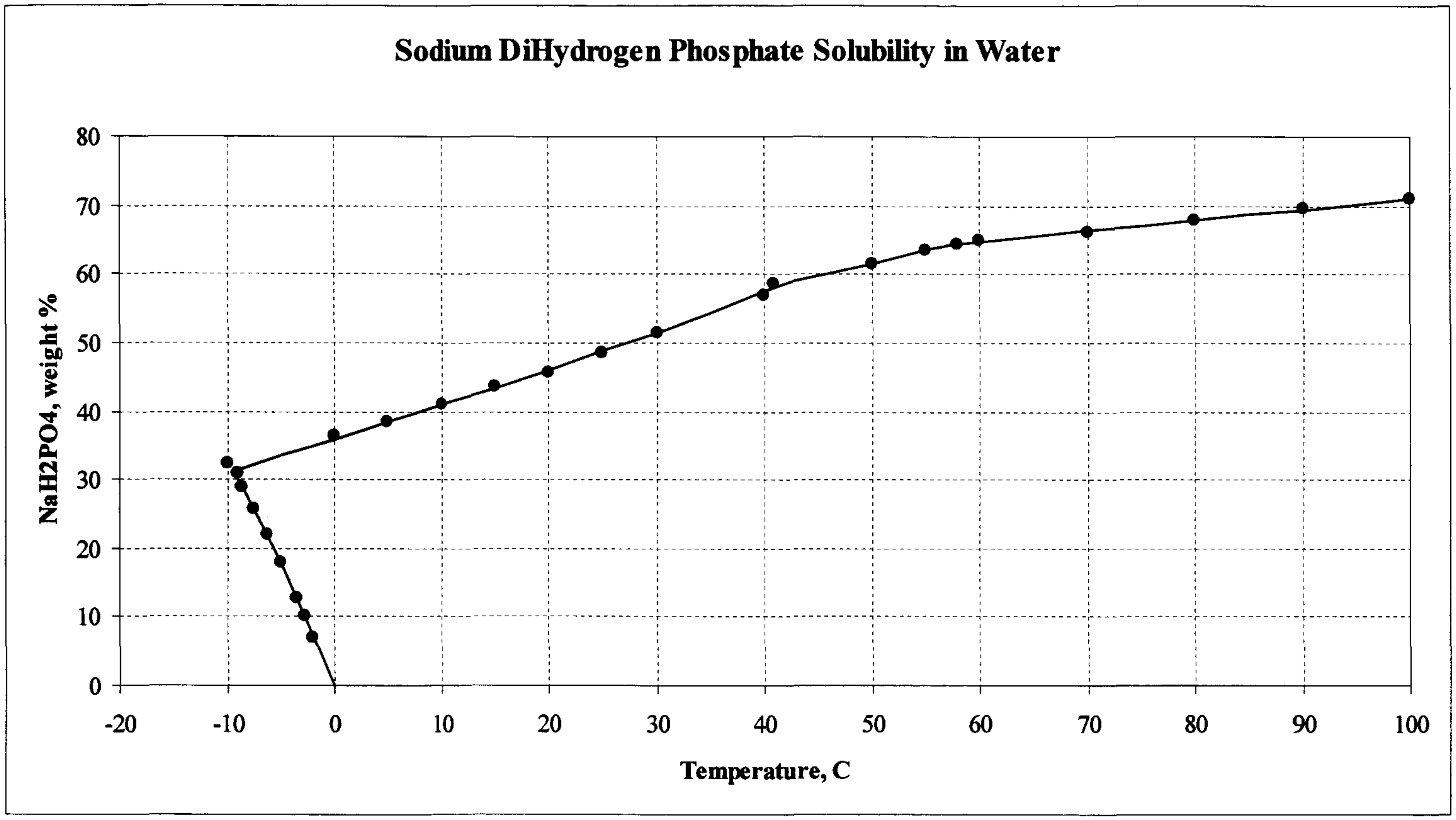
This figure has comparison of the solubilities in Al2(CO3)3-water and in Al(OH)3-water systems. The solid precipitations in both cases are Al(OH)3ppt and AlOOHppt

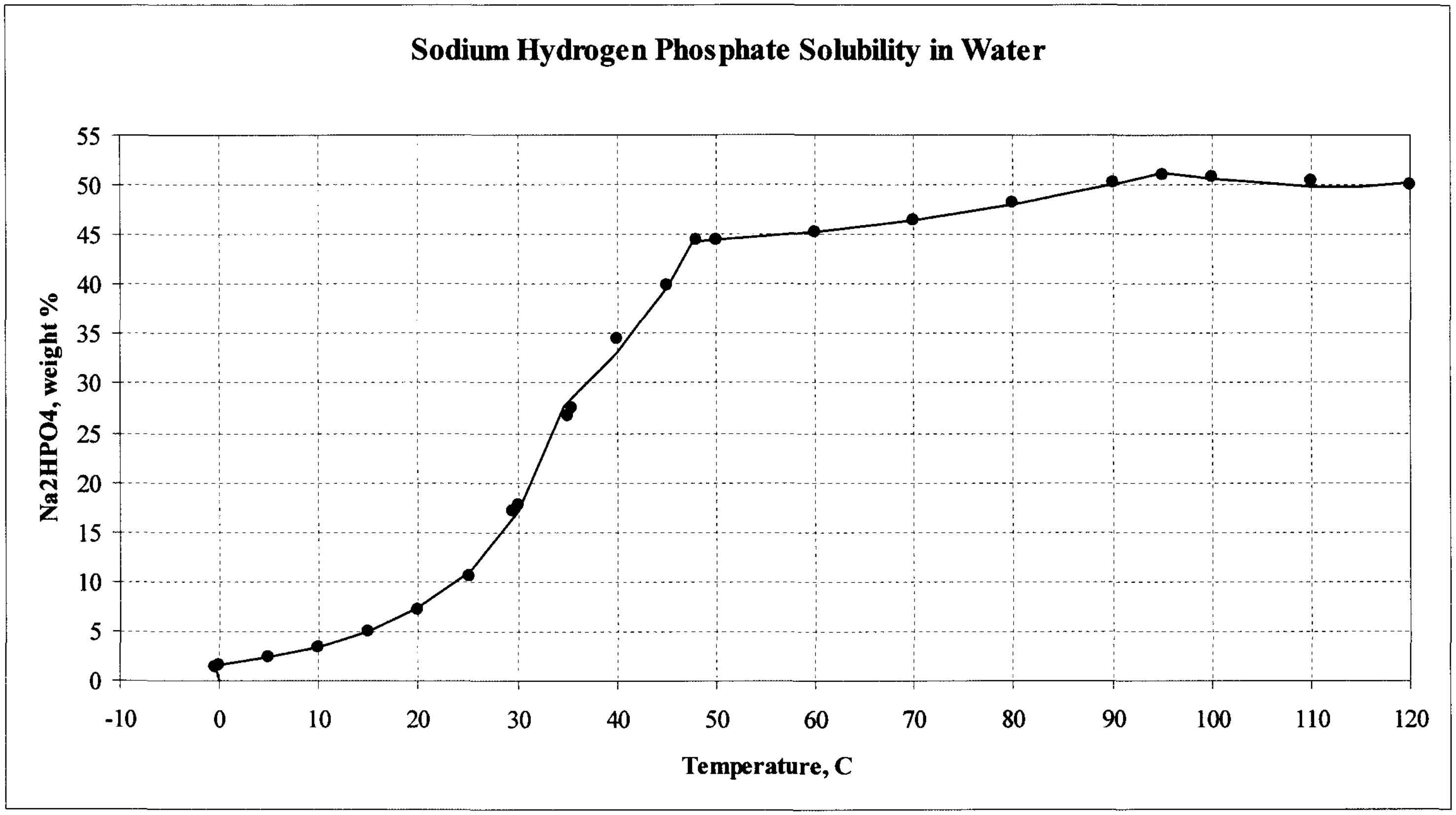


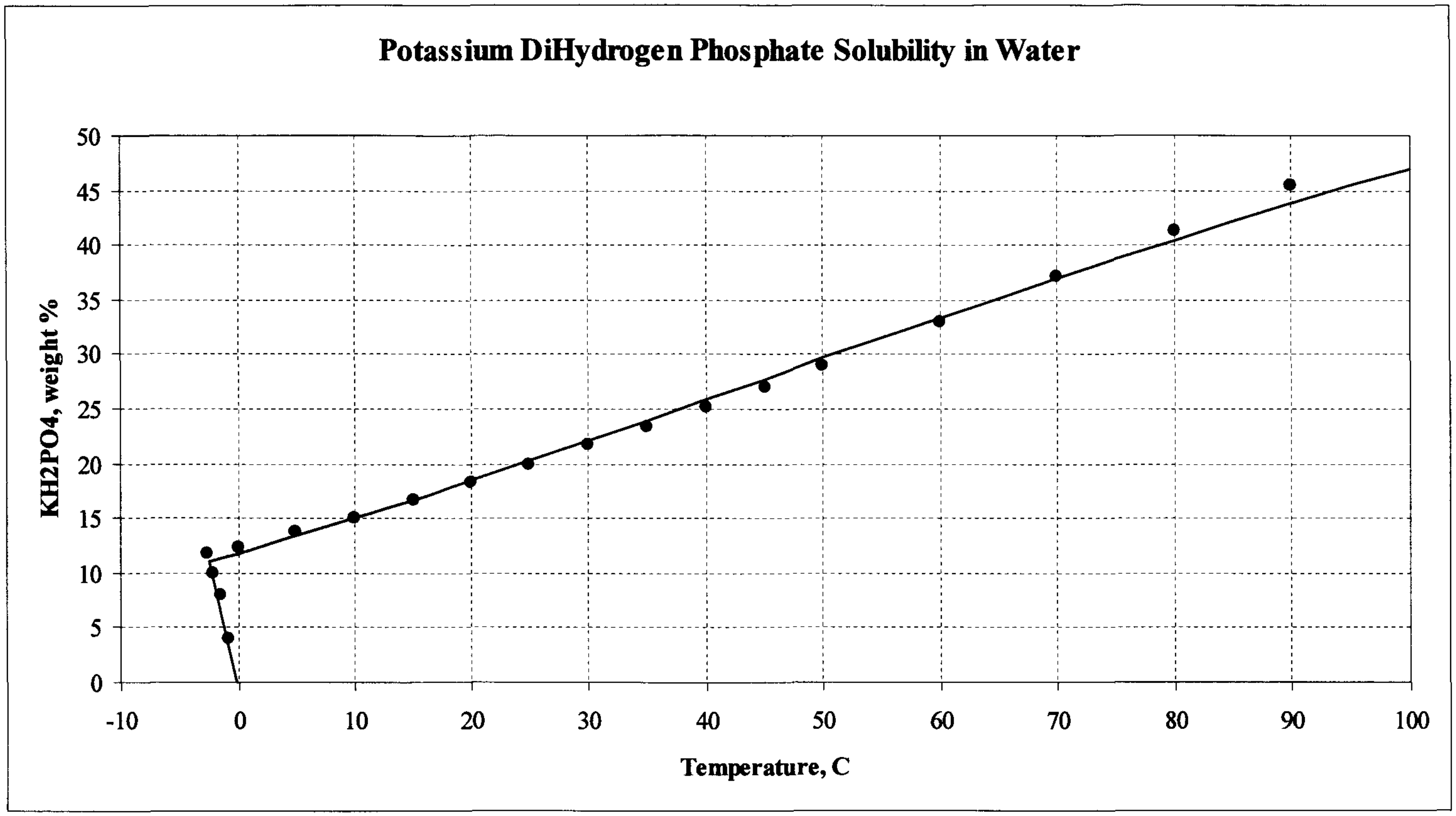
Phosphoric Acid Solubility in Water
H3PO4, weight %
100
90
80
70
60
50
40
30
20
10
0
-100
-90
-80
-70
-60
-50
-40
-30
-20
-10
0
10
20
30
40
50
Temperature, C

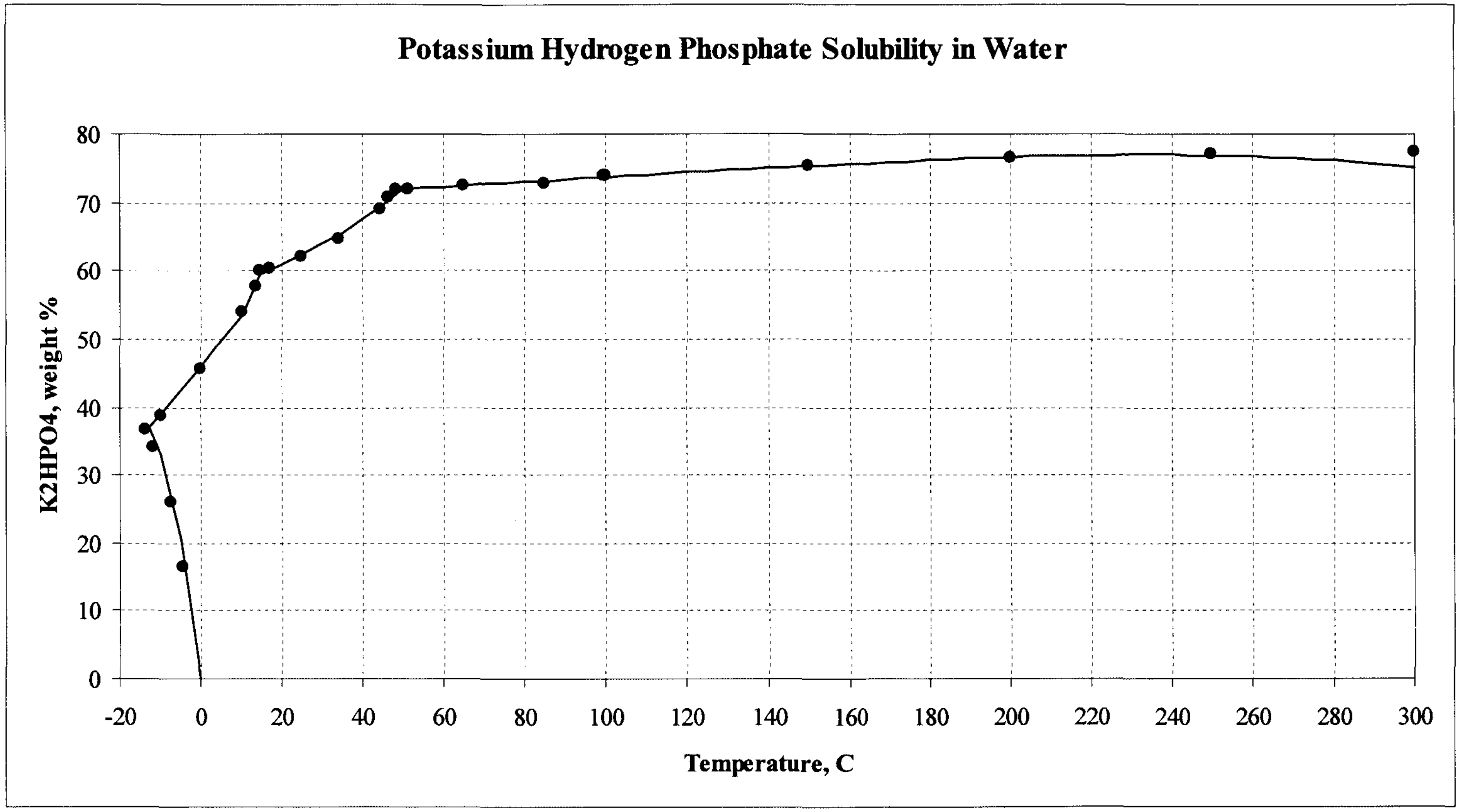

Sodium Phosphate Solubility in Water
Na3PO4, weight %
Temperature, C
50
45
40
35
30
25
20
15
10
5
0
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300


Potassium Phosphate Solubility in Water
K3PO4, weight %
Temperature, C
70
60
50
40
30
20
10
0
-30
-20
-10
0
10
20
30
40
50
60

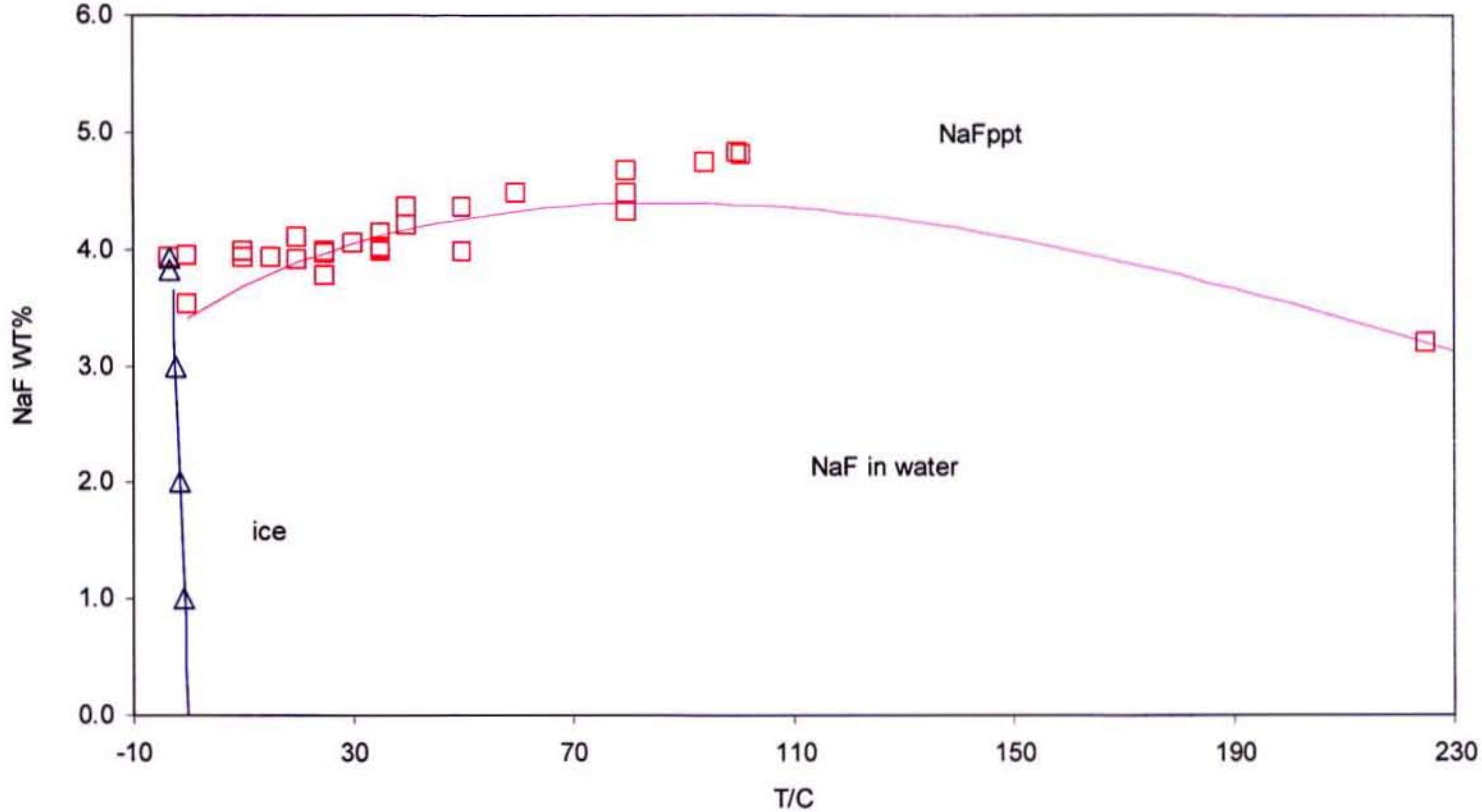

Sodium DiHydrogen Phosphate Solubility in Water
NaH2PO4, weight %
Temperature, C
0
10
20
30
40
50
60
70
80
-20
-10
0
10
20
30
40
50
60
70
80
90
100


Sodium Hydrogen Phosphate Solubility in Water
Na2HPO4, weight %
55
50
45
40
35
30
25
20
15
10
5
0
-10
0
10
20
30
40
50
60
70
80
90
100
110
120
Temperature, C

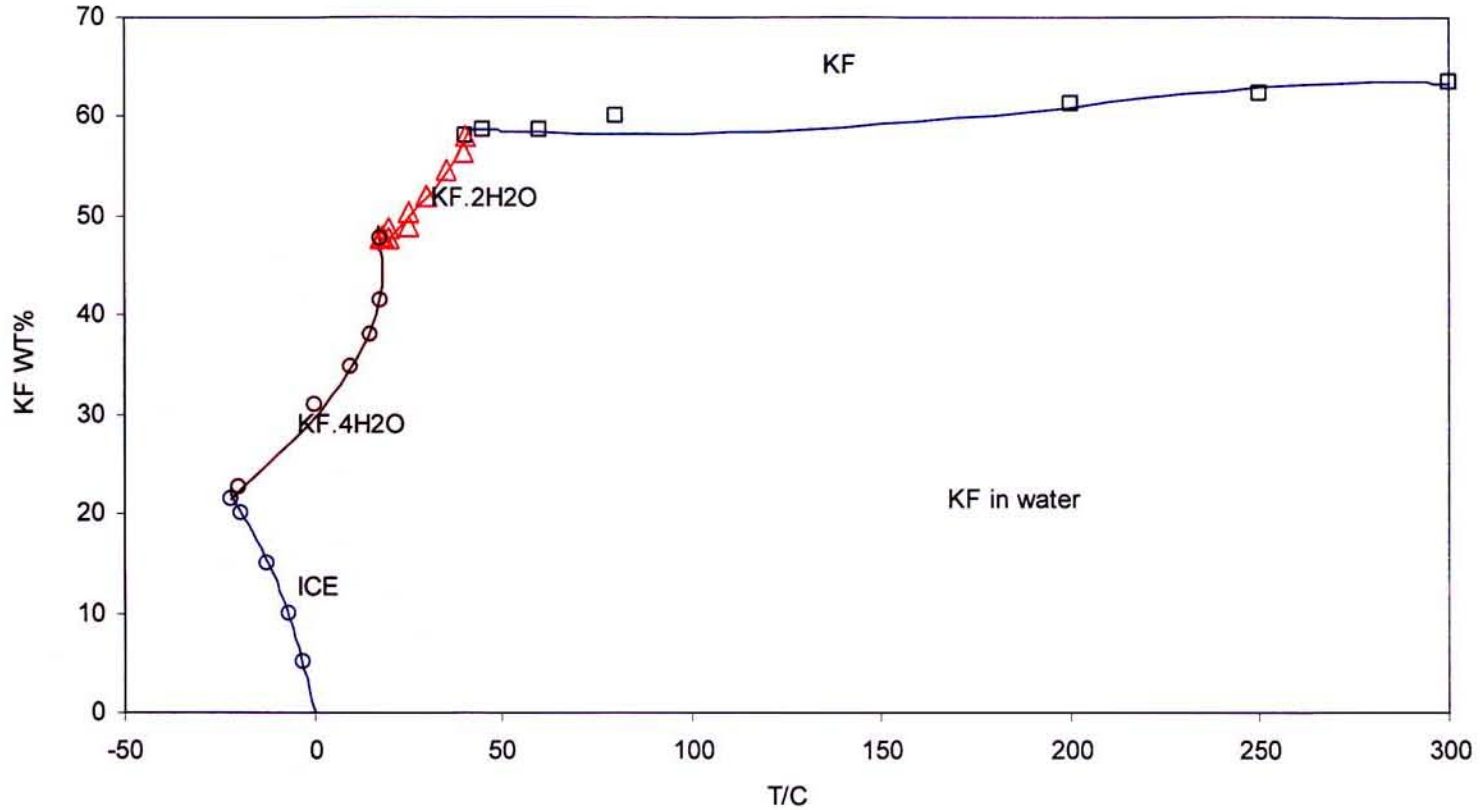

Potassium DiHydrogen Phosphate Solubility in Water
50
45
40
35
30
25
20
15
10
5
0
KH2PO4, weight %
-10
0
10
20
30
40
50
60
70
80
90
100
Temperature, C

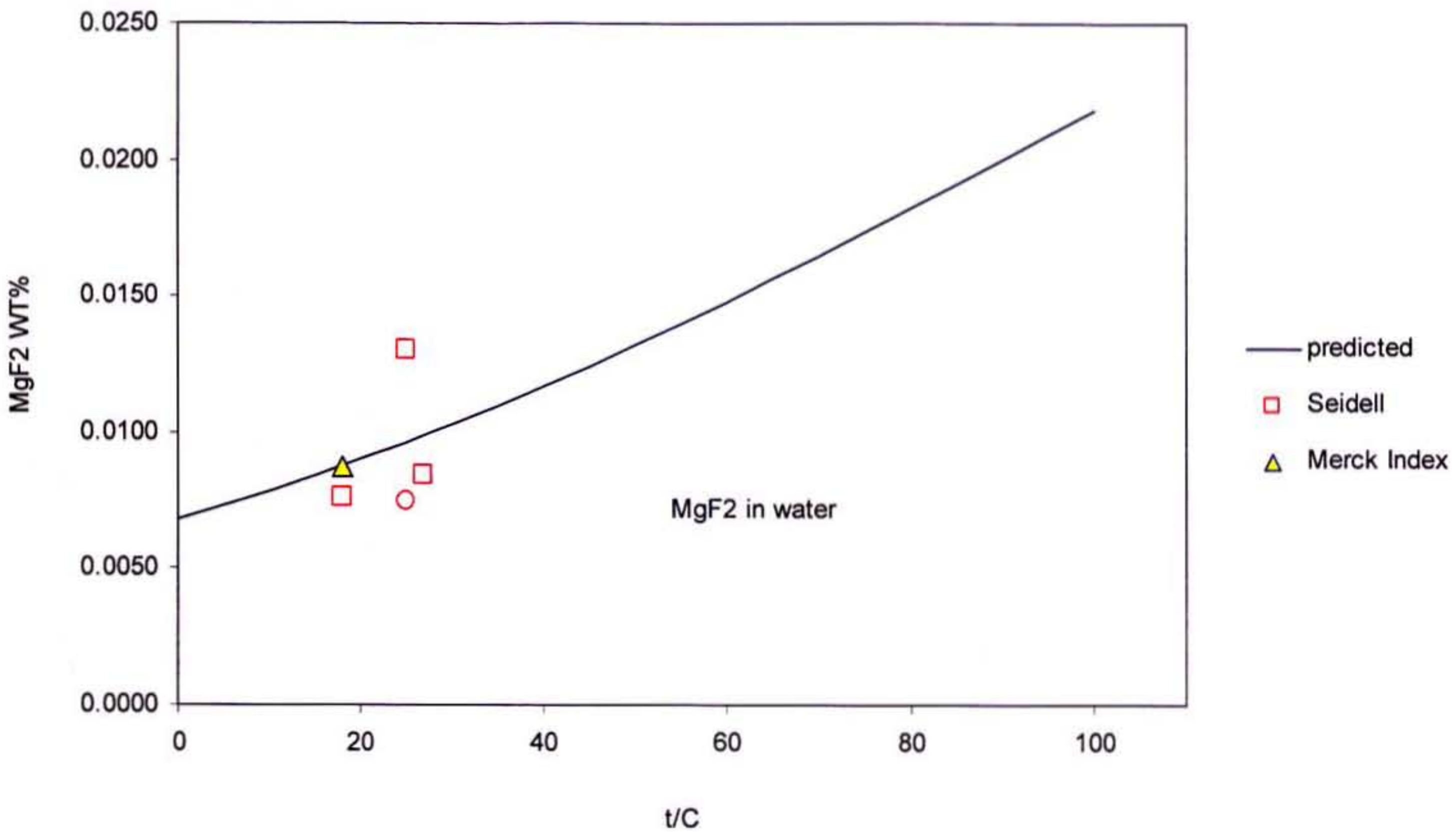


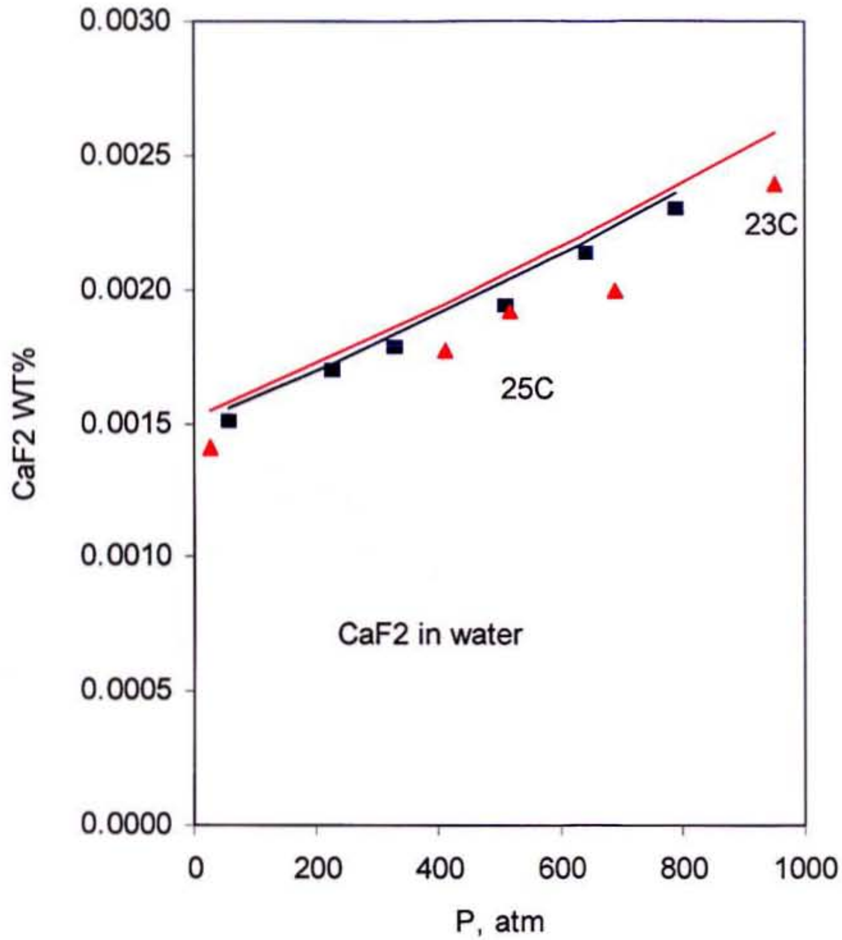
Potassium Hydrogen Phosphate Solubility in Water
K2HPO4, weight %
80
70
60
50
40
30
20
10
0
-20
0
20
40
60
80
100
120
140
160
180
200
220
240
260
280
300
Temperature, C



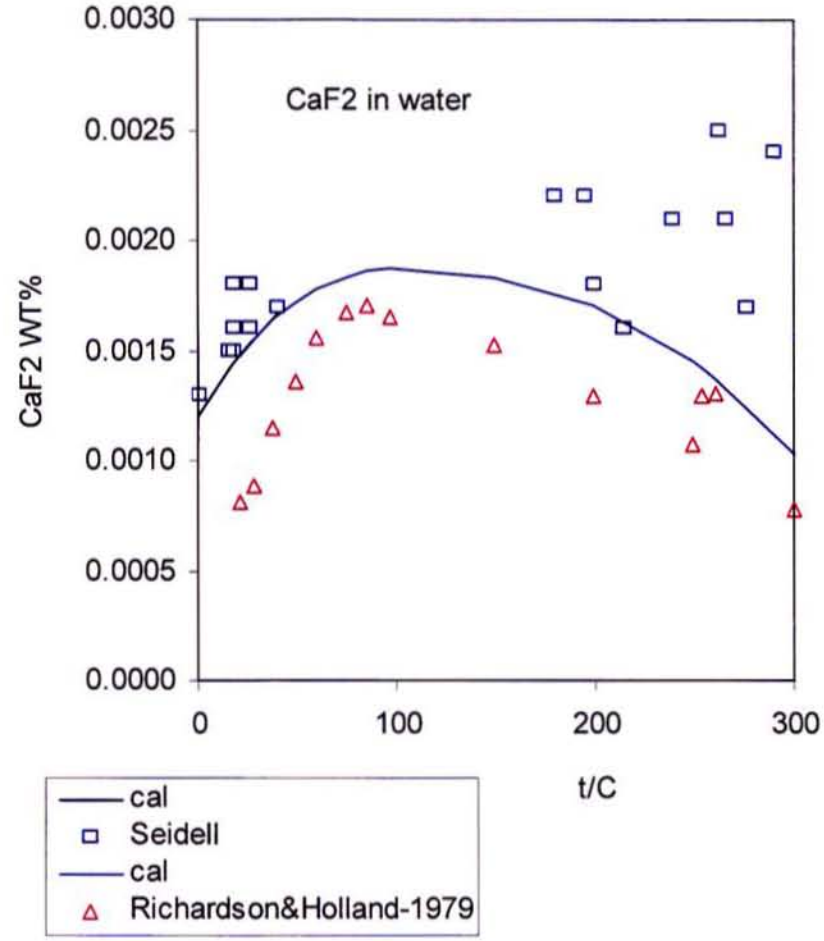
6.0
5.0
4.0
3.0
2.0
1.0
0.0
NaF WT%
-10
30
70
110
150
190
230
T/C
NaFppt
NaF in water
ice


70
60
50
40
30
20
10
0
KF WT%
-50
0
50
100
150
200
250
300
T/C
KF
KF.2H2O
KF.4H2O
ICE
KF in water

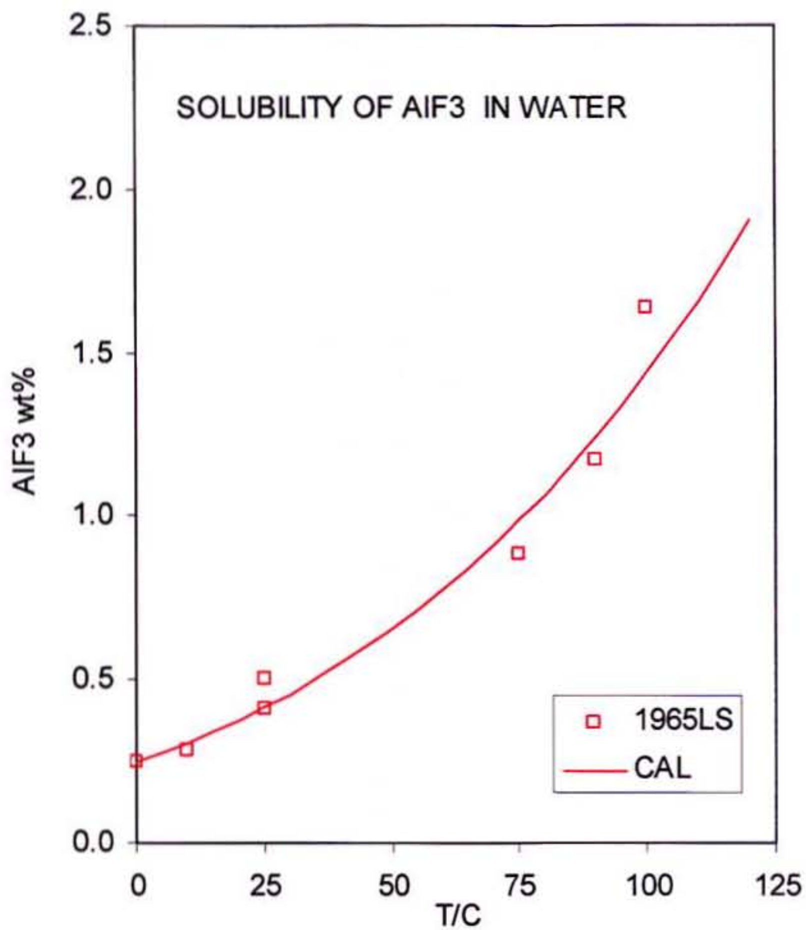

0.0250
0.0200
0.0150
0.0100
0.0050
0.0000
MgF2 WT%
0
20
40
60
80
100
t/C
MgF2 in water
predicted
Seidell
Merck Index

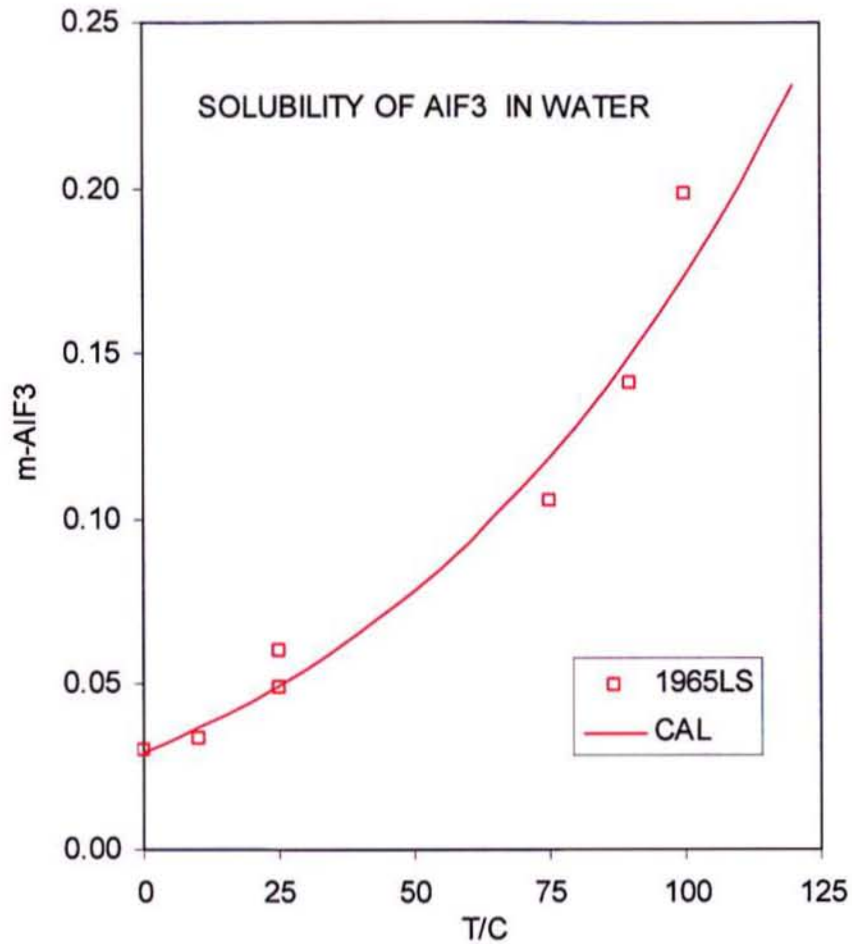


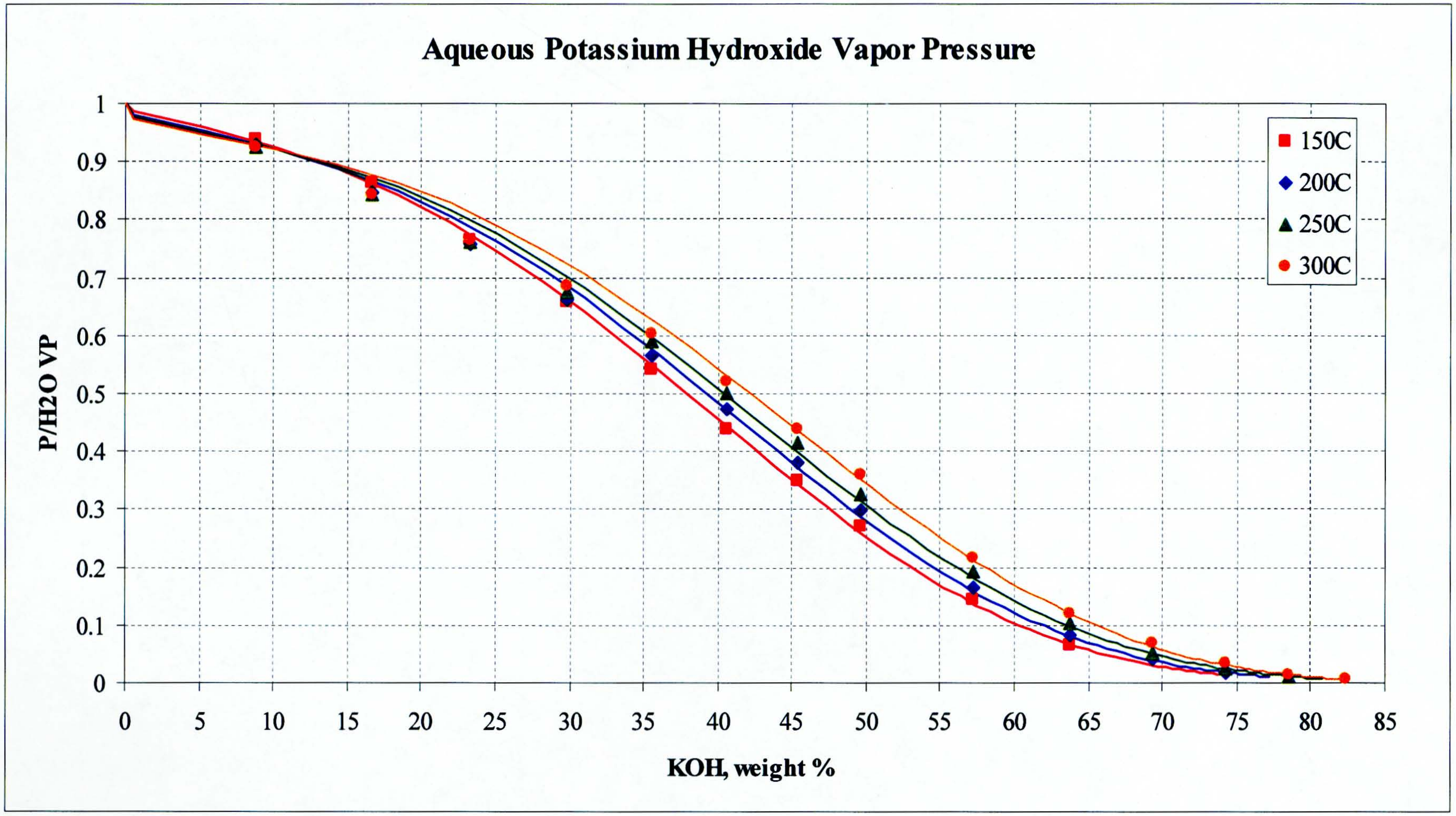
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
CaF2 WT%
23C
25C
CaF2 in water
0
200
400
600
800
1000
P, atm

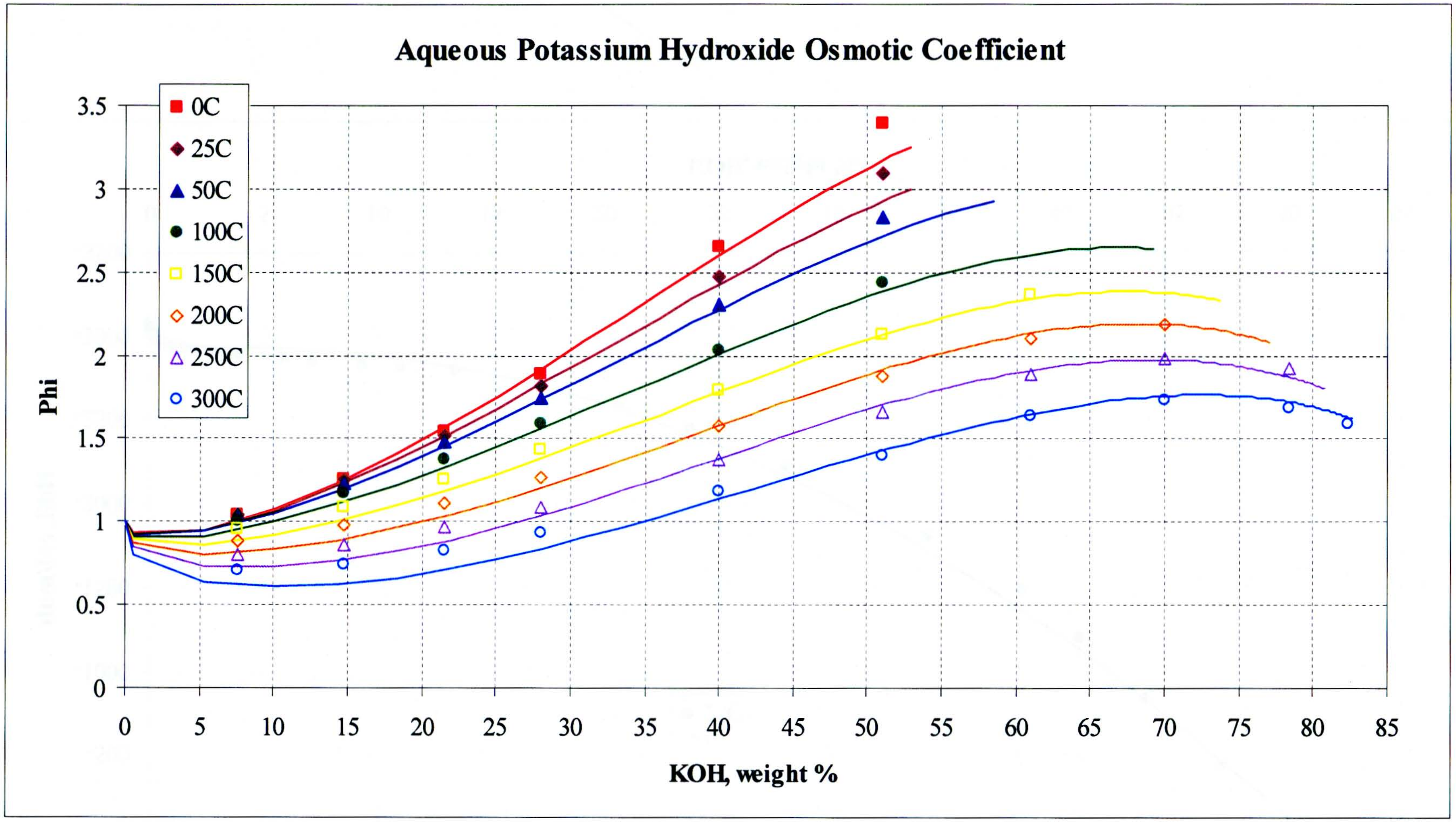


0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
CaF2 WT%
CaF2 in water
0
100
200
300
t/C
cal
Seidell
cal
Richardson&Holland-1979

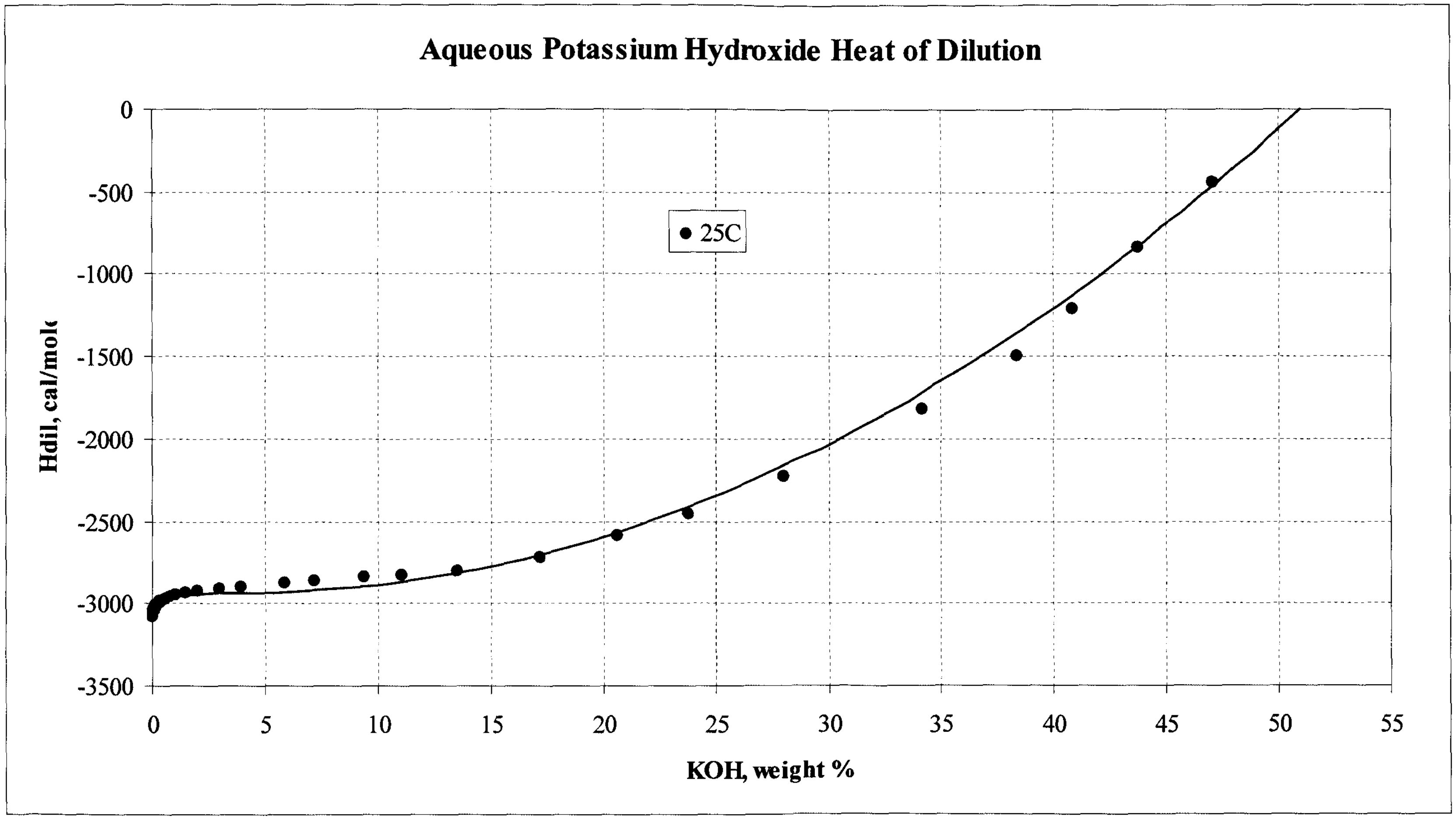

SOLUBILITY OF AlF3 IN WATER
AlF3 wt%
T/C
1965LS
CAL
0.0
0.5
1.0
1.5
2.0
2.5
0
25
50
75
100
125

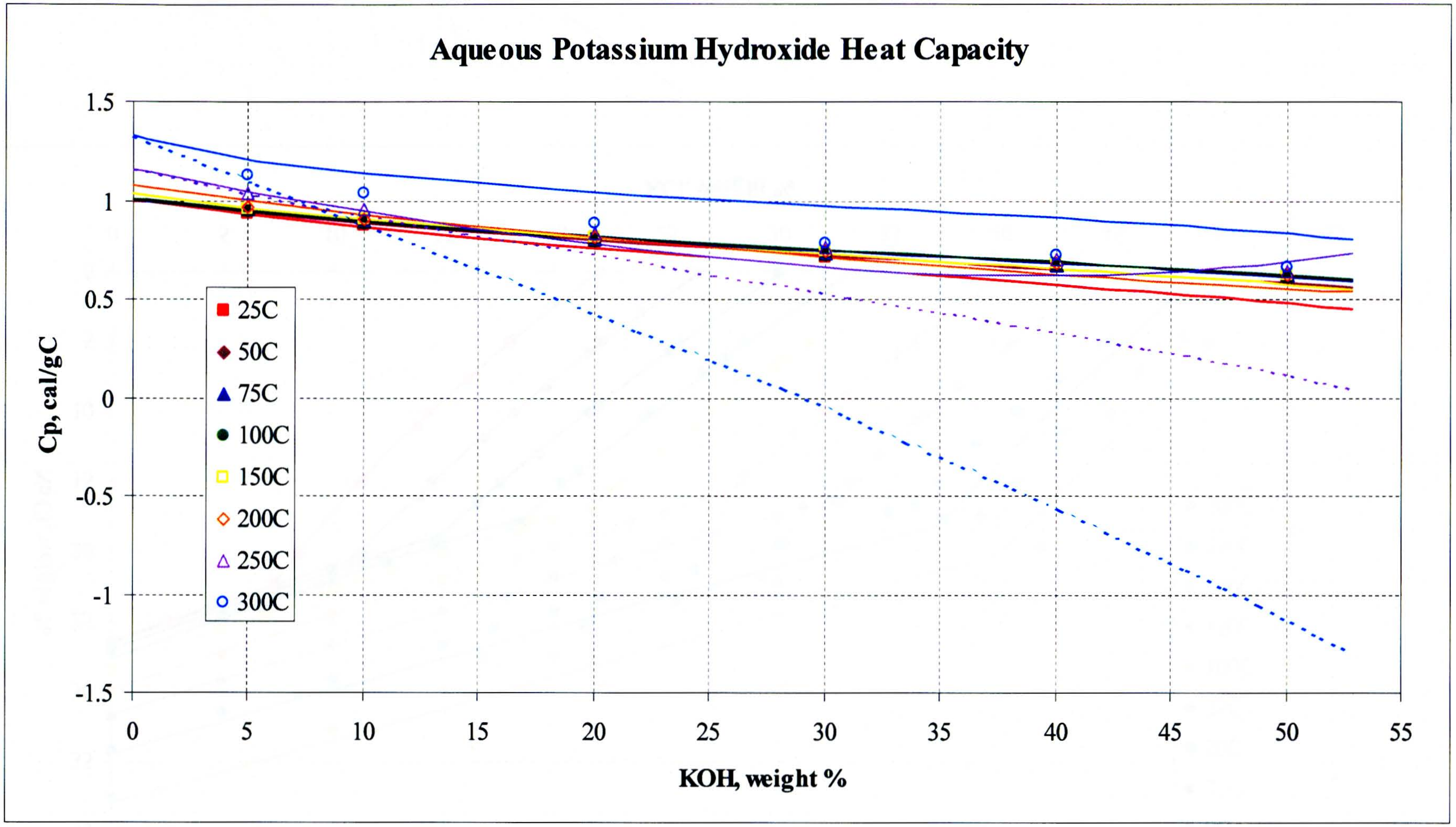

SOLUBILITY OF AlF3 IN WATER
m-AlF3
T/C
1965LS
CAL
0.00
0.05
0.10
0.15
0.20
0.25
0
25
50
75
100
125

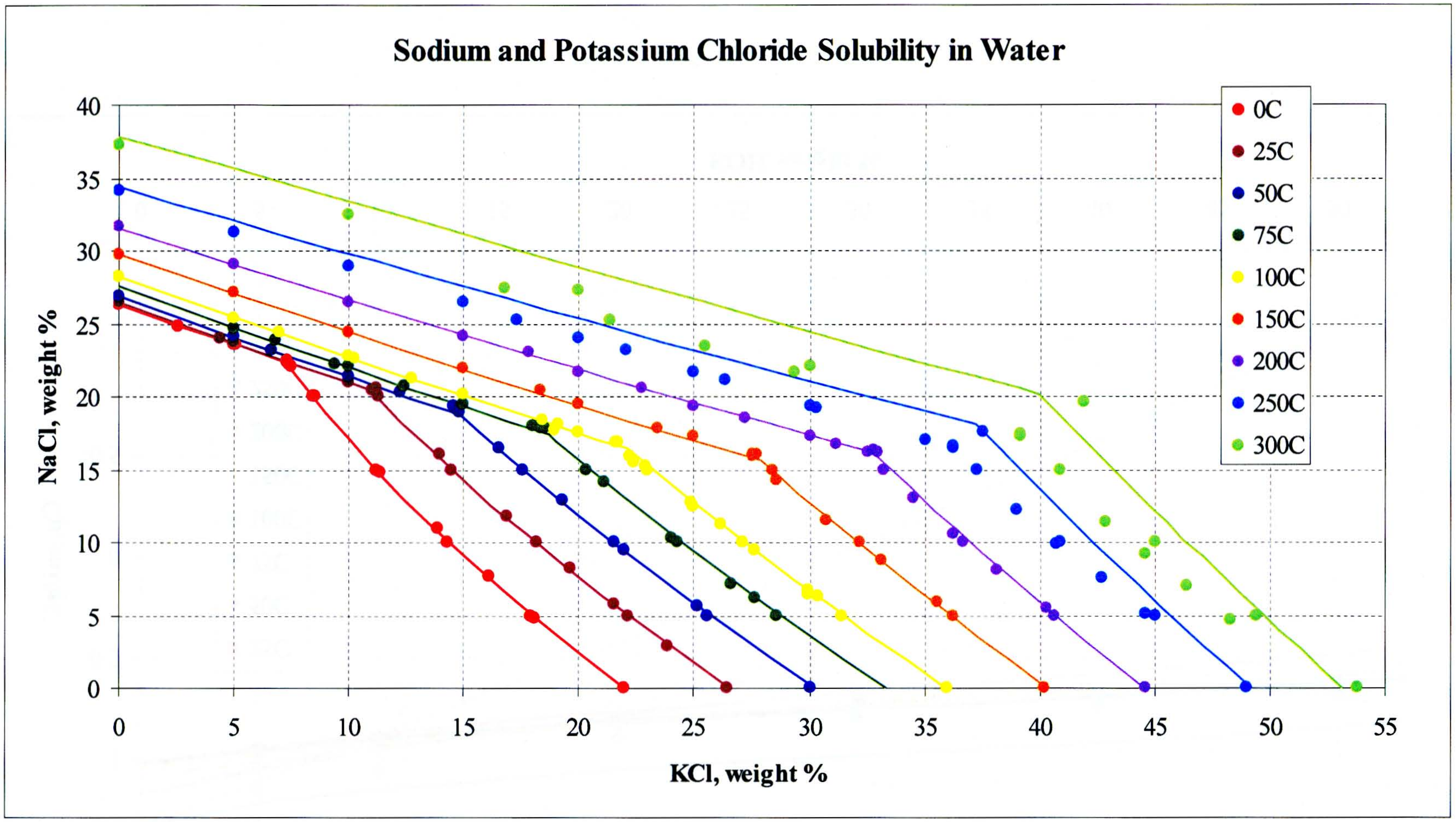

Aqueous Potassium Hydroxide Vapor Pressure
P/H2O VP
KOH, weight %
150C
200C
250C
300C
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85

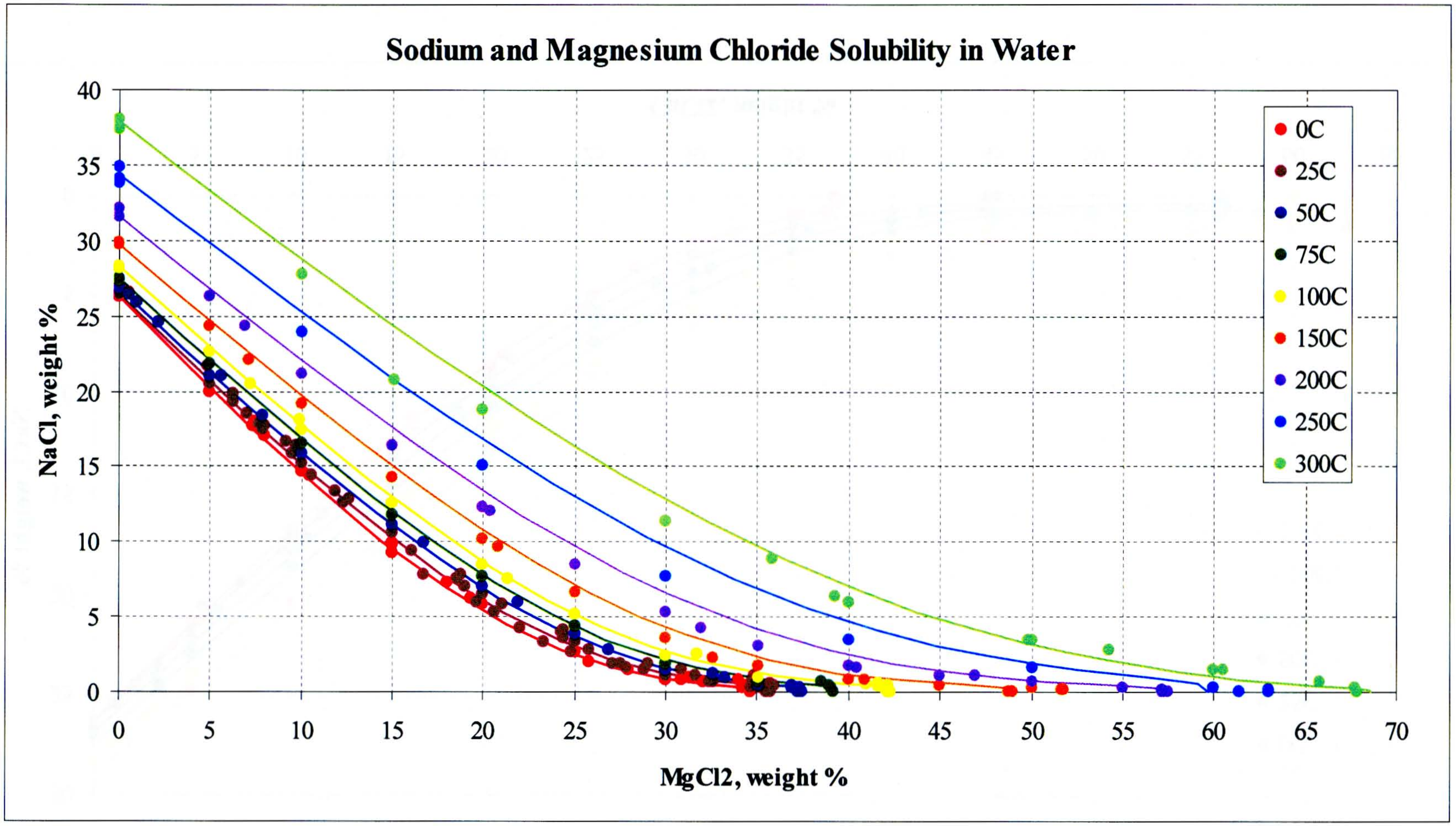


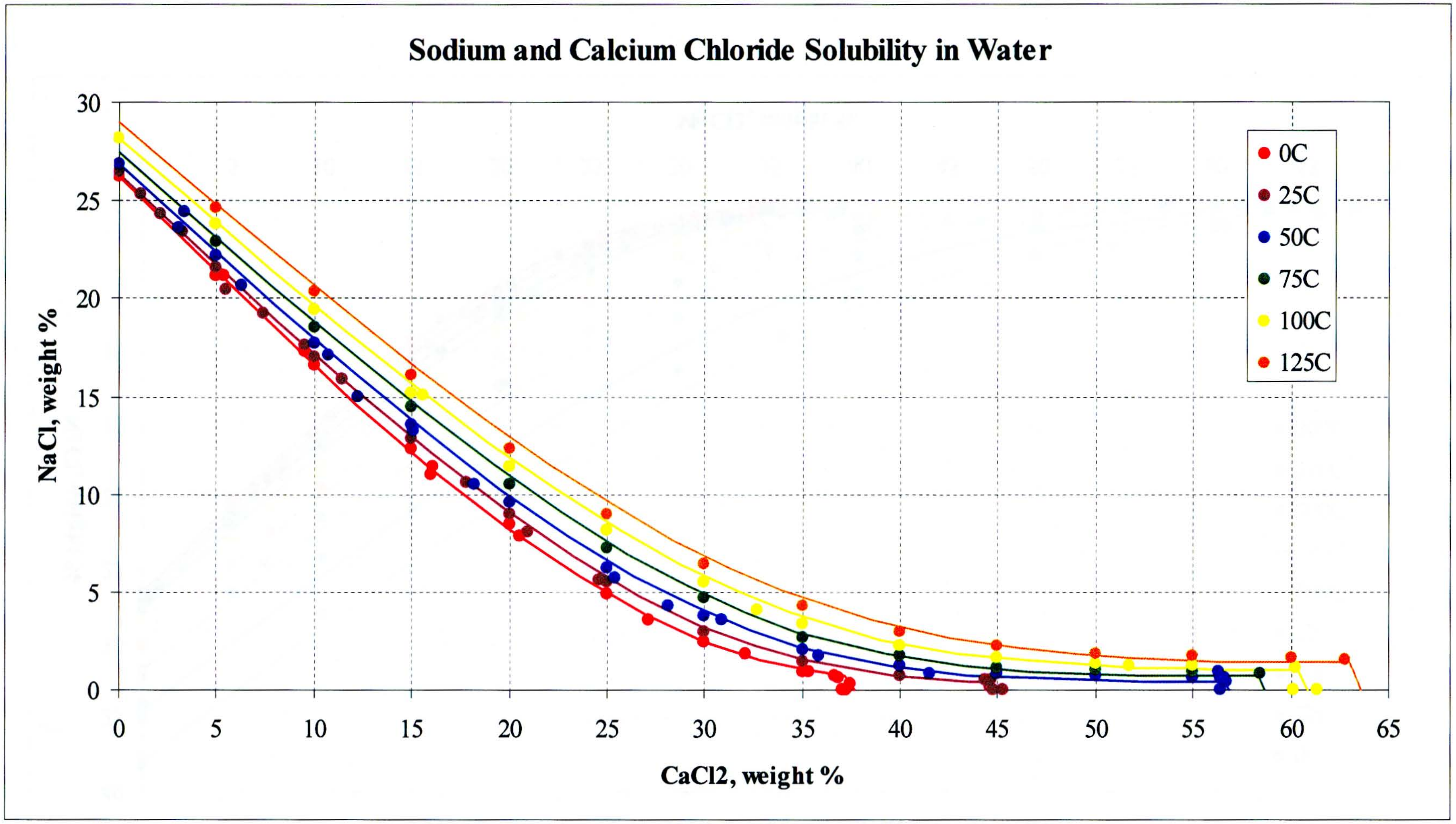
Aqueous Potassium Hydroxide Osmotic Coefficient
0C
25C
50C
100C
150C
200C
250C
300C
Phi
3.5
3
2.5
2
1.5
1
0.5
0
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
KOH, weight %

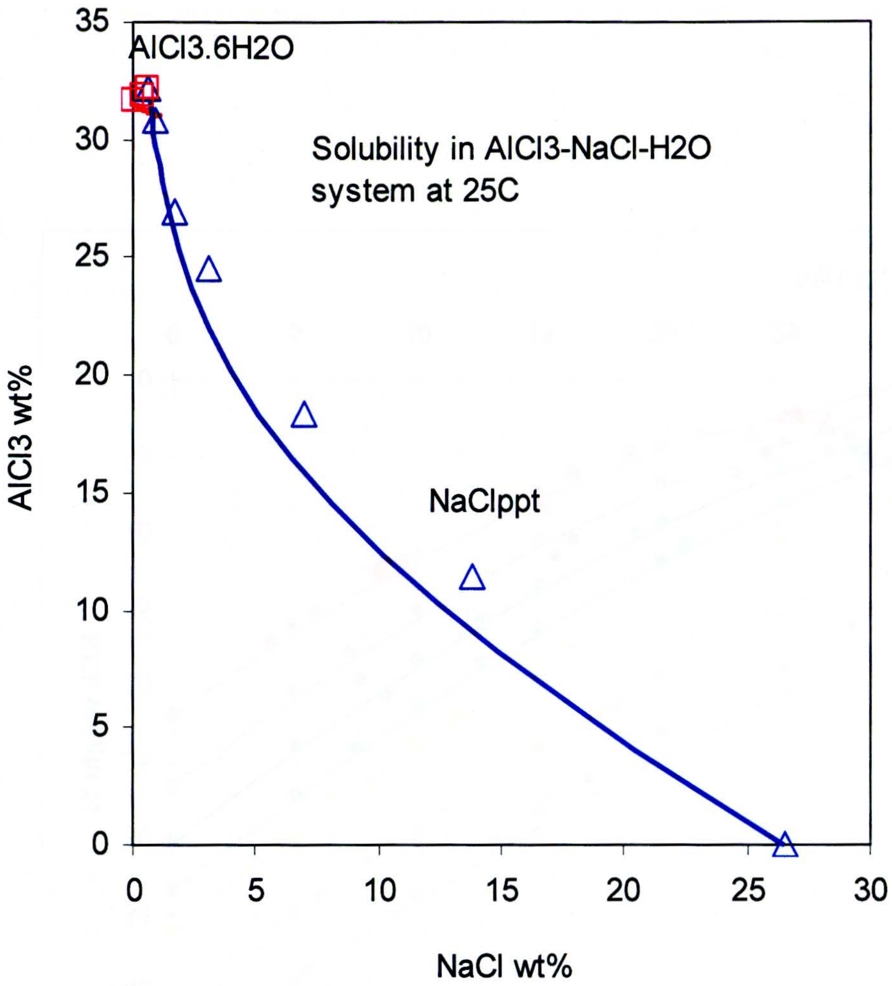

Aqueous Potassium Hydroxide Heat of Dilution
0
-500
-1000
-1500
-2000
-2500
-3000
-3500
Hdil, cal/mol
25C
0
5
10
15
20
25
30
35
40
45
50
55
KOH, weight %

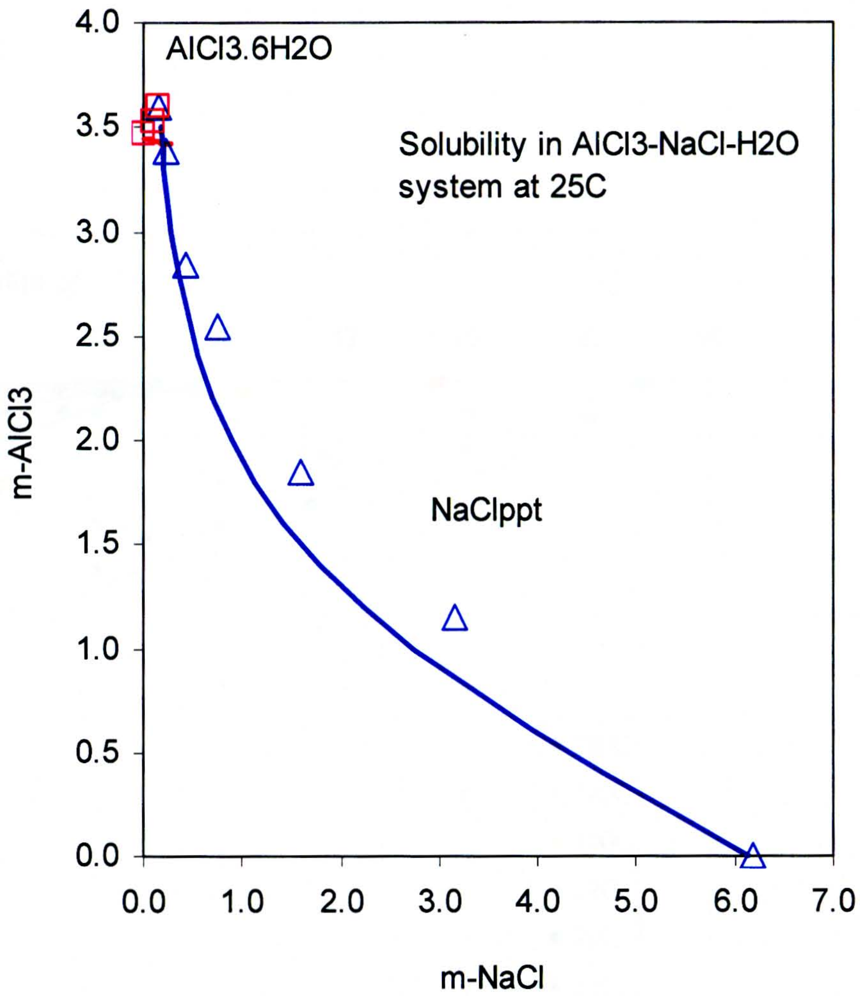

Aqueous Potassium Hydroxide Heat Capacity
1.5
1
0.5
0
-0.5
-1
-1.5
Cp, cal/gC
0
5
10
15
20
25
30
35
40
45
50
55
KOH, weight %
25C
50C
75C
100C
150C
200C
250C
300C

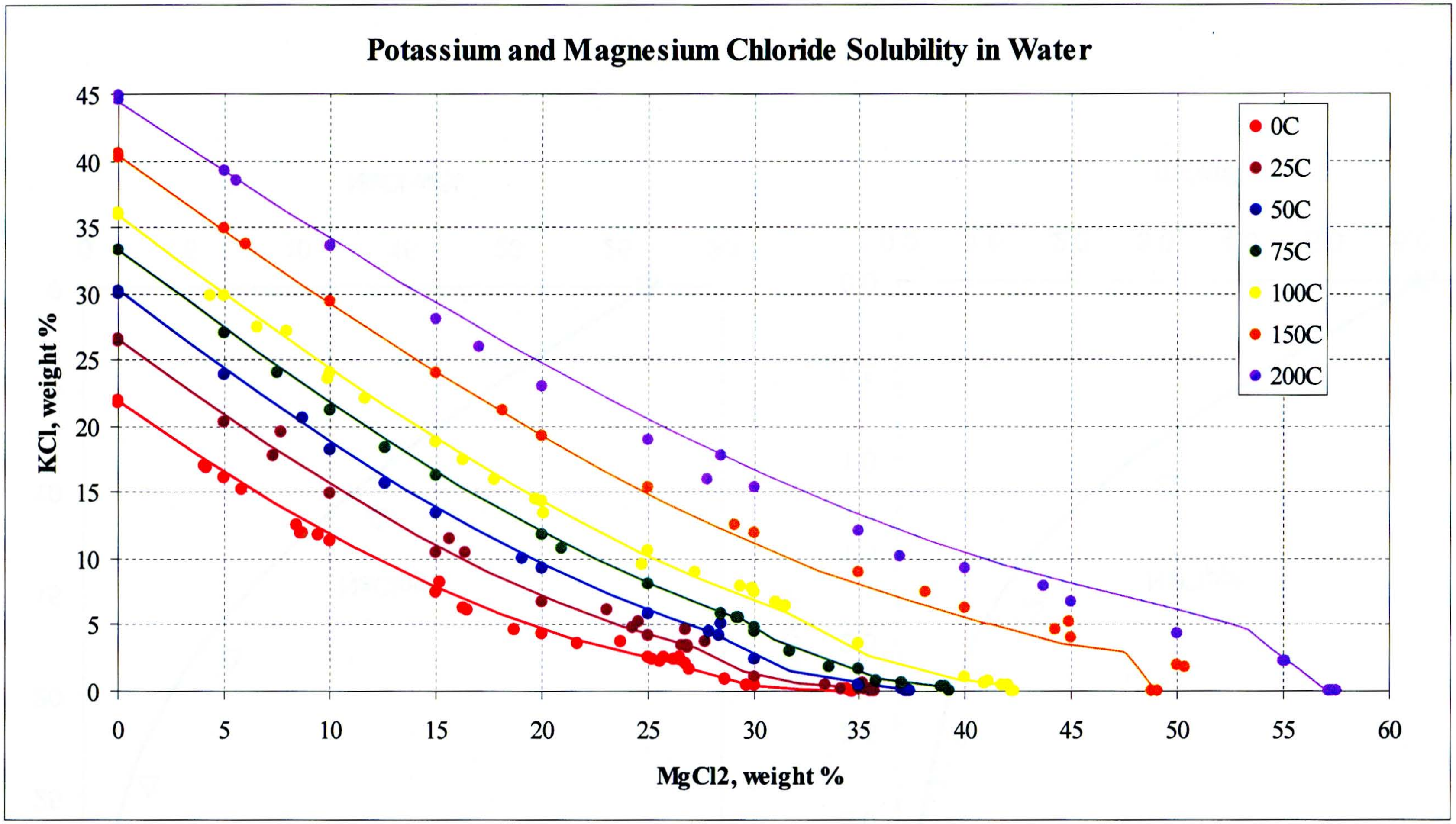

Sodium and Potassium Chloride Solubility in Water
NaCl, weight %
KCl, weight %
0C
25C
50C
75C
100C
150C
200C
250C
300C
0
5
10
15
20
25
30
35
40
45
50
55

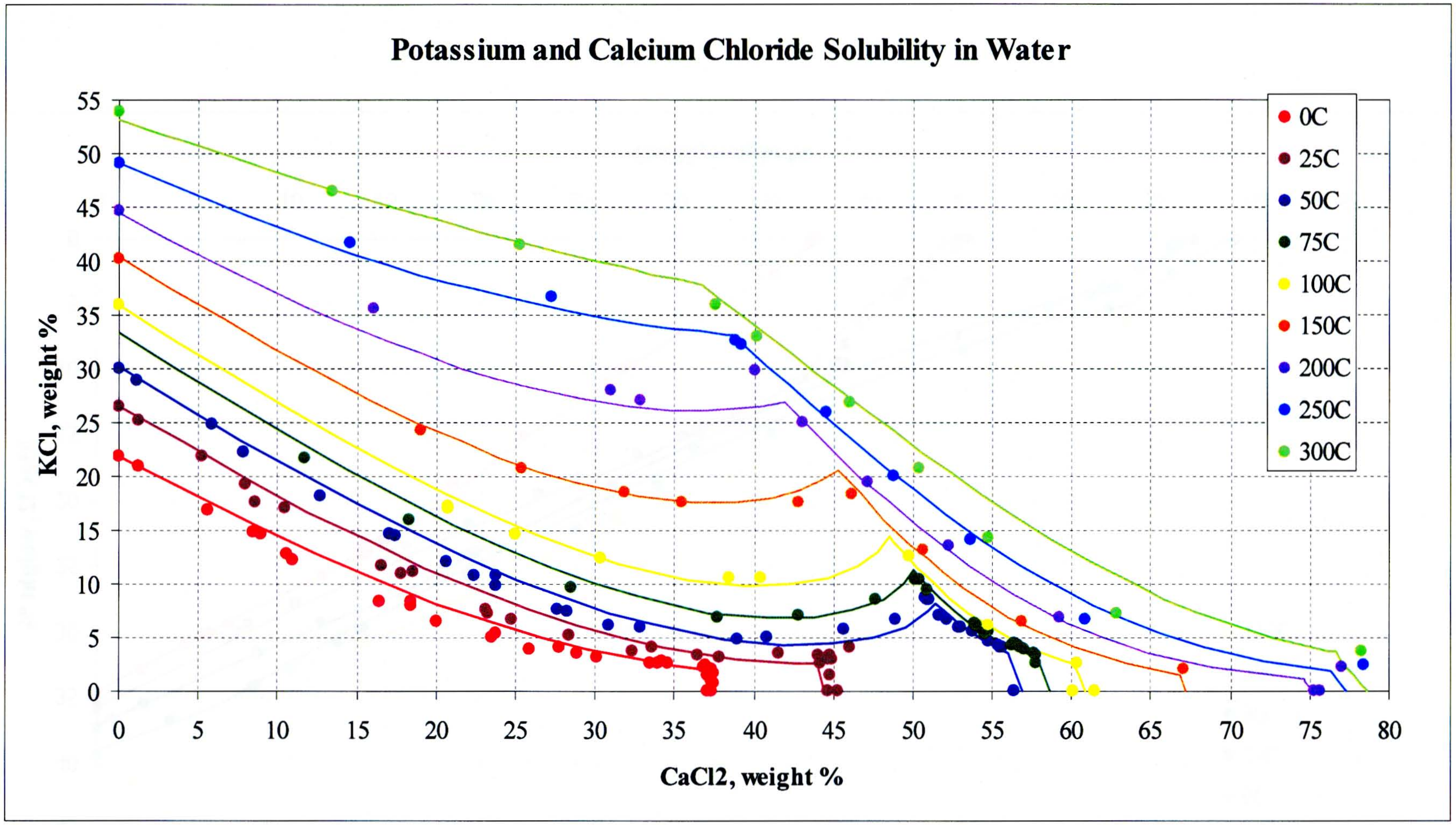

Sodium and Magnesium Chloride Solubility in Water
NaCl, weight %
MgCl2, weight %
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
0C
25C
50C
75C
100C
150C
200C
250C
300C

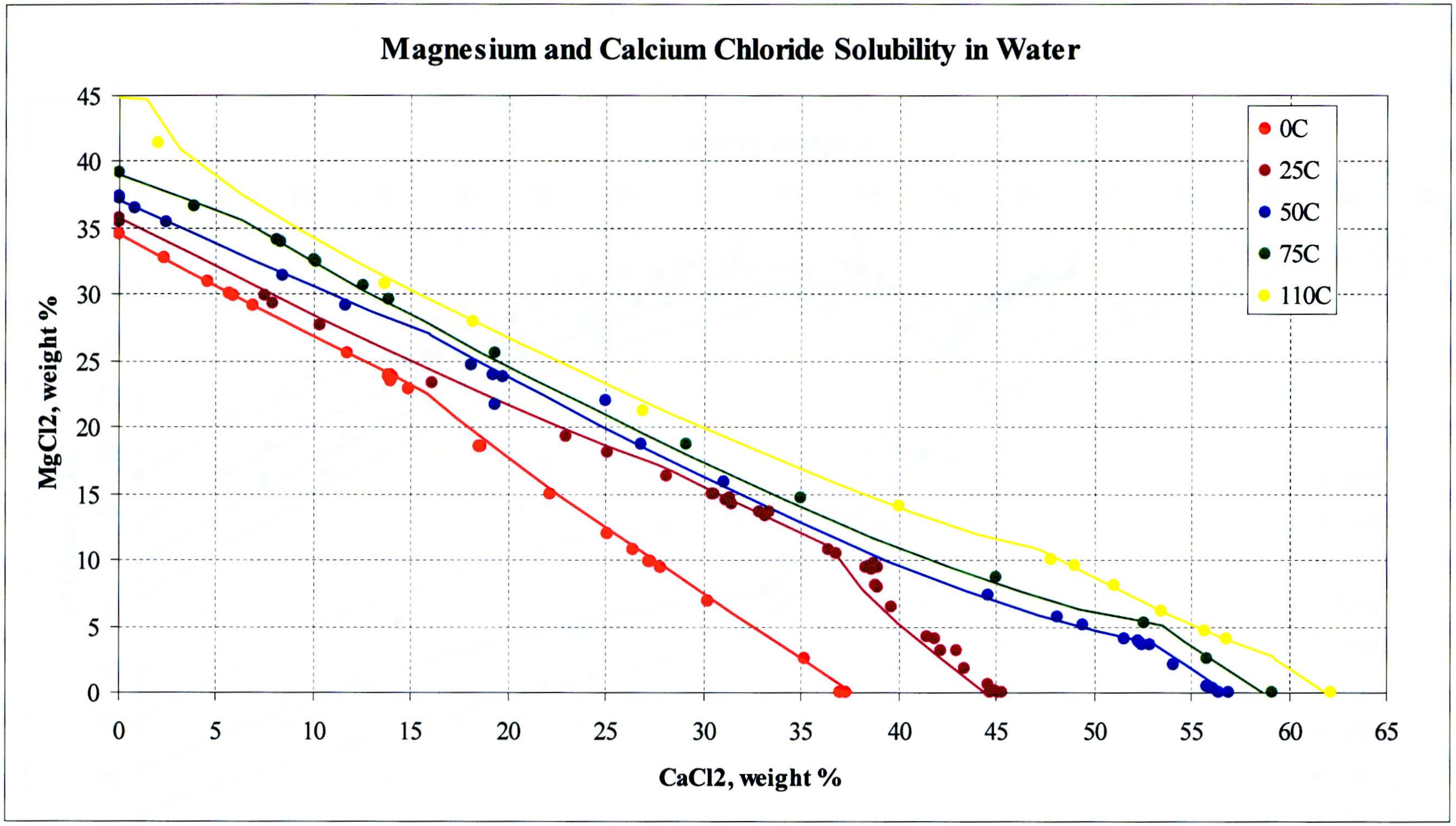

Sodium and Calcium Chloride Solubility in Water
NaCl, weight %
CaCl2, weight %
0 5 10 15 20 25 30 35 40 45 50 55 60 65
0 5 10 15 20 25 30
0C
25C
50C
75C
100C
125C


AlCl3.6H2O
Solubility in AlCl3-NaCl-H2O system at 25C
NaClppt
AlCl3 wt%
NaCl wt%
0
5
10
15
20
25
30
35

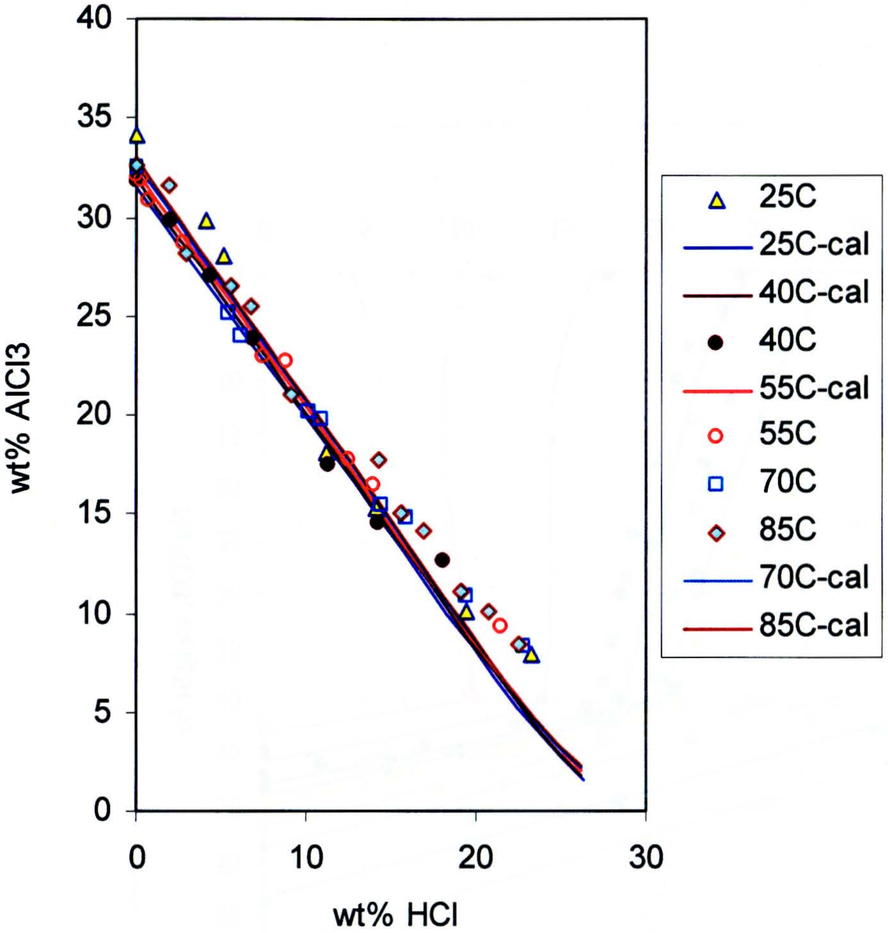

AlCl3.6H2O
Solubility in AlCl3-NaCl-H2O system at 25C
NaClppt
m-AlCl3
m-NaCl
0.0
1.0
2.0
3.0
4.0
5.0
6.0
7.0

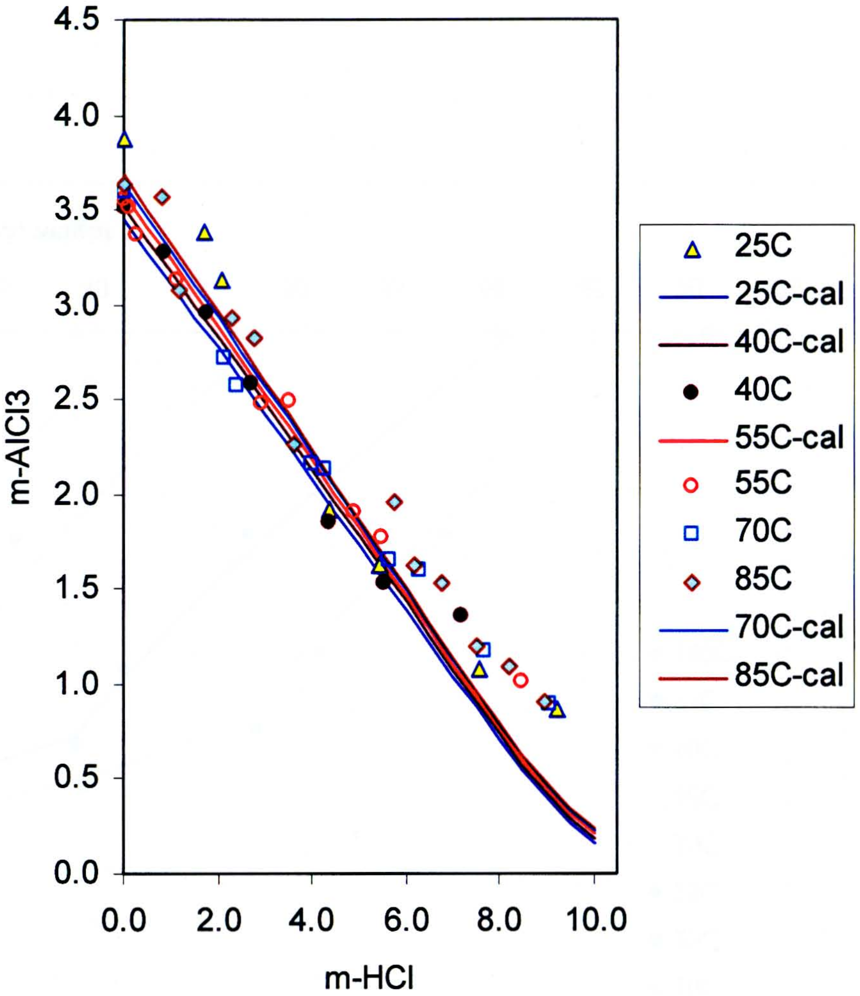

Potassium and Magnesium Chloride Solubility in Water
KCl, weight %
MgCl2, weight %
0C
25C
50C
75C
100C
150C
200C
0
5
10
15
20
25
30
35
40
45
50
55
60

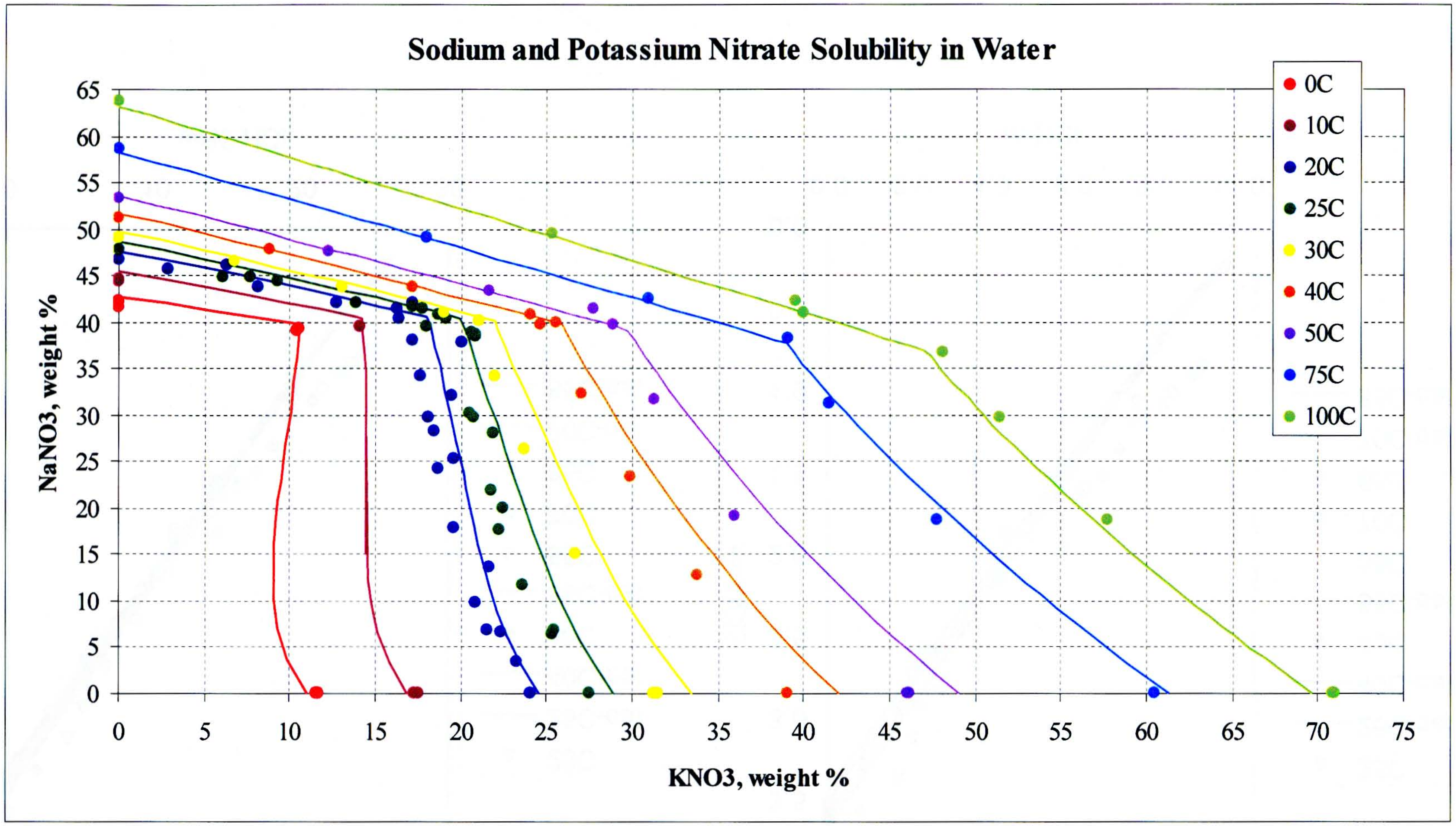

Potassium and Calcium Chloride Solubility in Water
KCl, weight %
CaCl2, weight %
0
5
10
15
20
25
30
35
40
45
50
55
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
0C
25C
50C
75C
100C
150C
200C
250C
300C

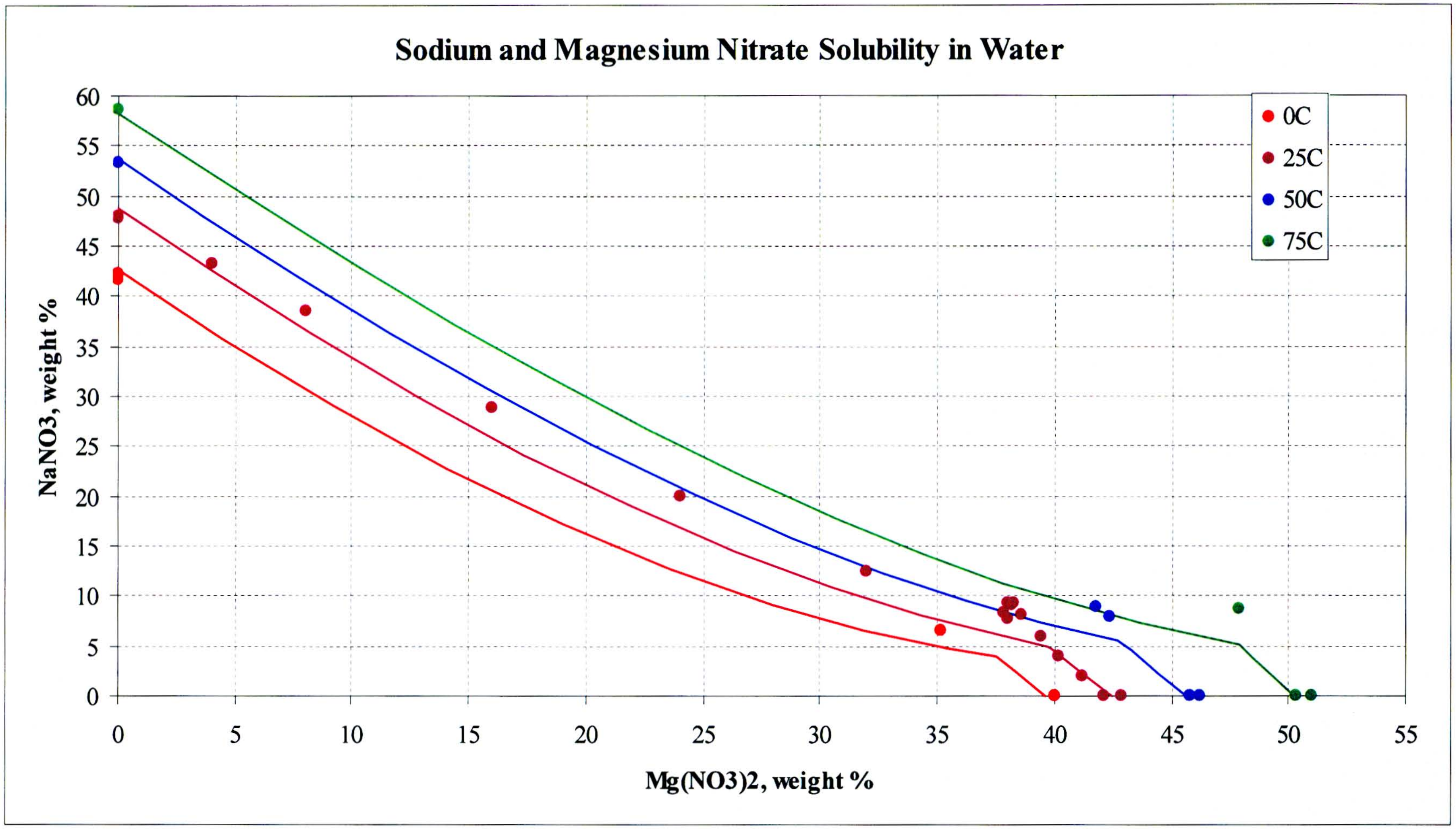


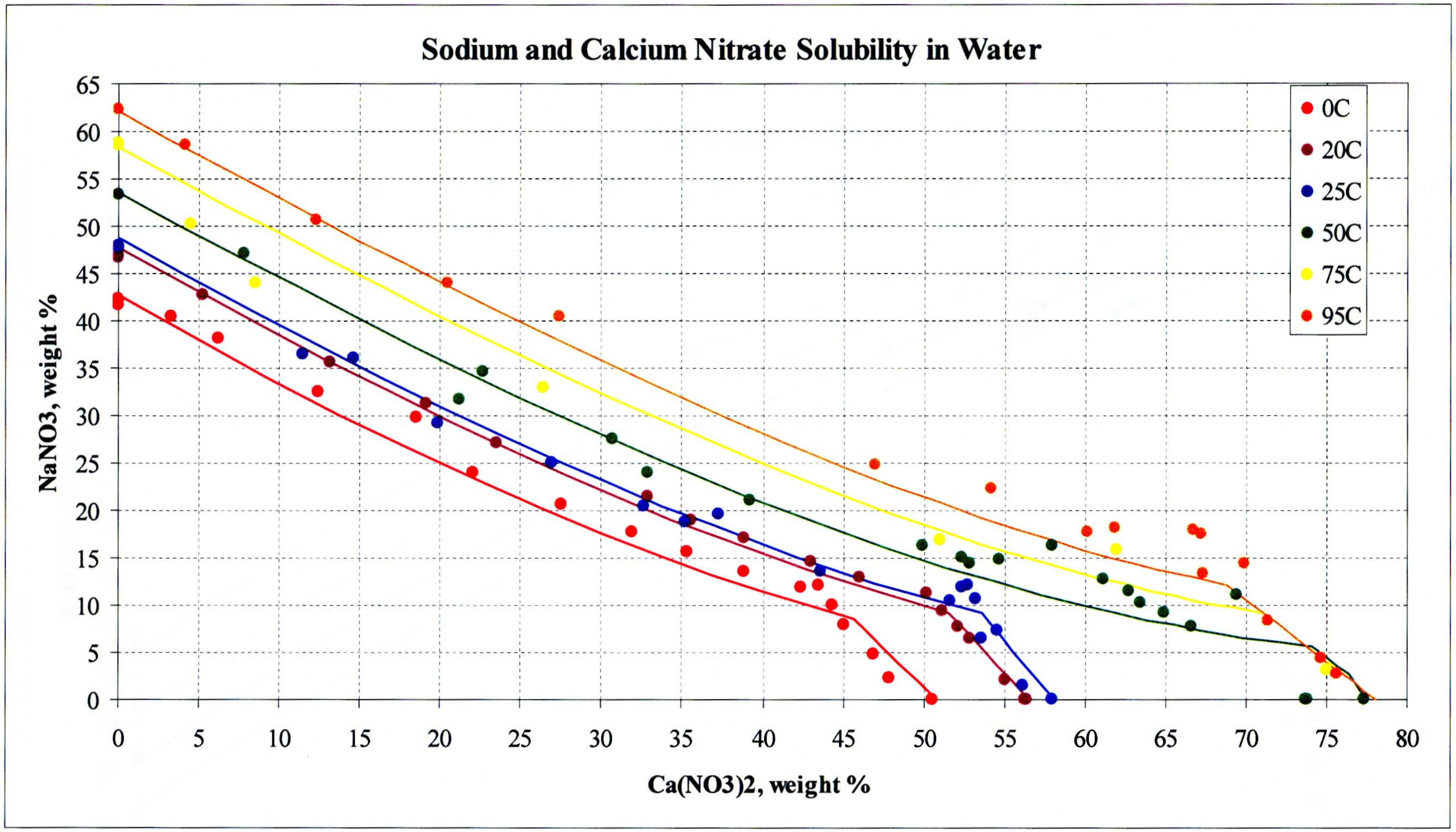
Magnesium and Calcium Chloride Solubility in Water
MgCl2, weight %
CaCl2, weight %
0C
25C
50C
75C
110C
0
5
10
15
20
25
30
35
40
45
50
55
60
65


40
35
30
25
20
15
10
5
0
wt% AlCl3
0
10
20
30
wt% HCl
25C
25C-cal
40C-cal
40C
55C-cal
55C
70C
85C
70C-cal
85C-cal

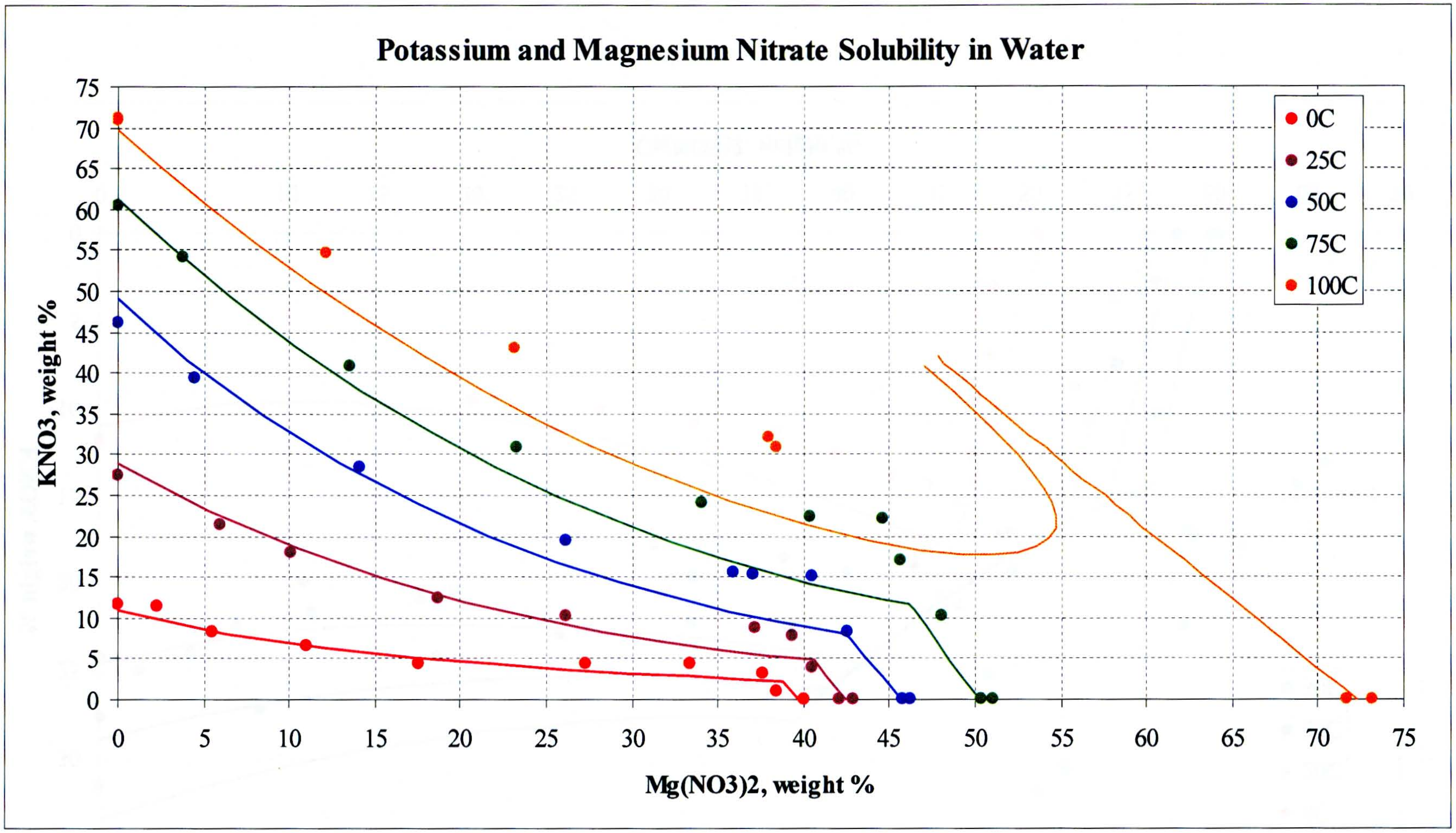

4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
m-AlCl3
0.0
2.0
4.0
6.0
8.0
10.0
m-HCl
25C
25C-cal
40C-cal
40C
55C-cal
55C
70C
85C
70C-cal
85C-cal

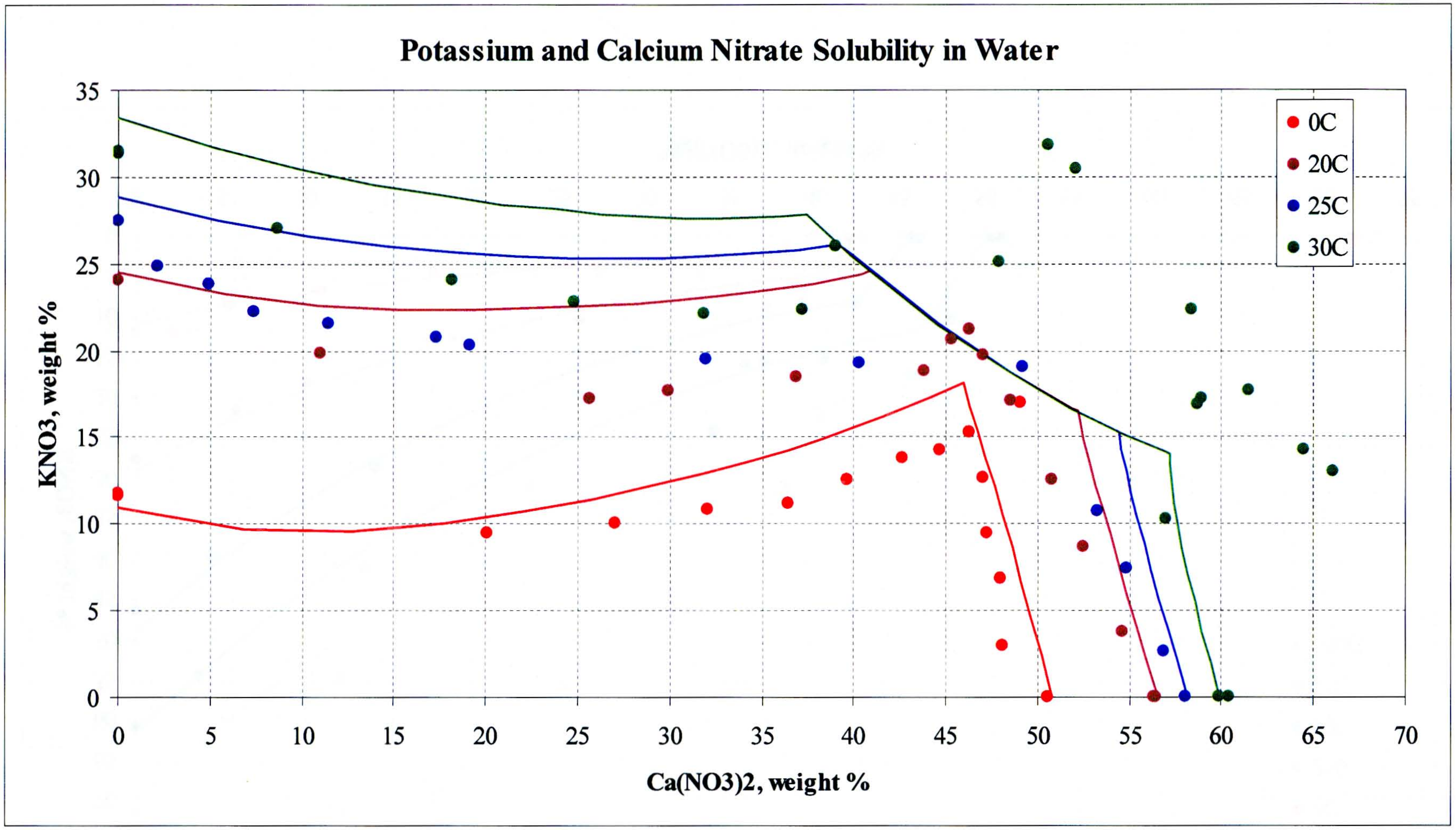

Sodium and Potassium Nitrate Solubility in Water
NaNO3, weight %
KNO3, weight %
0C
10C
20C
25C
30C
40C
50C
75C
100C
65
60
55
50
45
40
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75

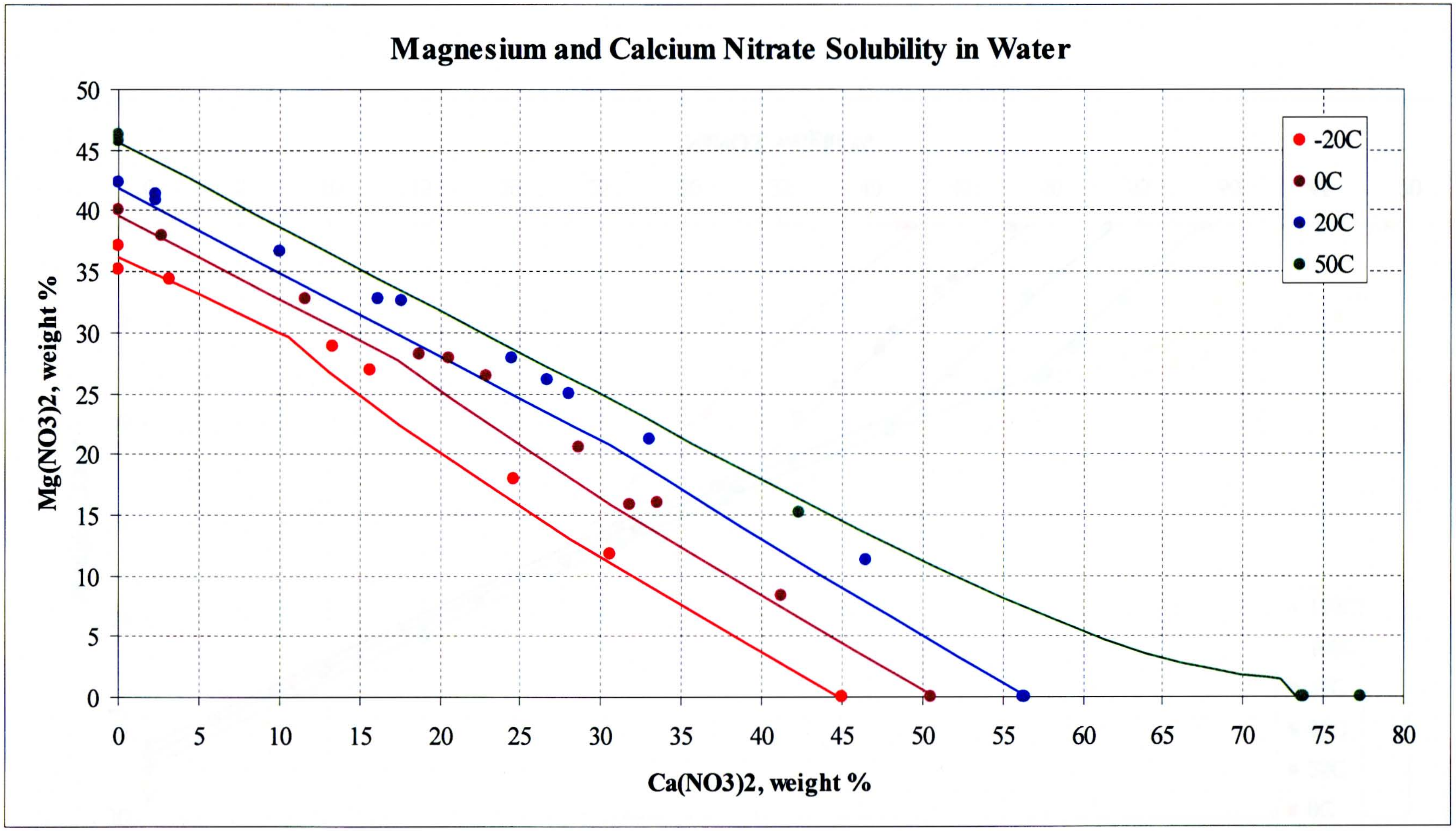

Sodium and Magnesium Nitrate Solubility in Water
NaNO3, weight %
Mg(NO3)2, weight %
60
55
50
45
40
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30
35
40
45
50
55
0C
25C
50C
75C

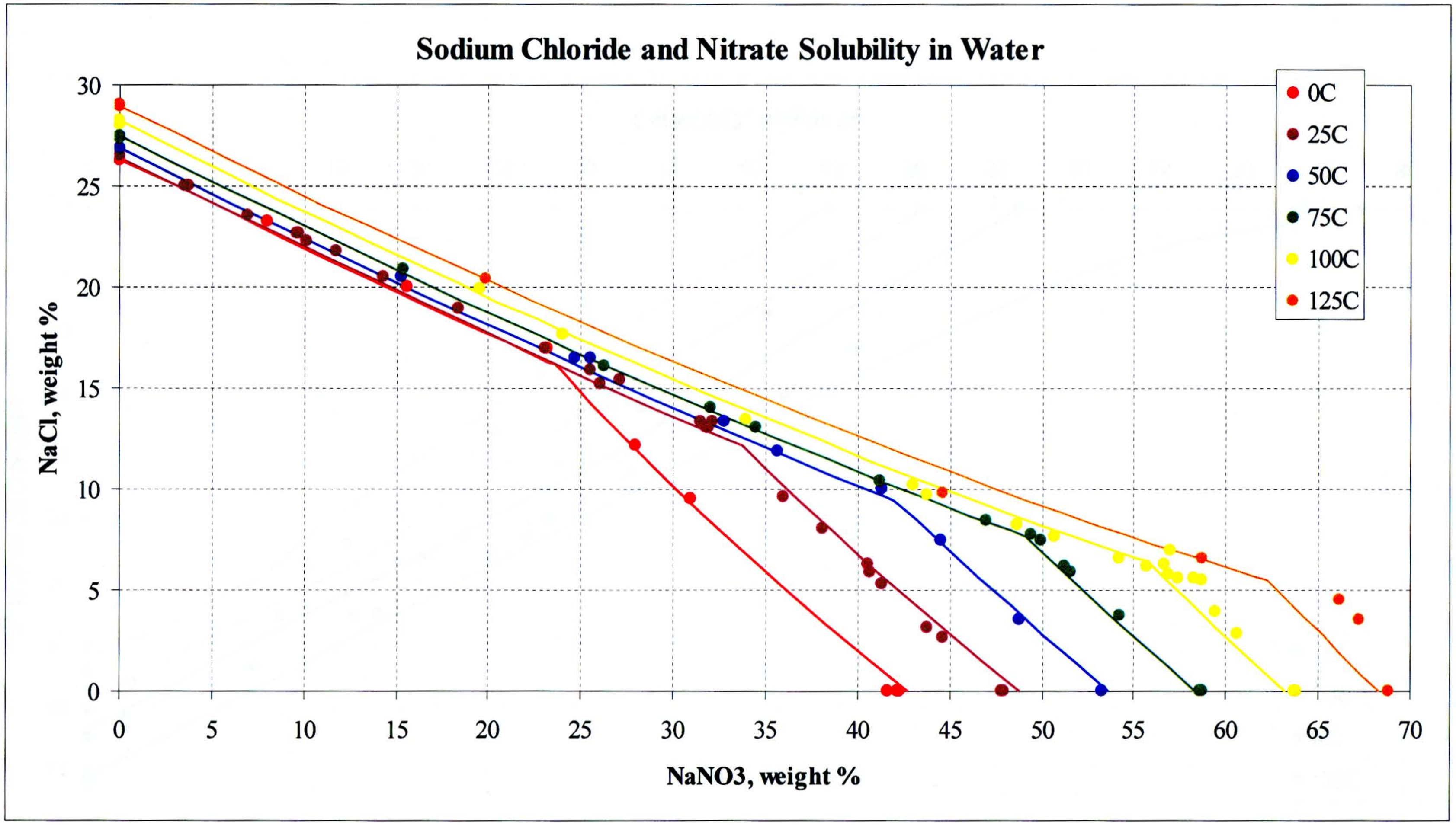


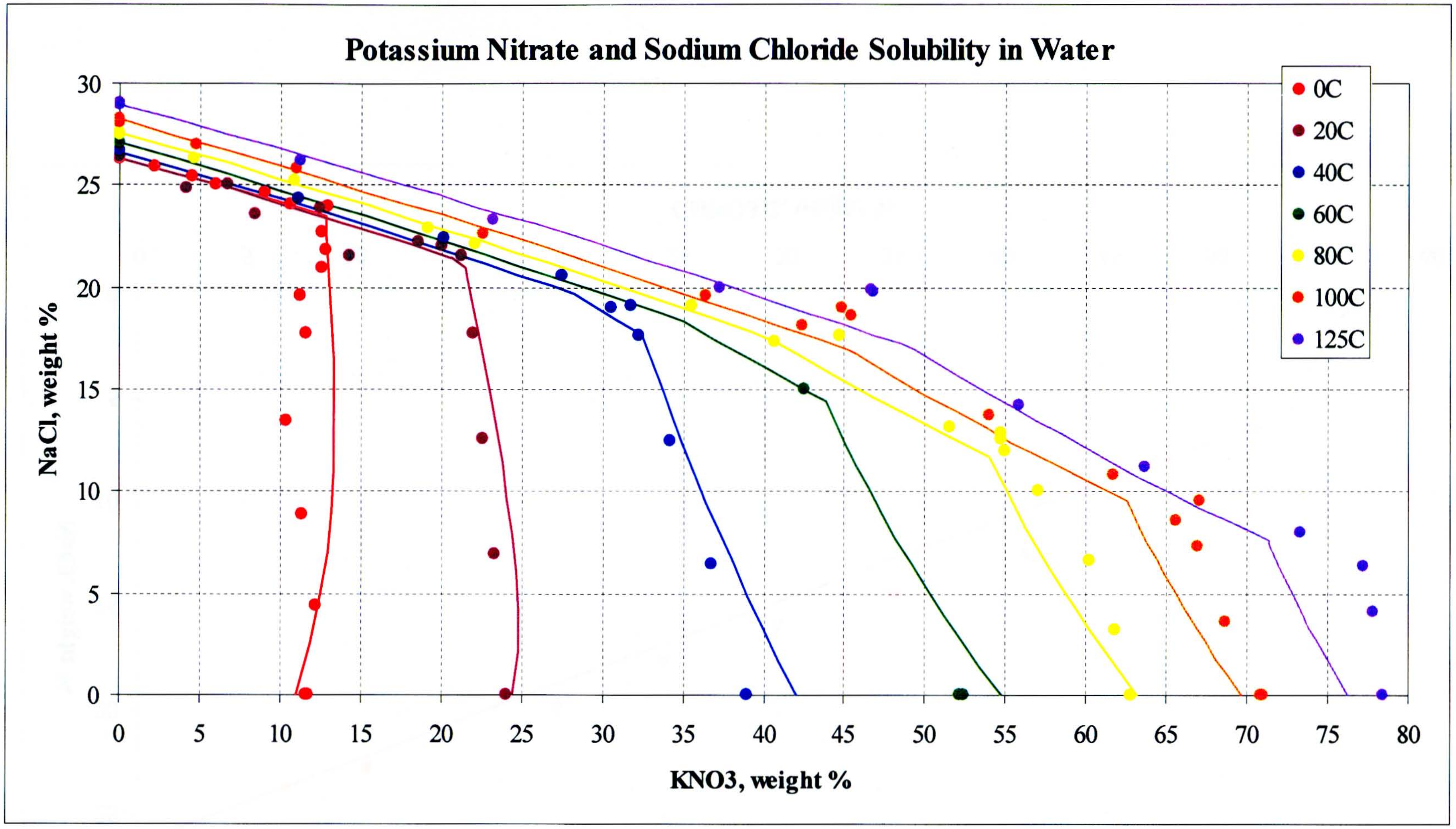
Sodium and Calcium Nitrate Solubility in Water
NaNO3, weight %
Ca(NO3)2, weight %
0C
20C
25C
50C
75C
95C
65
60
55
50
45
40
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80

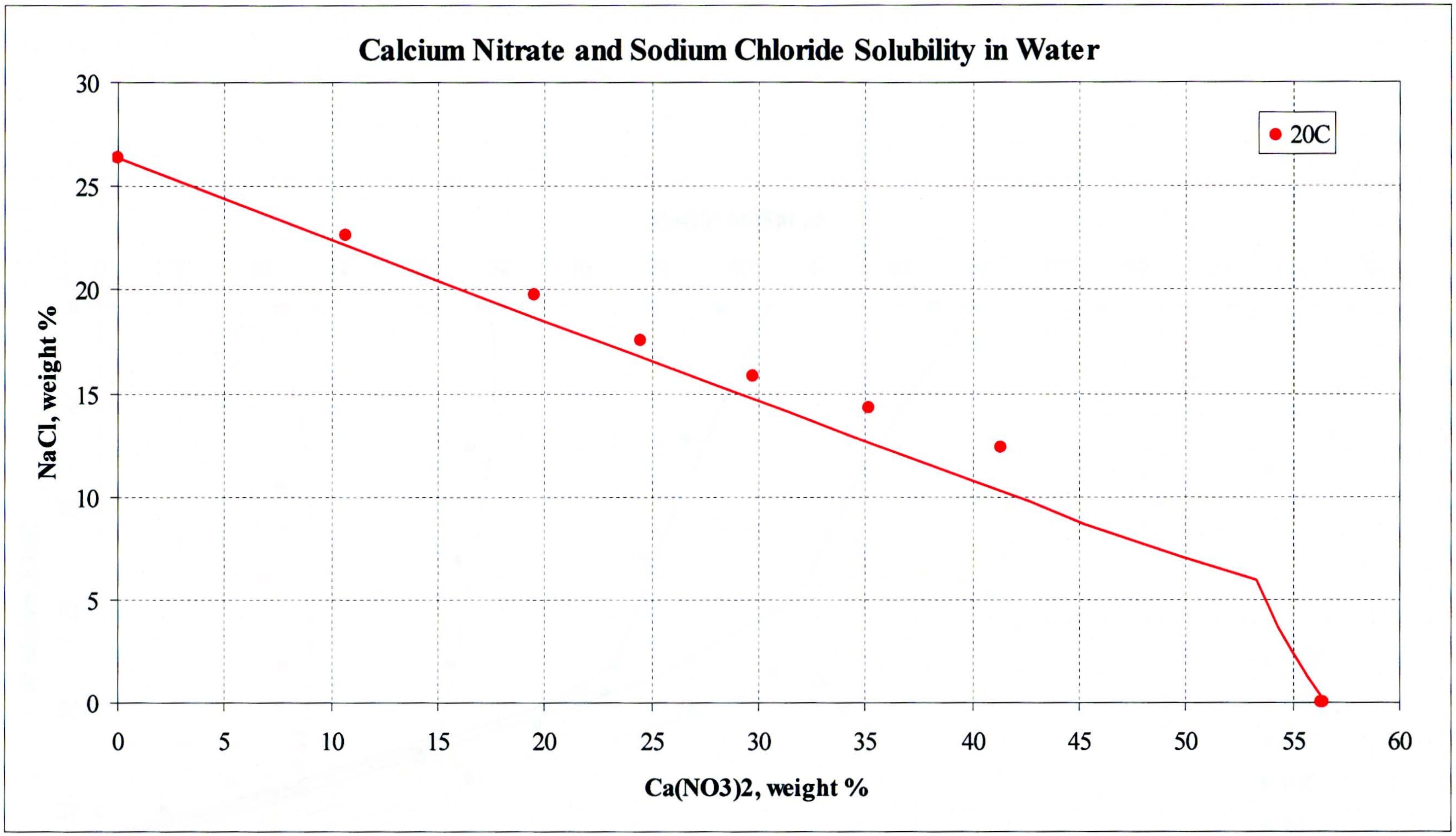

Potassium and Magnesium Nitrate Solubility in Water
KNO3, weight %
Mg(NO3)2, weight %
0C
25C
50C
75C
100C
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75

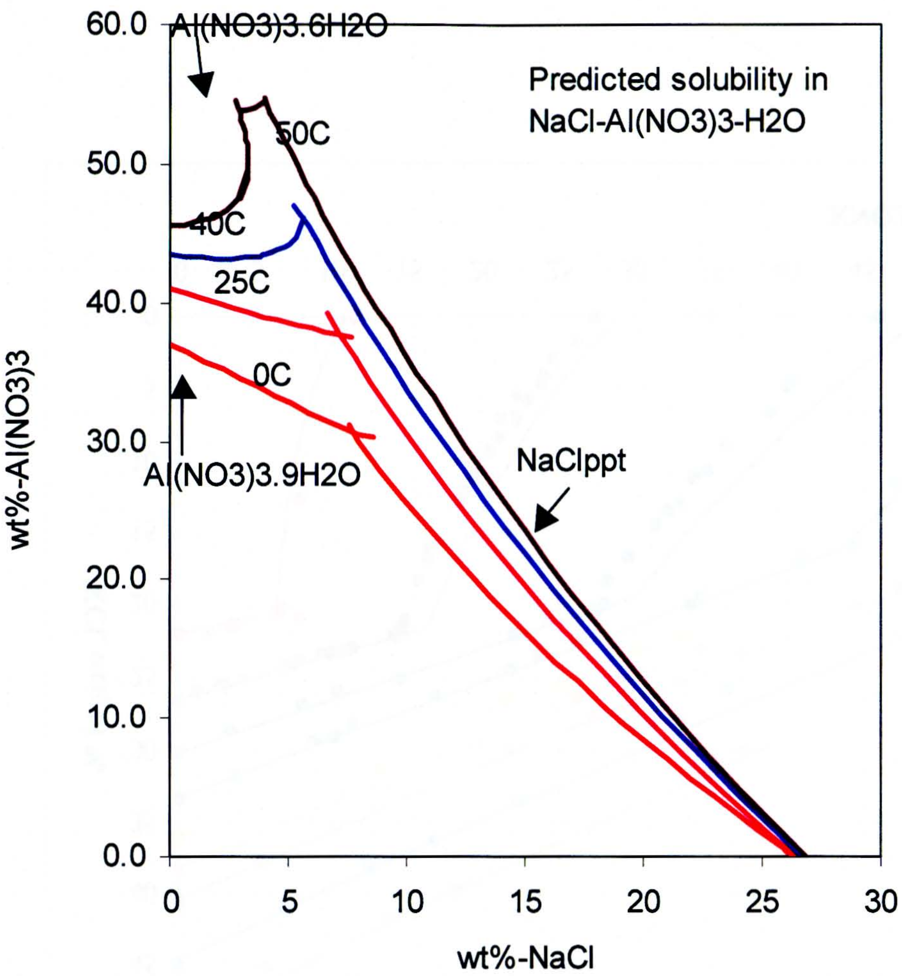

Potassium and Calcium Nitrate Solubility in Water
KNO3, weight %
Ca(NO3)2, weight %
0C
20C
25C
30C
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70

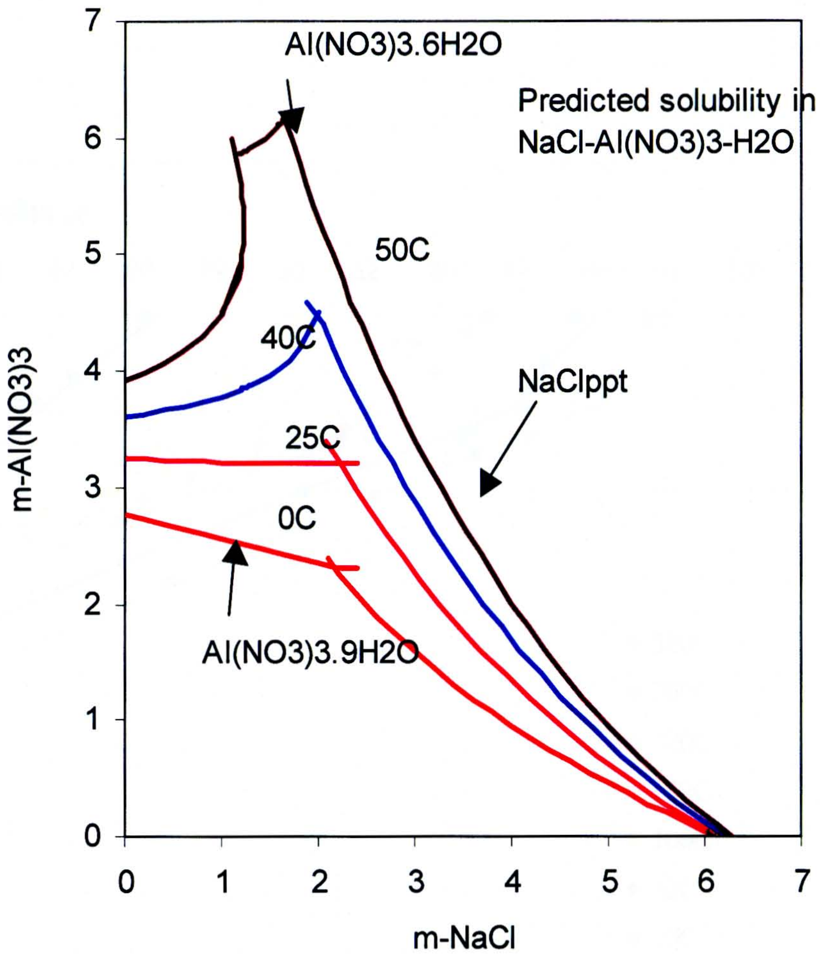

Magnesium and Calcium Nitrate Solubility in Water
Mg(NO3)2, weight %
Ca(NO3)2, weight %
-20C
0C
20C
50C
0
5
10
15
20
25
30
35
40
45
50
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80

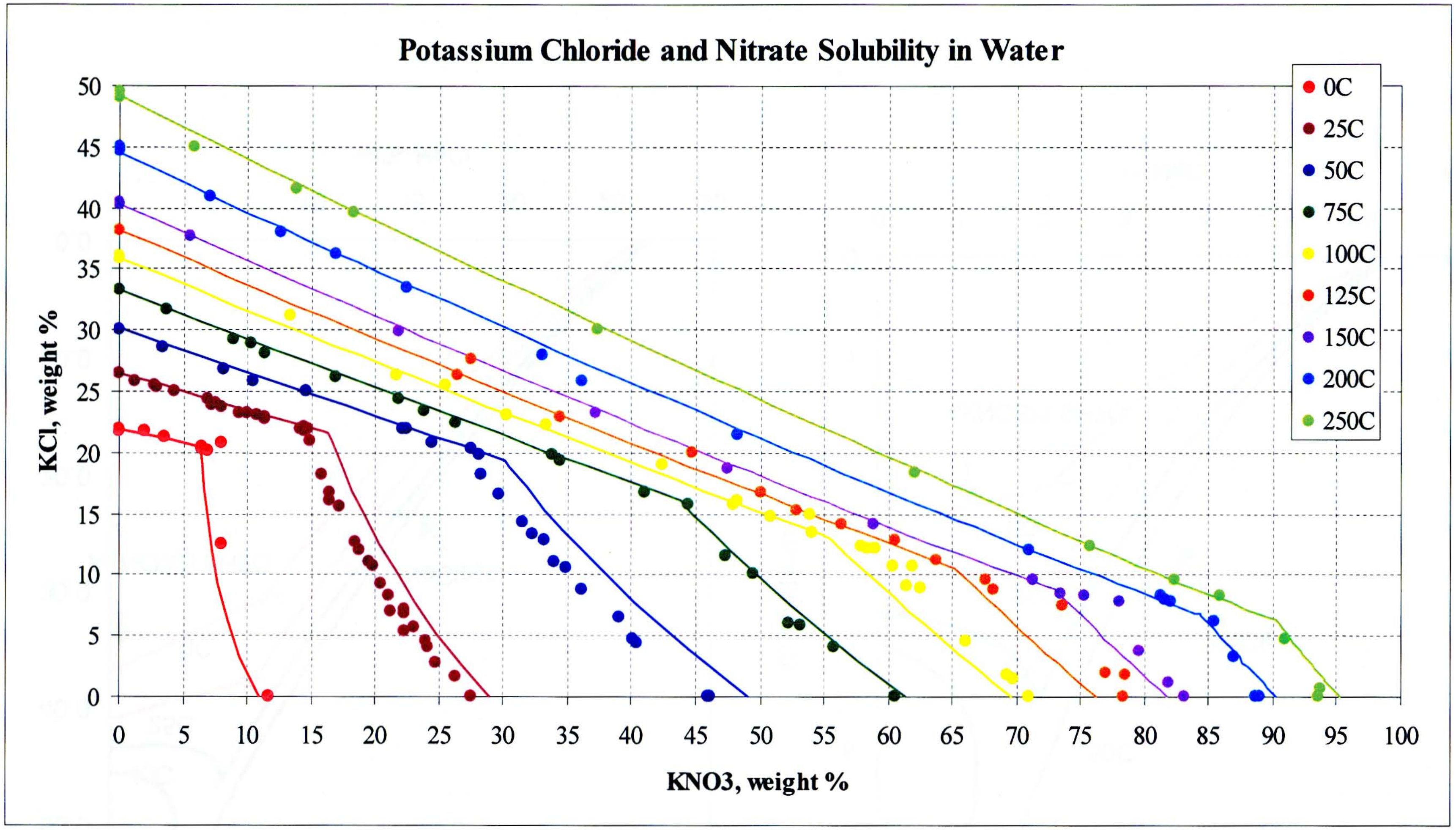

Sodium Chloride and Nitrate Solubility in Water
NaCl, weight %
NaNO3, weight %
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
0C
25C
50C
75C
100C
125C

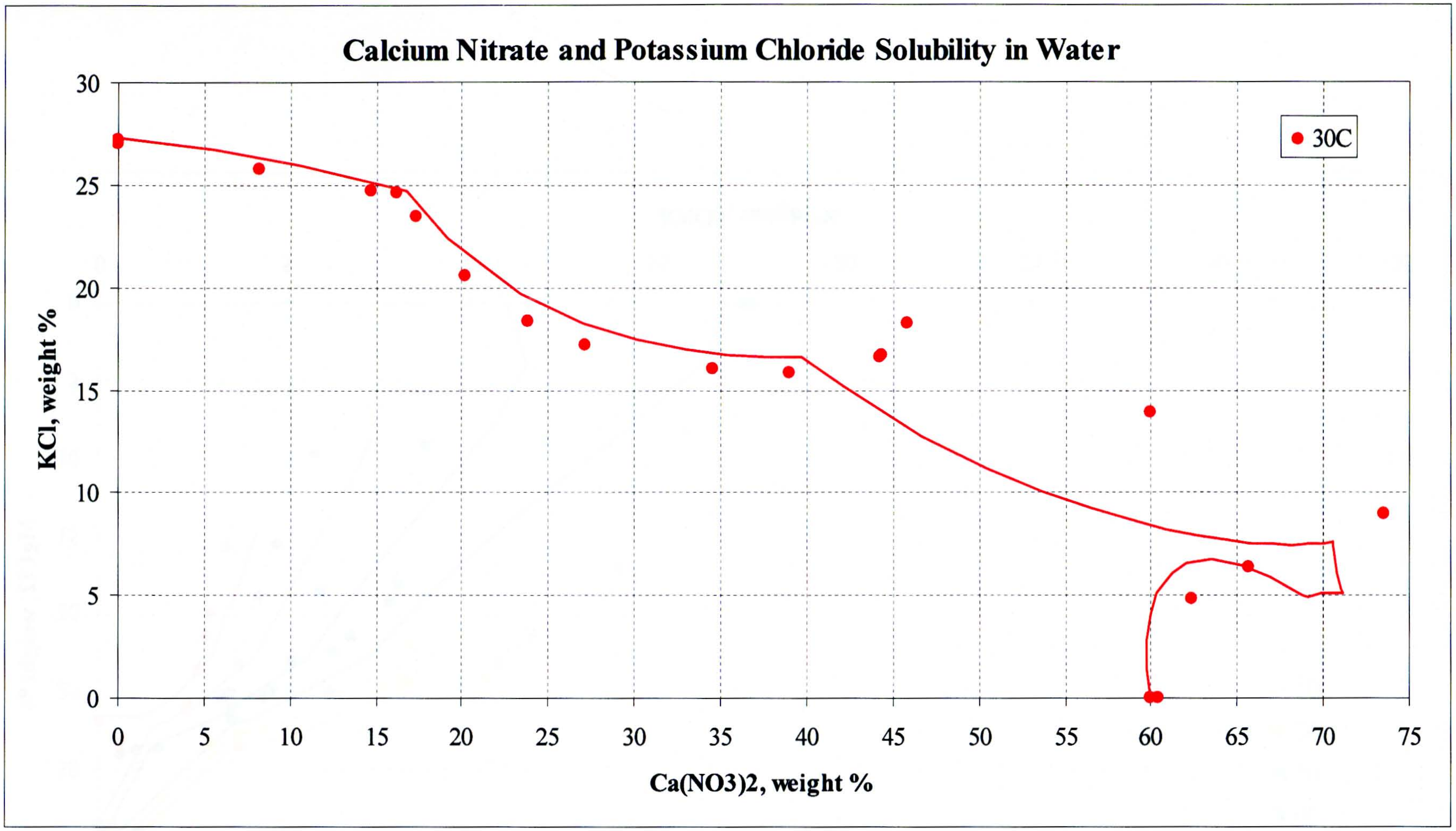

Potassium Nitrate and Sodium Chloride Solubility in Water
0C
20C
40C
60C
80C
100C
125C
NaCl, weight %
KNO3, weight %
0
5
10
15
20
25
30
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80

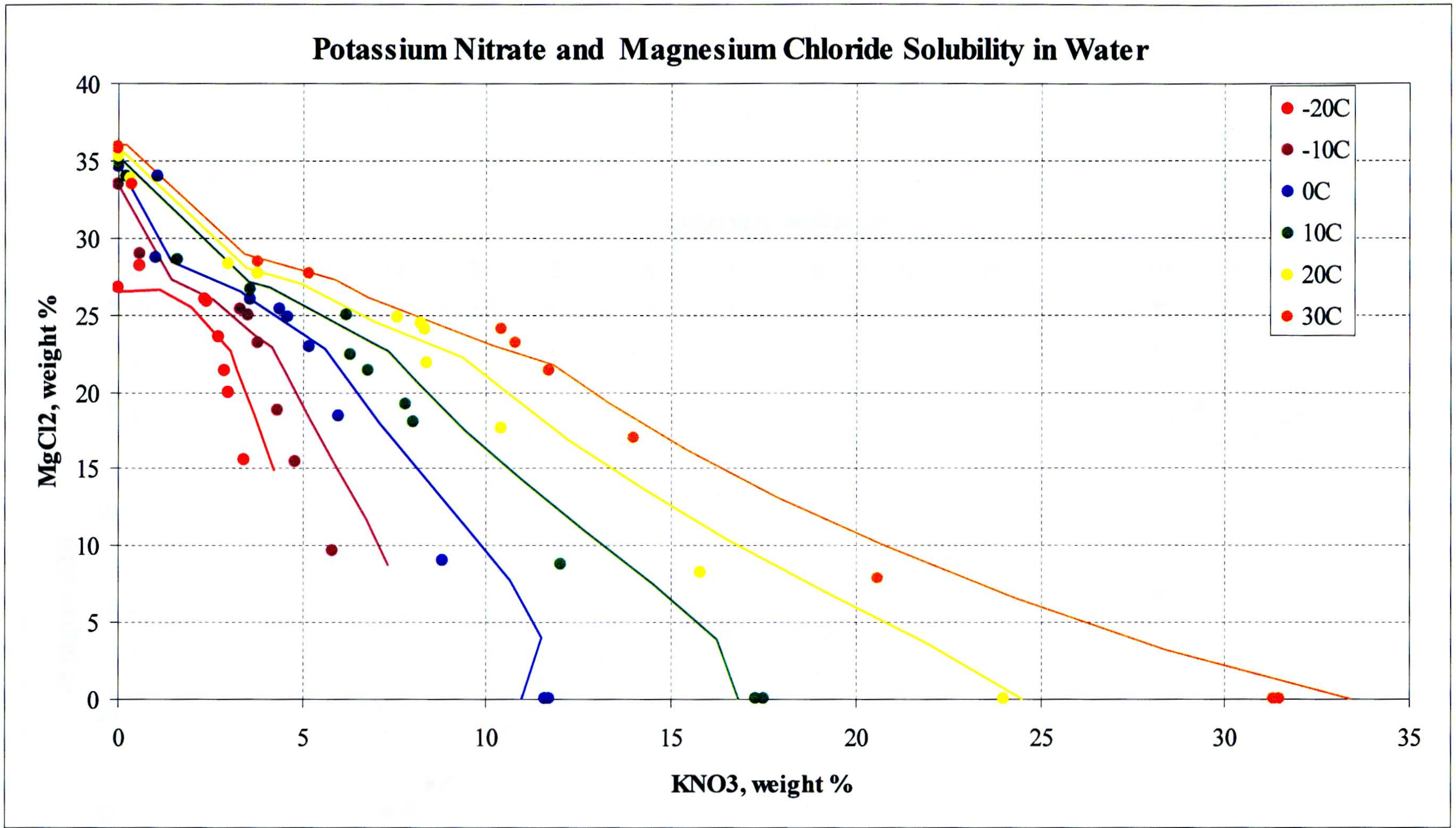

Calcium Nitrate and Sodium Chloride Solubility in Water
30
25
20
15
10
5
0
NaCl, weight %
0
5
10
15
20
25
30
35
40
45
50
55
60
Ca(NO3)2, weight %
20C


Predicted solubility in
NaCl-Al(NO3)3-H2O
Al(NO3)3.6H2O
50C
40C
25C
0C
NaClppt
Al(NO3)3.9H2O
wt%-Al(NO3)3
wt%-NaCl

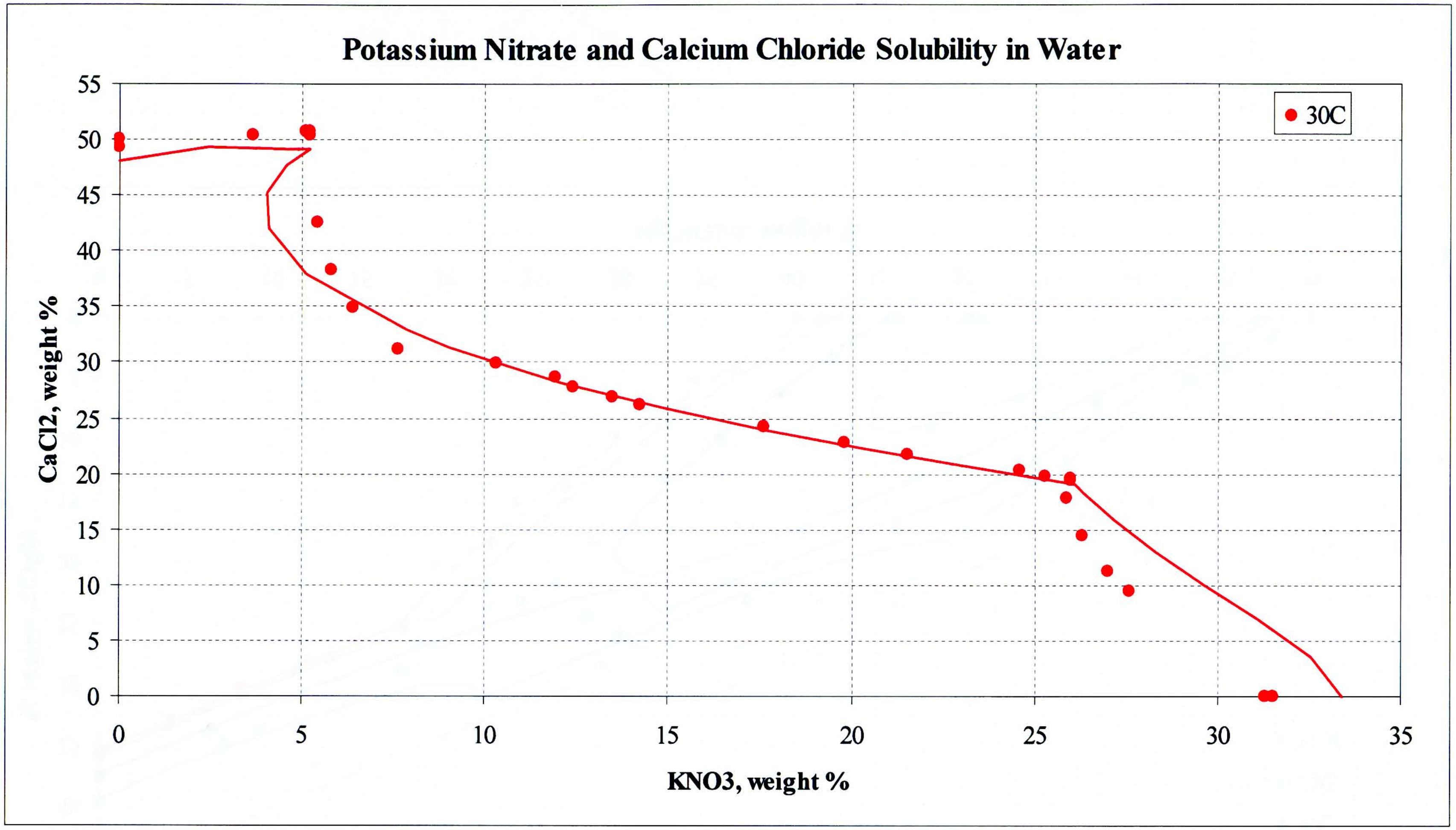

Al(NO3)3.6H2O
Predicted solubility in
NaCl-Al(NO3)3-H2O
50C
40C
NaClppt
25C
0C
Al(NO3)3.9H2O
m-Al(NO3)3
m-NaCl

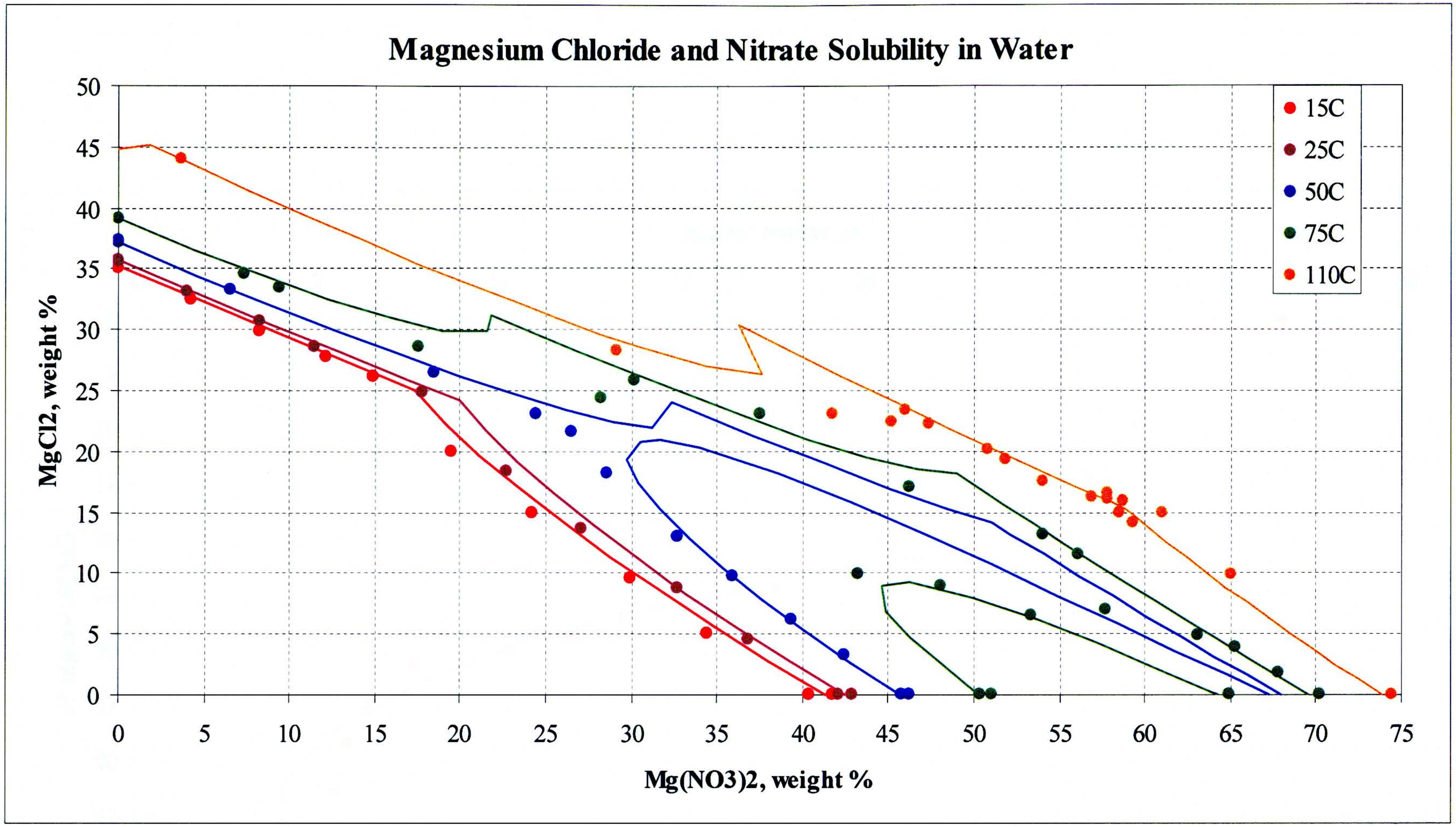

Potassium Chloride and Nitrate Solubility in Water
KCl, weight %
KNO3, weight %
0C
25C
50C
75C
100C
125C
150C
200C
250C
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100

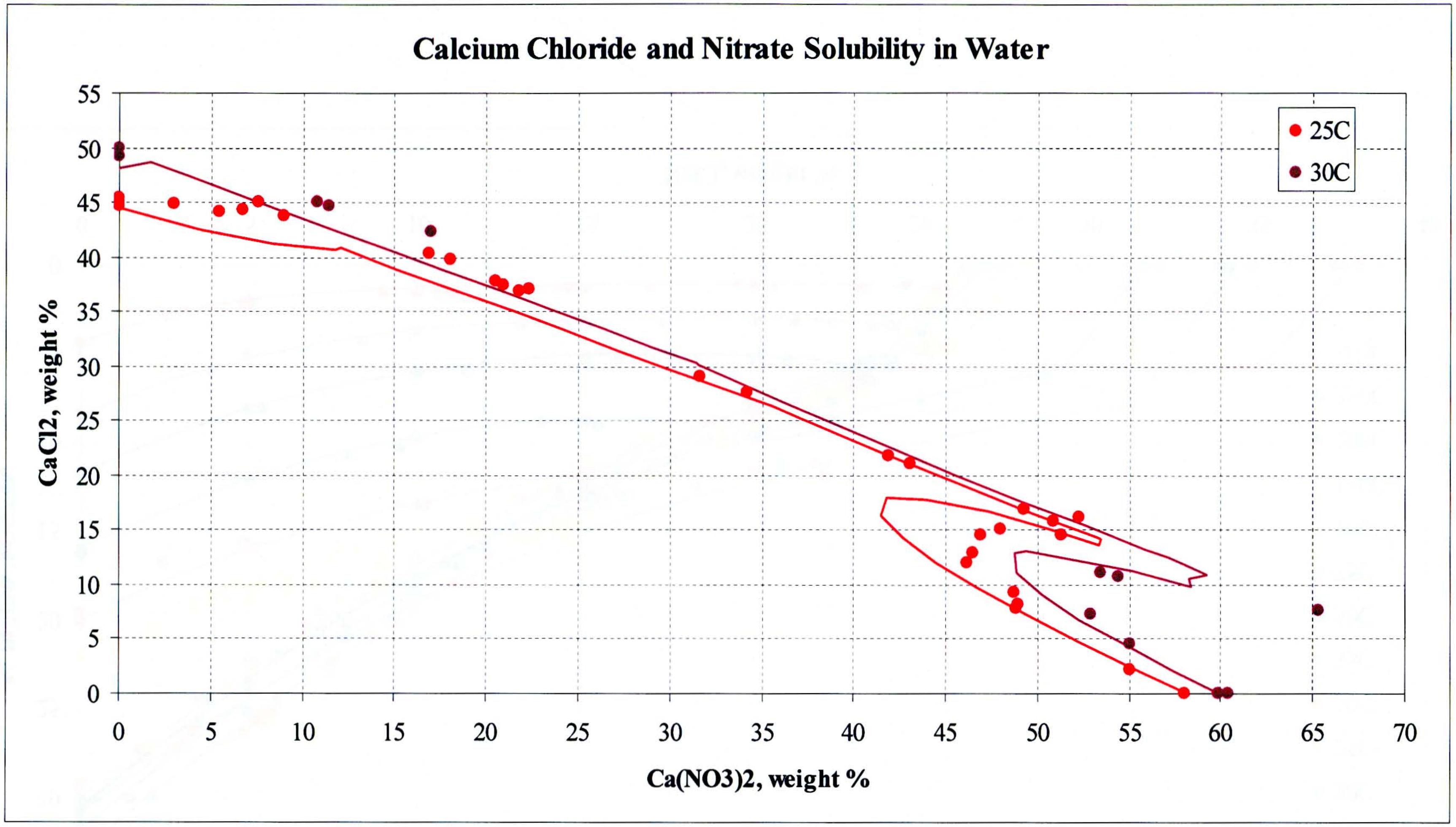

Calcium Nitrate and Potassium Chloride Solubility in Water
30C
KCl, weight %
Ca(NO3)2, weight %
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75



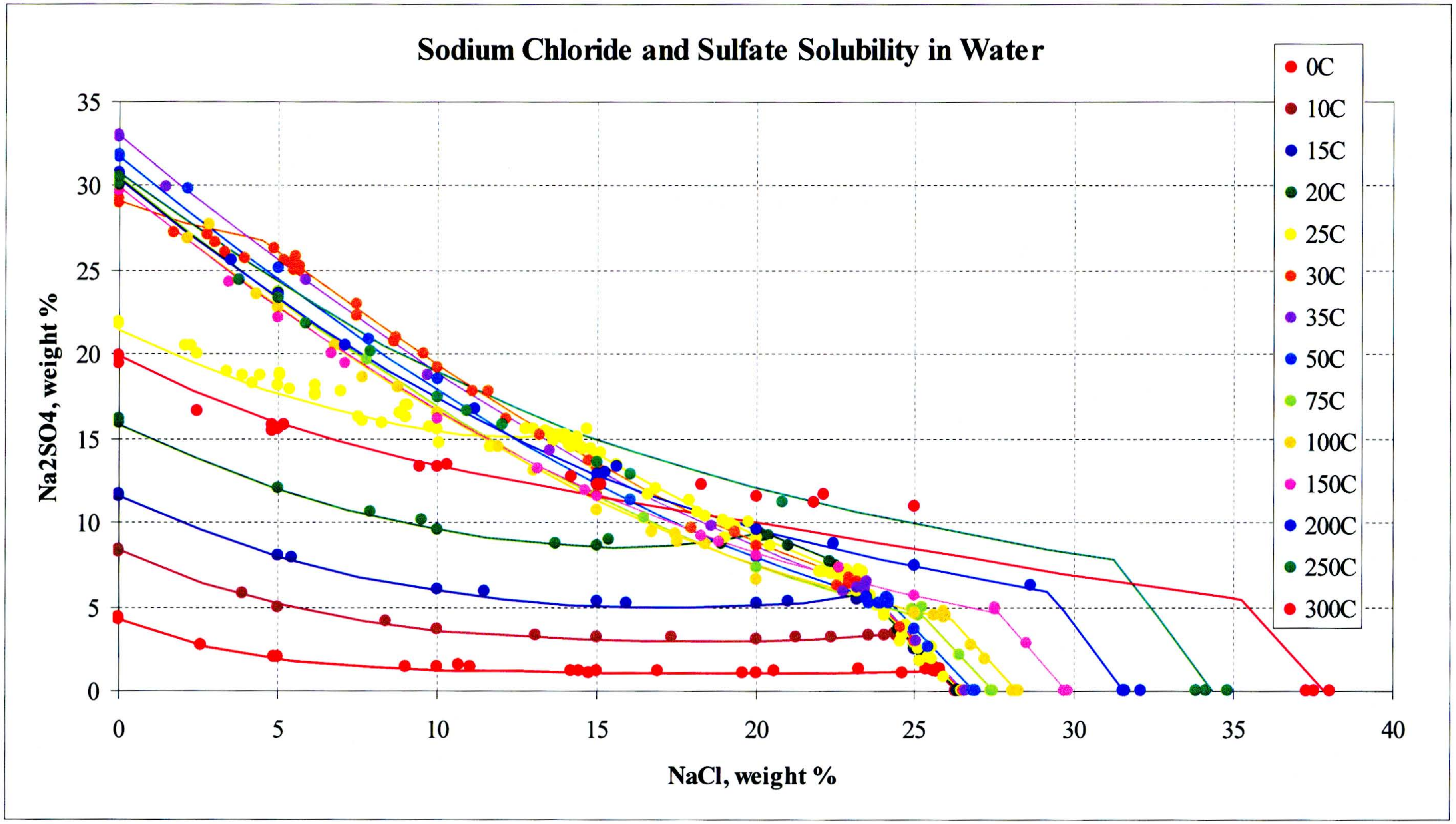
Potassium Nitrate and Magnesium Chloride Solubility in Water
MgCl2, weight %
KNO3, weight %
-20C
-10C
0C
10C
20C
30C
0
5
10
15
20
25
30
35
40


Potassium Nitrate and Calcium Chloride Solubility in Water
30C
CaCl2, weight %
KNO3, weight %
55
50
45
40
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30
35

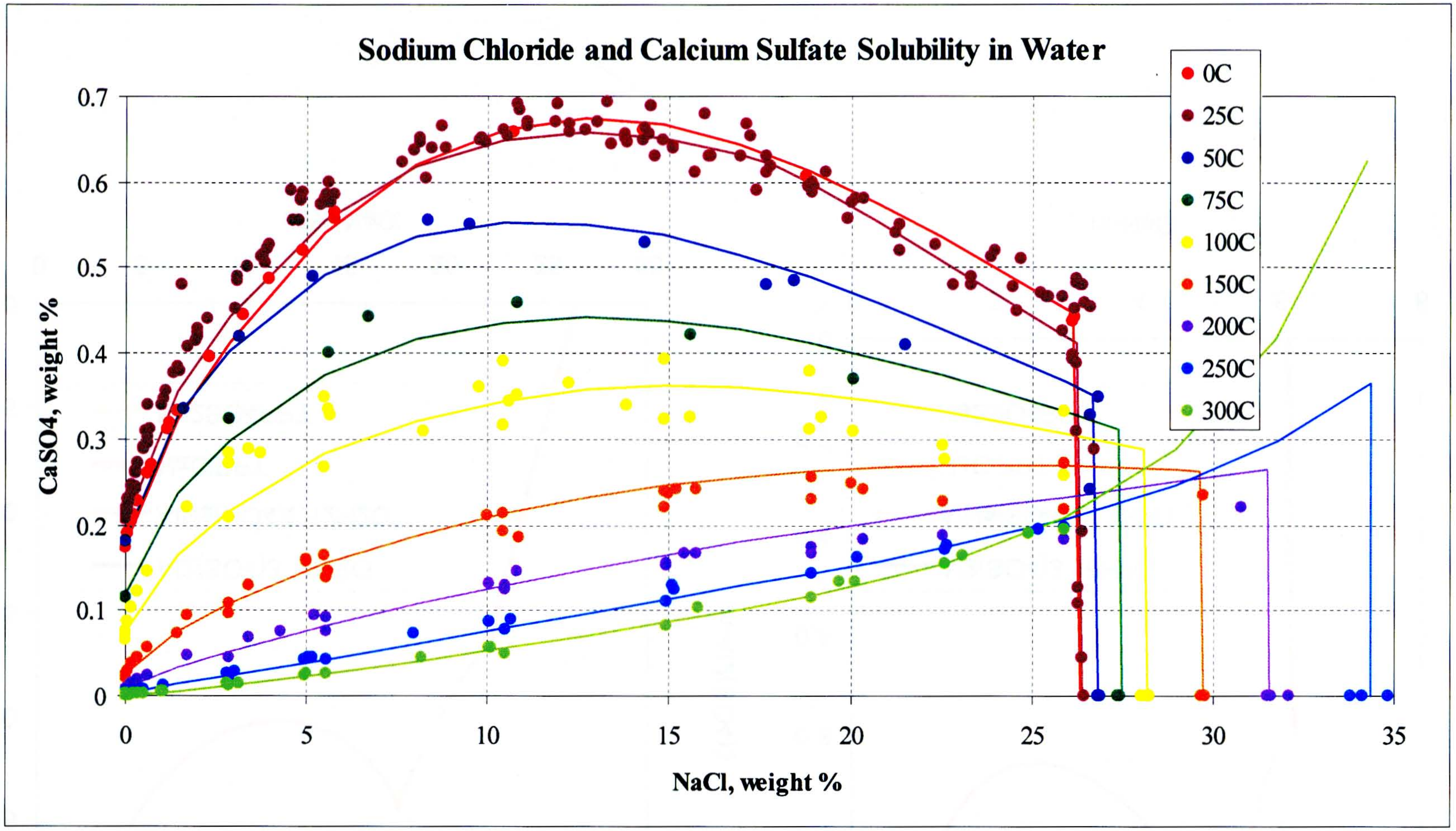

Magnesium Chloride and Nitrate Solubility in Water
15C
25C
50C
75C
110C
MgCl2, weight %
Mg(NO3)2, weight %
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75

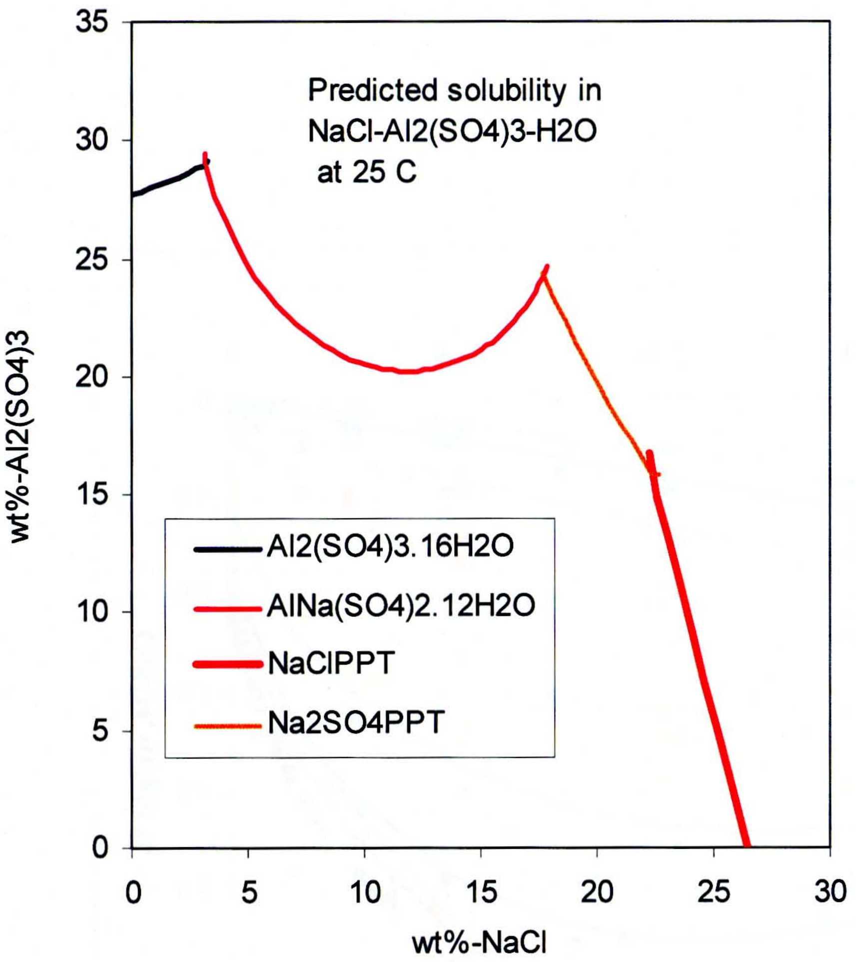


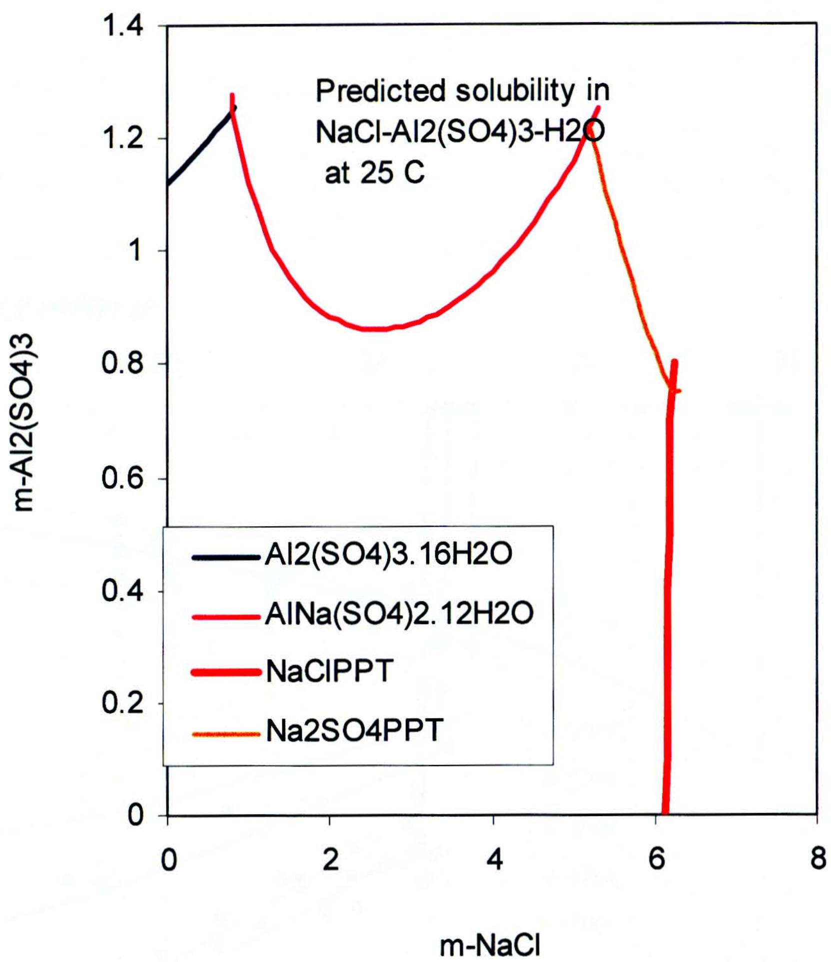
Calcium Chloride and Nitrate Solubility in Water
CaCl2, weight %
Ca(NO3)2, weight %
25C
30C
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70

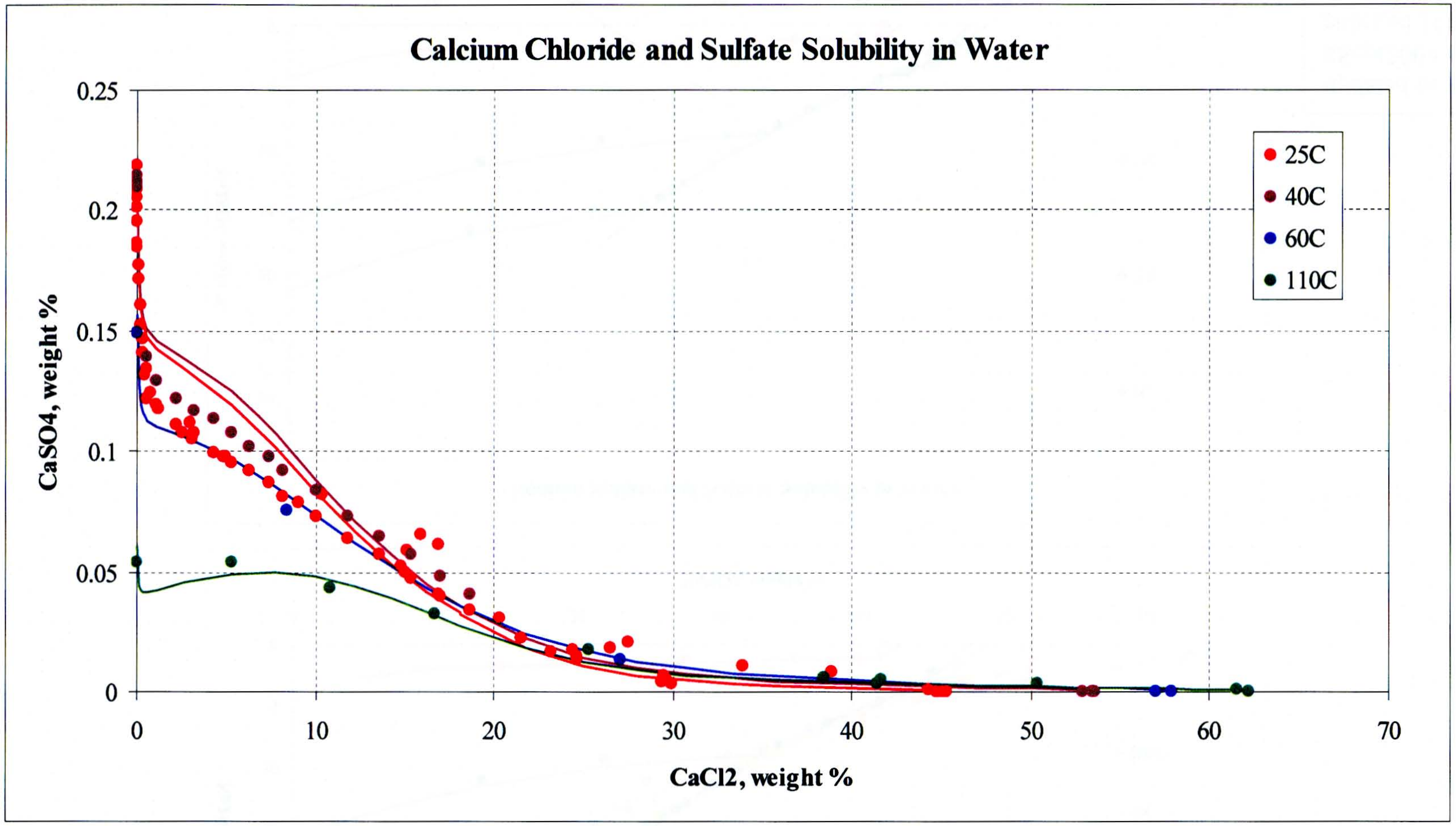


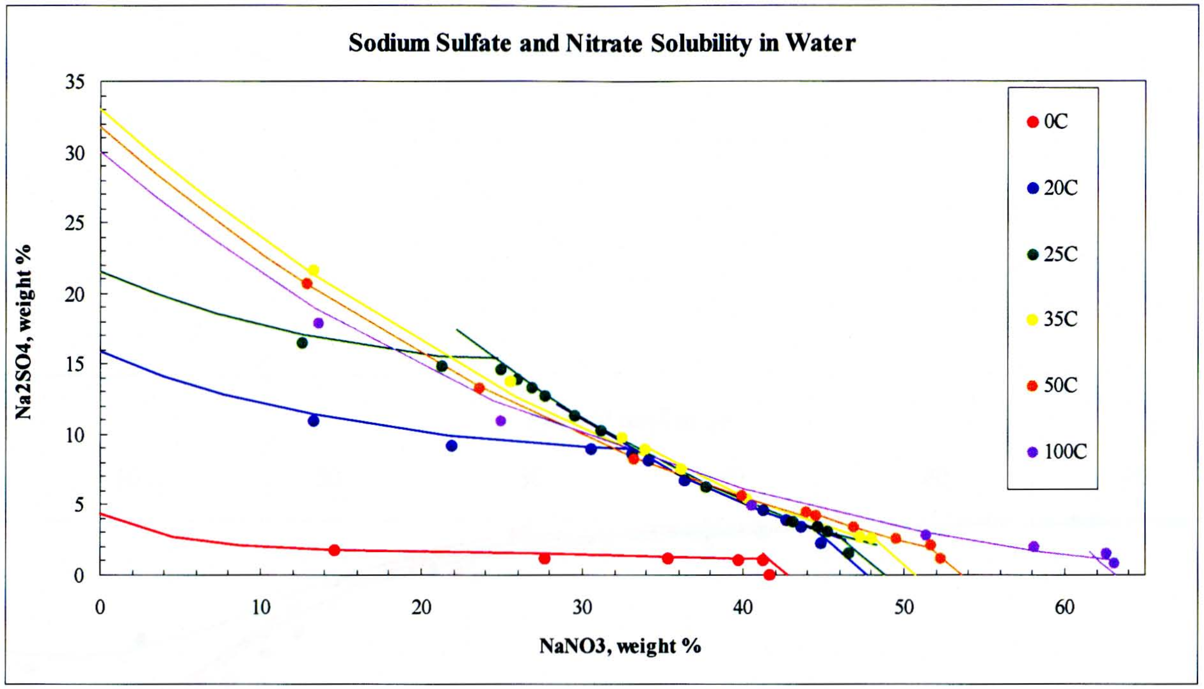
Sodium Chloride and Sulfate Solubility in Water
Na2SO4, weight %
NaCl, weight %
0
5
10
15
20
25
30
35
40
0C
10C
15C
20C
25C
30C
35C
50C
75C
100C
150C
200C
250C
300C

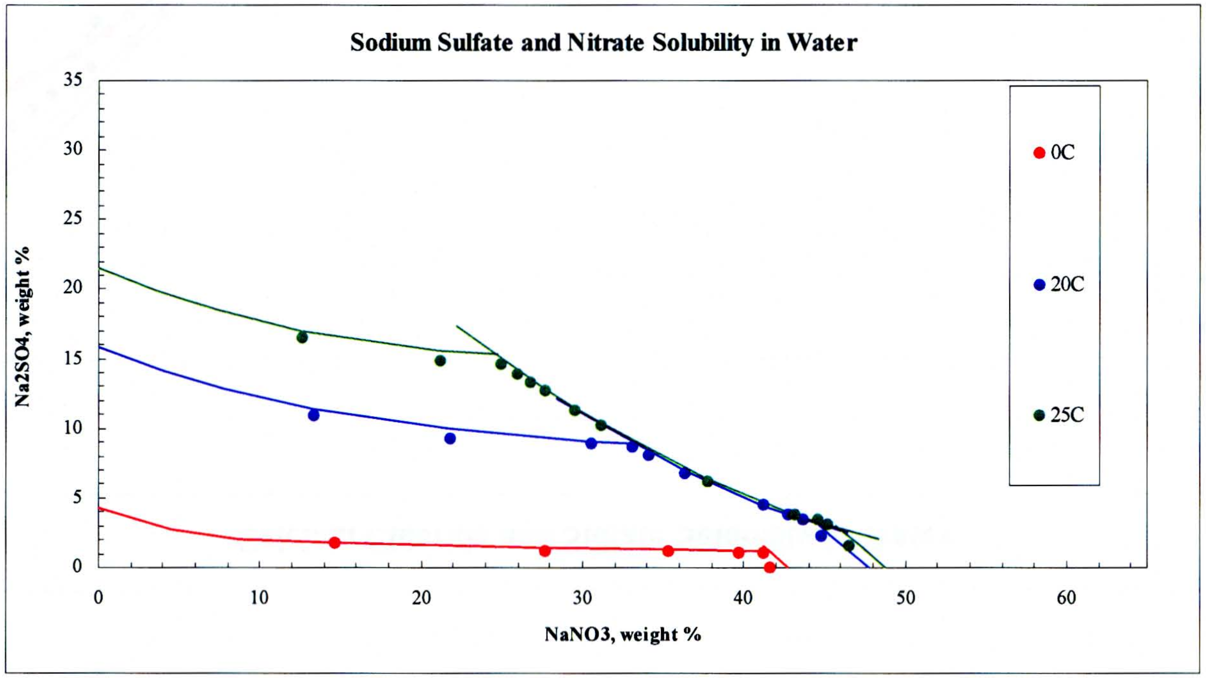

Sodium Chloride and Calcium Sulfate Solubility in Water
0C
25C
50C
75C
100C
150C
200C
250C
300C
CaSO4, weight %
NaCl, weight %
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
5
10
15
20
25
30
35


Predicted solubility in
NaCl-Al2(SO4)3-H2O
at 25 C
wt%-Al2(SO4)3
wt%-NaCl
Al2(SO4)3.16H2O
AlNa(SO4)2.12H2O
NaClPPT
Na2SO4PPT
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30

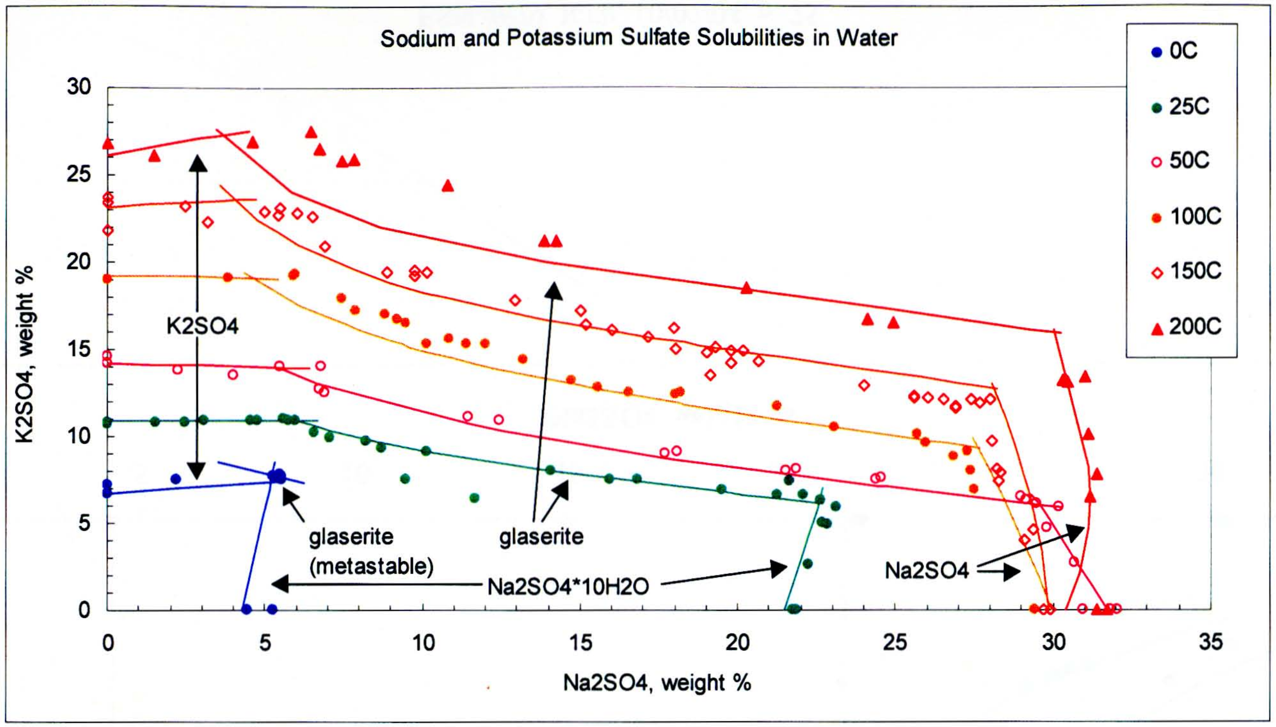

Predicted solubility in
NaCl-Al2(SO4)3-H2O
at 25 C
m-Al2(SO4)3
m-NaCl
Al2(SO4)3.16H2O
AlNa(SO4)2.12H2O
NaClPPT
Na2SO4PPT
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
2
4
6
8

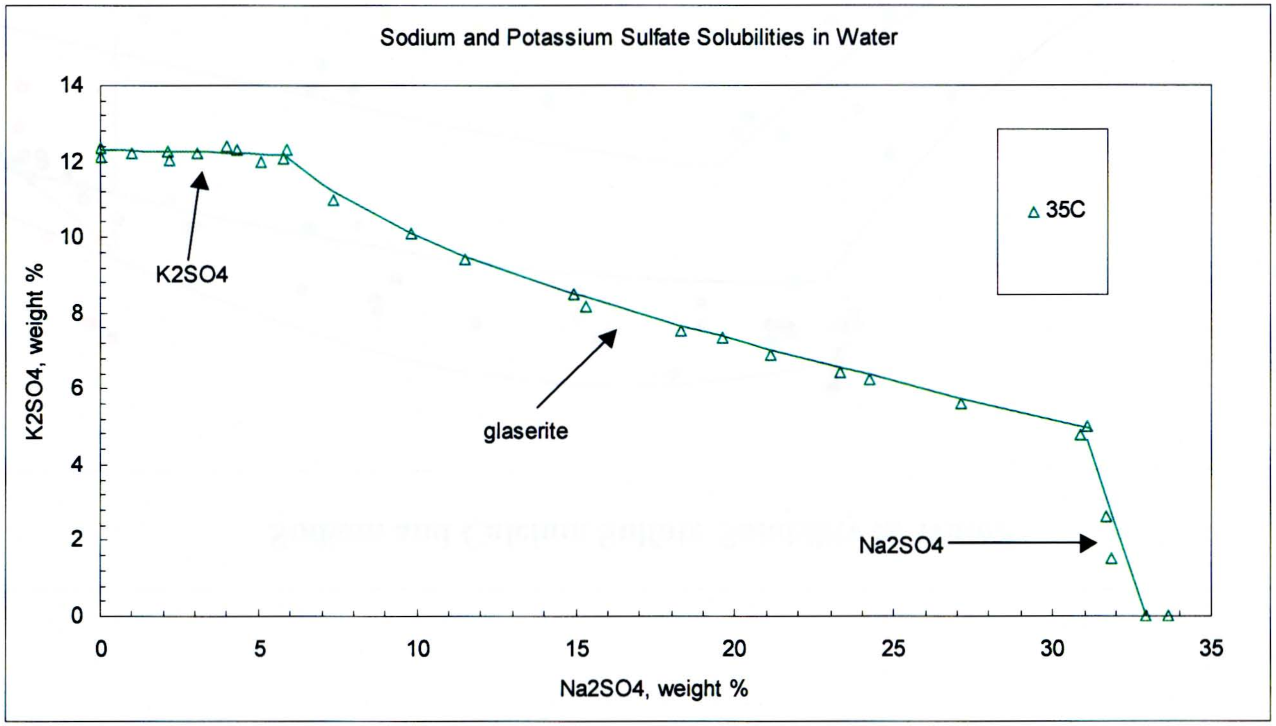

Calcium Chloride and Sulfate Solubility in Water
0.25
0.2
0.15
0.1
0.05
0
0
10
20
30
40
50
60
70
CaSO4, weight %
CaCl2, weight %
25C
40C
60C
110C

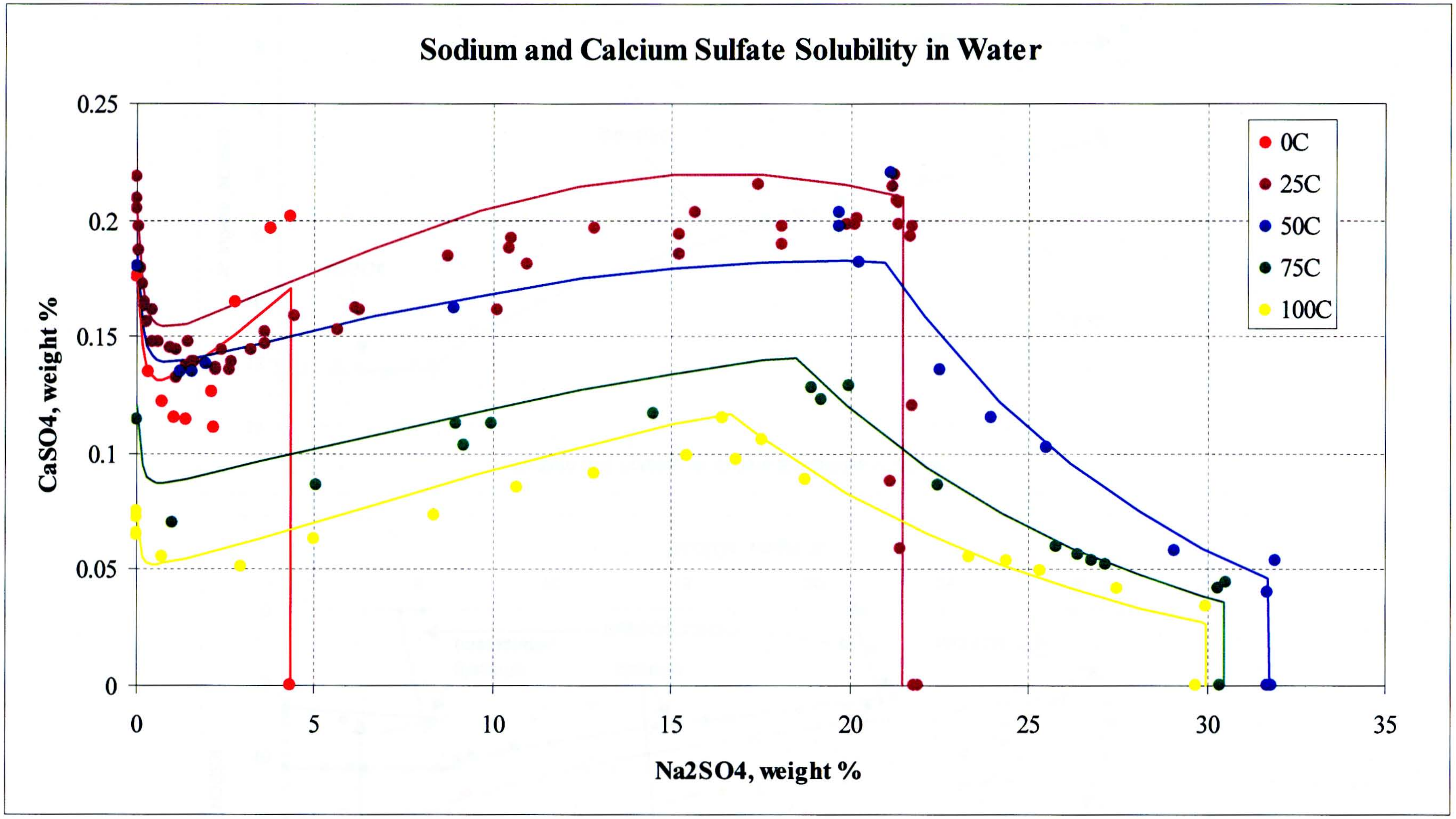


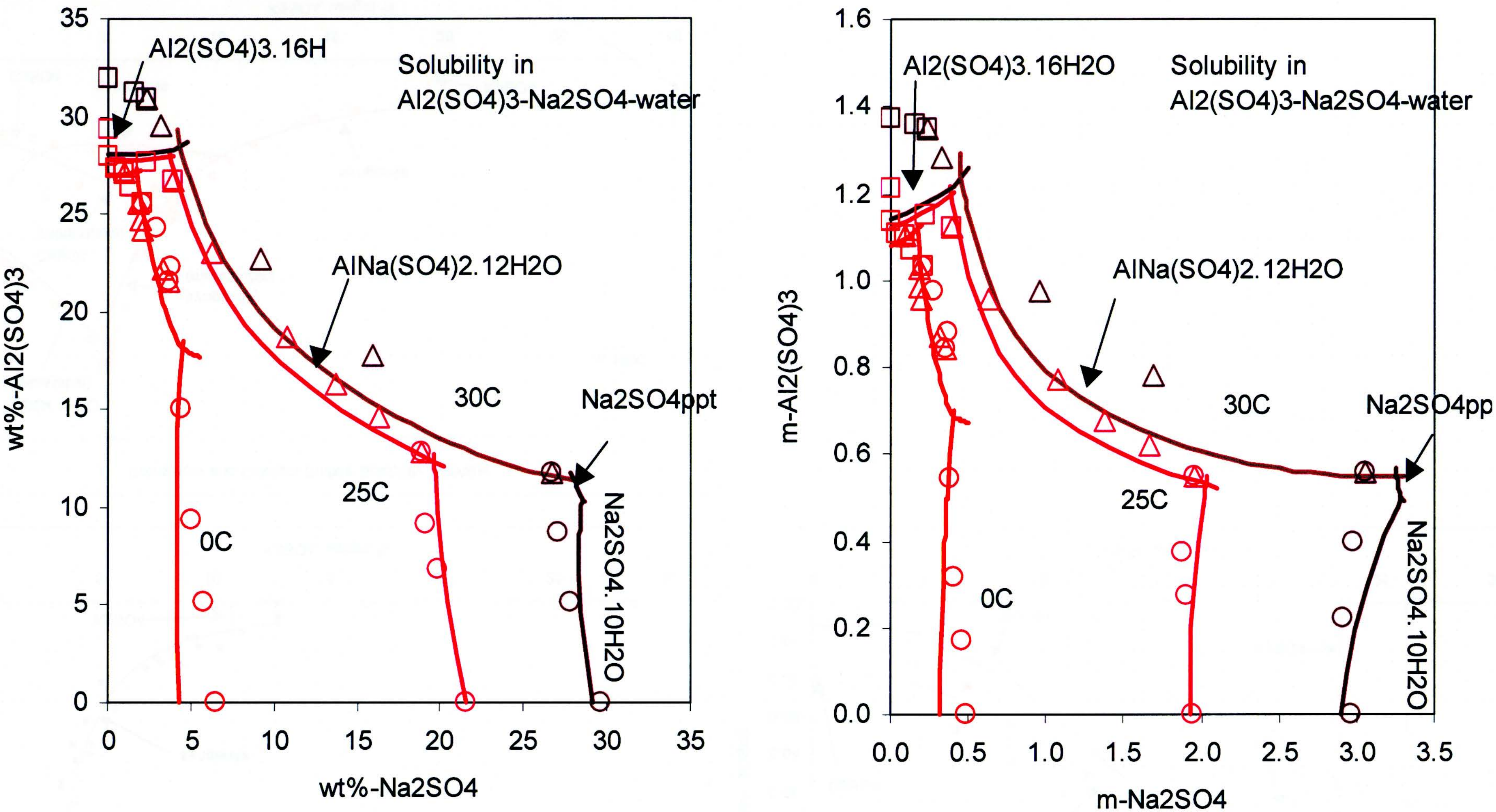


updated by CSO 8Sept2004 and checked 1Oct2004 darapskite (NaNO3*Na2SO4*H

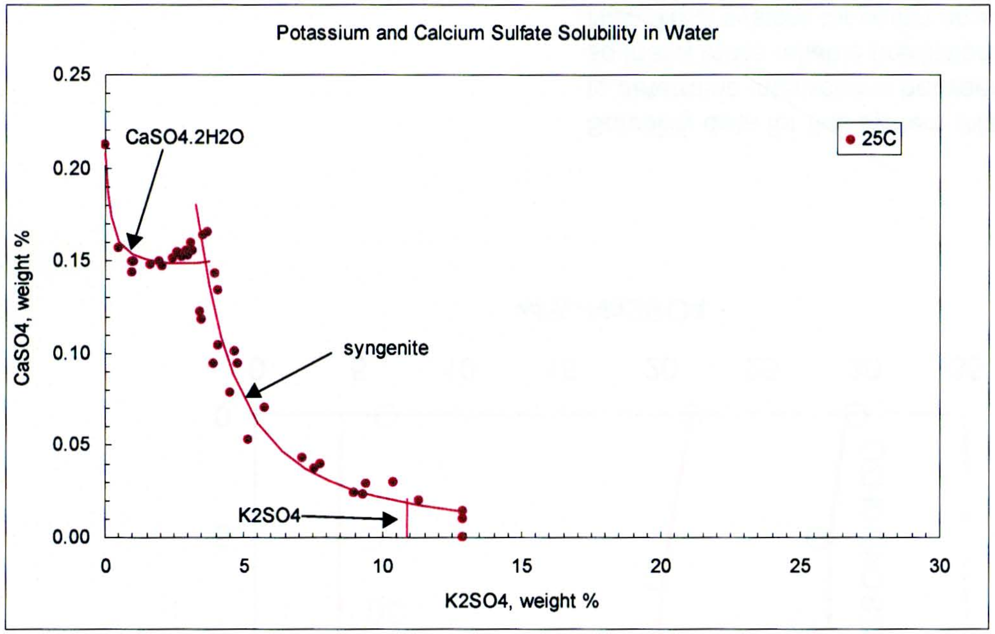

Sodium and Potassium Sulfate Solubilities in Water
0C
25C
50C
100C
150C
200C
K2SO4, weight %
Na2SO4, weight %
K2SO4
glaserite
(metastable)
glaserite
Na2SO4*10H2O
Na2SO4

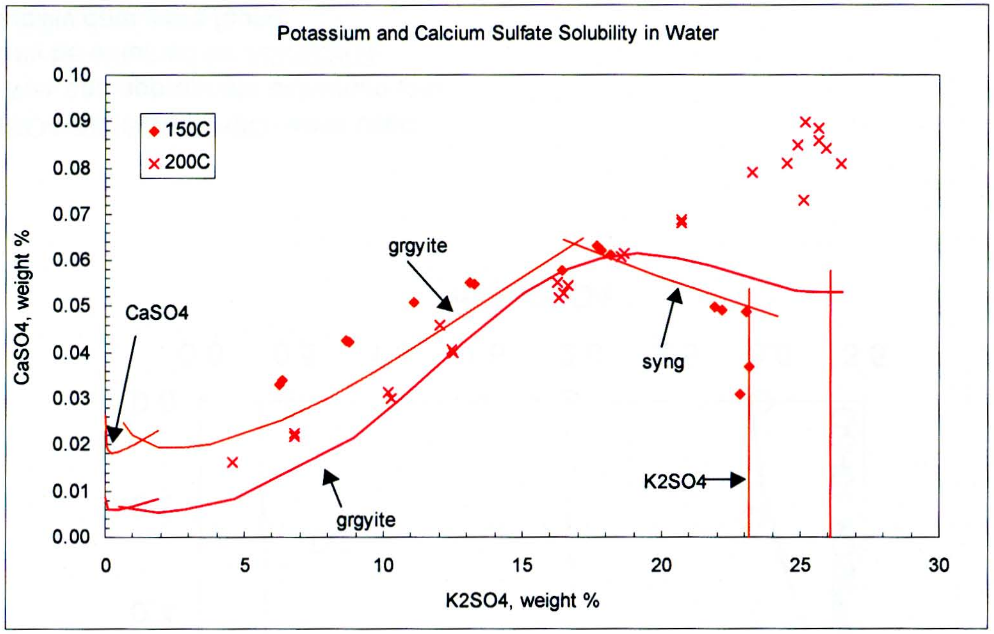

Sodium and Potassium Sulfate Solubilities in Water
35C
K2SO4, weight %
Na2SO4, weight %
K2SO4
glaserite
Na2SO4

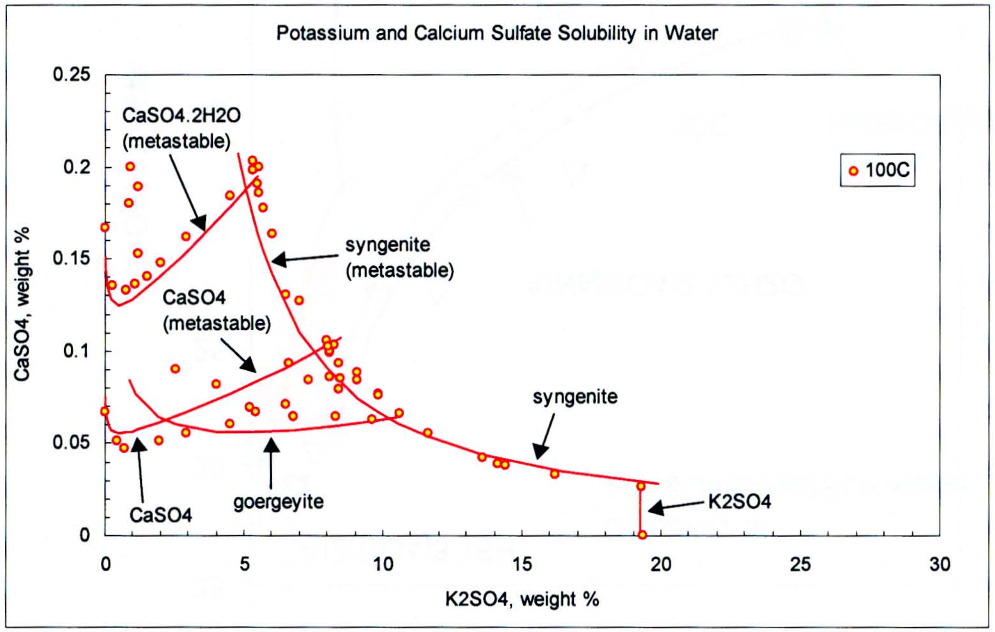

Sodium and Calcium Sulfate Solubility in Water
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
30
35
CaSO4, weight %
Na2SO4, weight %
0C
25C
50C
75C
100C

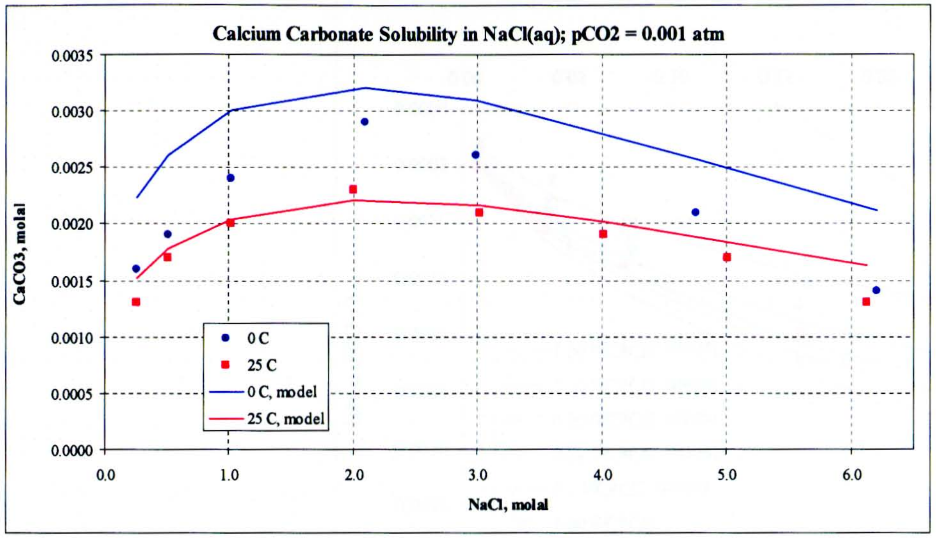


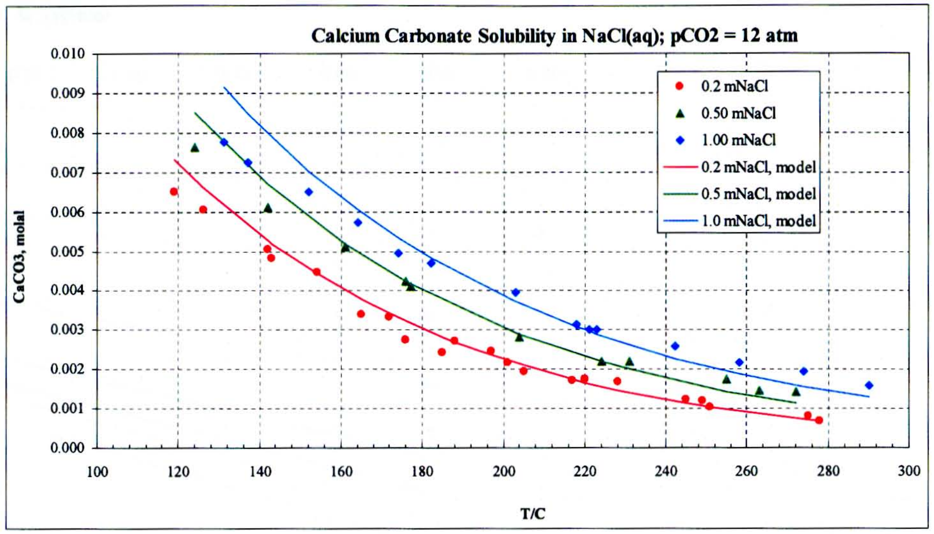
Solubility data for this system (Na2SO4-Al2(SO4)3-H2O) were used to determine interactions between Na+ and appropriate aluminum ions so that a more reliable prediction may be obtained for Al2(SO4)3-NaCl-H2O system for which no solubility data were found.

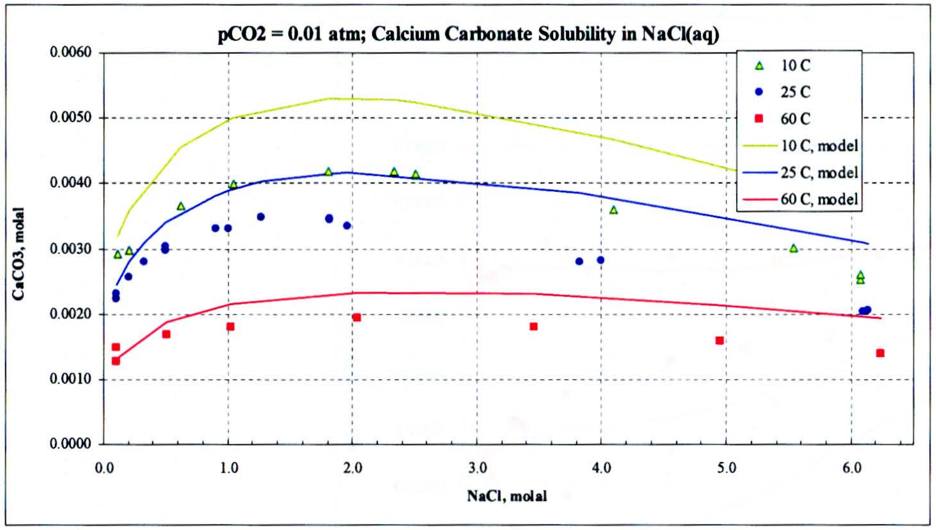

Potassium and Calcium Sulfate Solubility in Water
CaSO4, weight %
K2SO4, weight %
25C
CaSO4.2H2O
syngenite
K2SO4
0.25
0.20
0.15
0.10
0.05
0.00
0
5
10
15
20
25
30

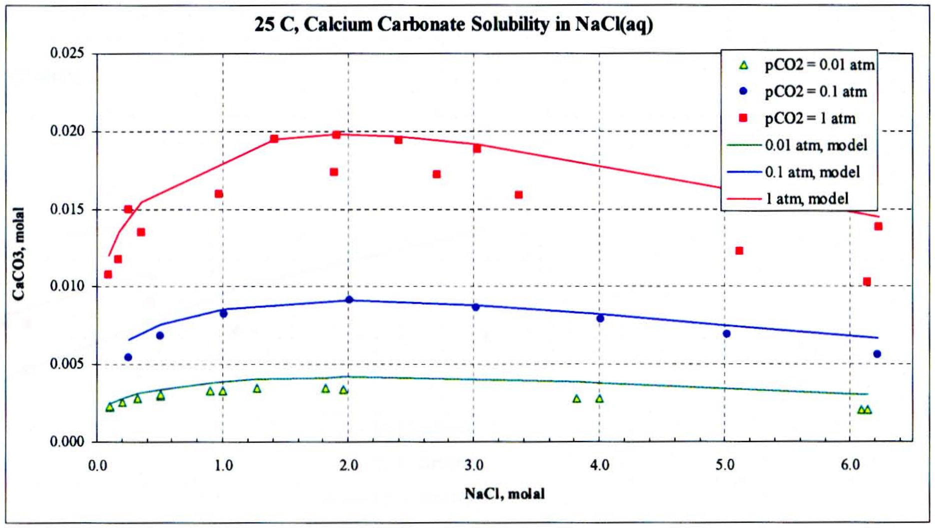

Potassium and Calcium Sulfate Solubility in Water
CaSO4, weight %
K2SO4, weight %
150C
200C
grgyite
CaSO4
syng
grgyite
K2SO4
0.10
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
0
5
10
15
20
25
30

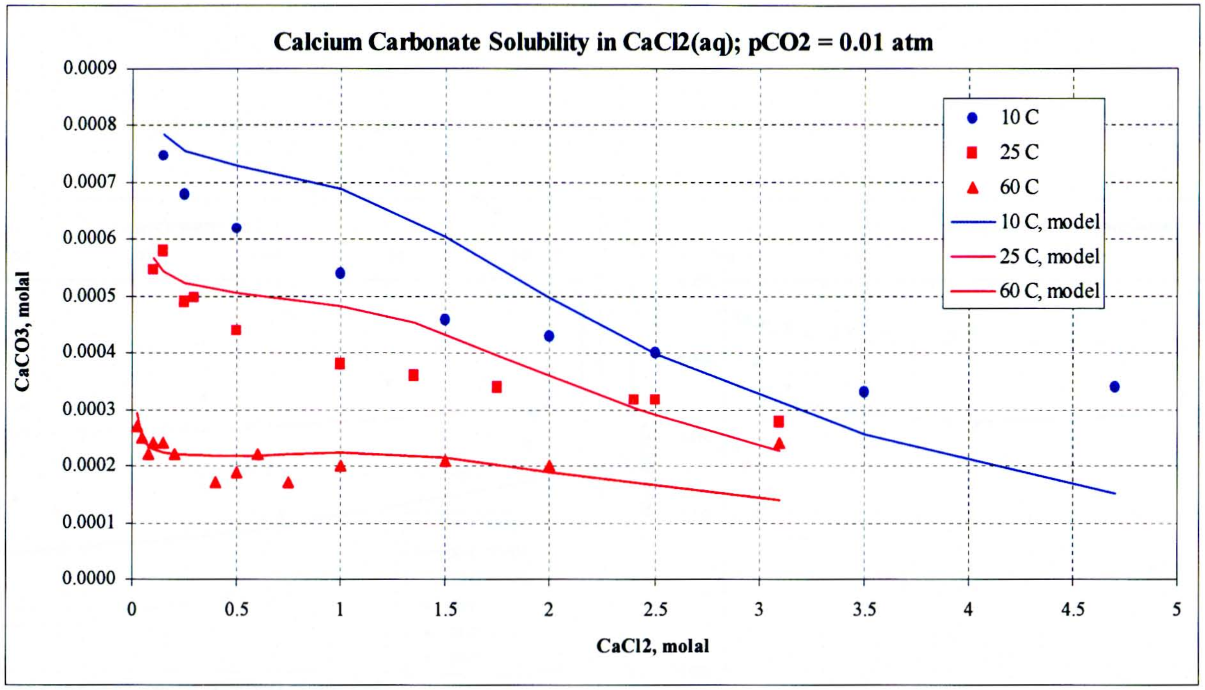

Potassium and Calcium Sulfate Solubility in Water
CaSO4, weight %
K2SO4, weight %
100C
CaSO4.2H2O
(metastable)
syngenite
(metastable)
CaSO4
(metastable)
syngenite
CaSO4
goergeyite
K2SO4
0.25
0.2
0.15
0.1
0.05
0
0
5
10
15
20
25
30

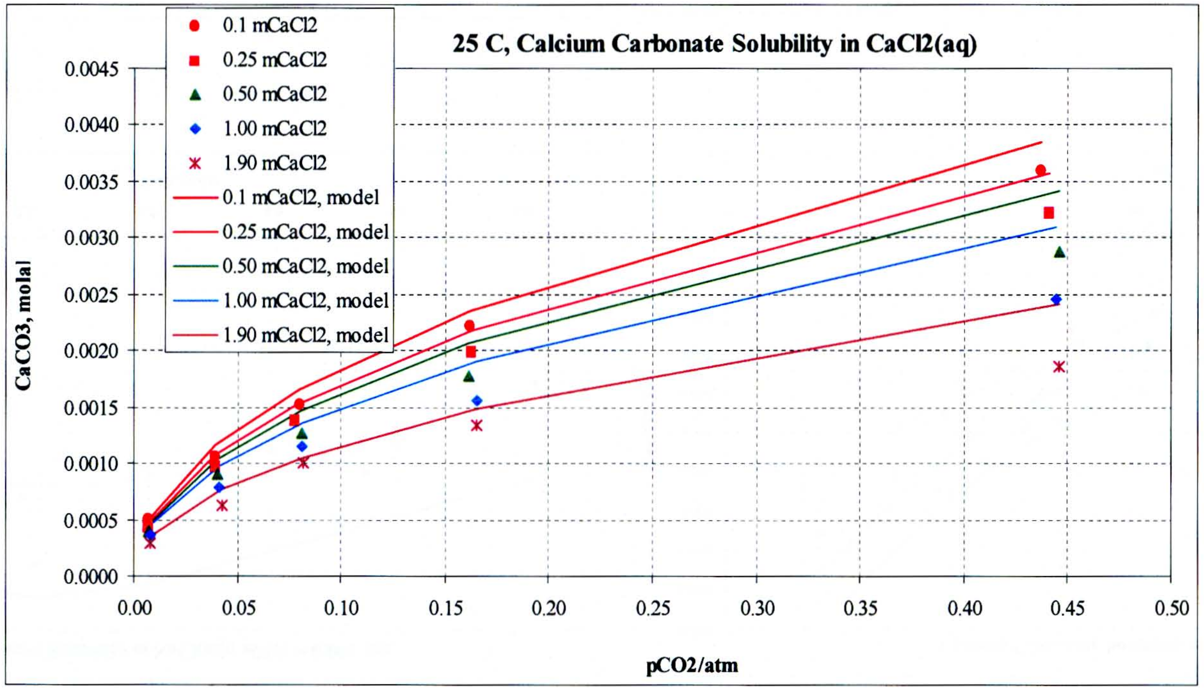

Calcium Carbonate Solubility in NaCl(aq); pCO2 = 0.001 atm
CaCO3, molal
NaCl, molal
0 C
25 C
0 C, model
25 C, model

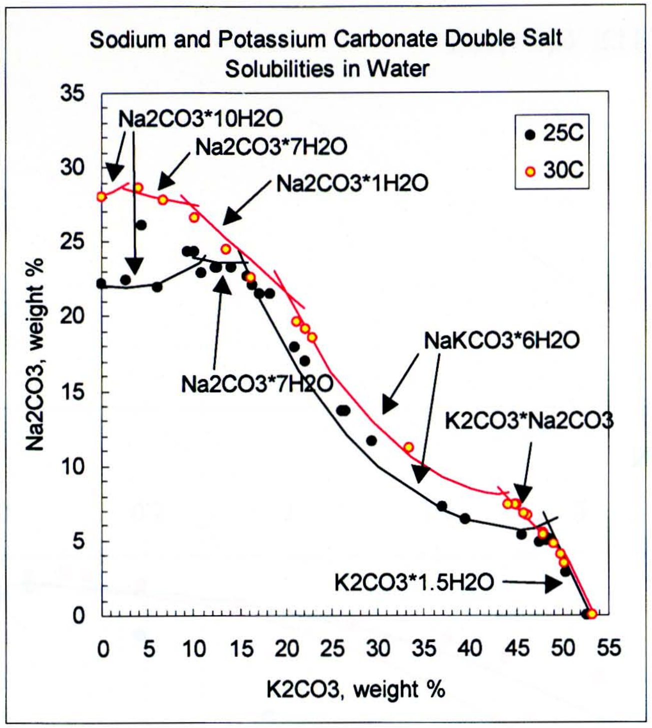

Calcium Carbonate Solubility in NaCl(aq); pCO2 = 12 atm
CaCO3, molal
T/C
0.2 mNaCl
0.50 mNaCl
1.00 mNaCl
0.2 mNaCl, model
0.5 mNaCl, model
1.0 mNaCl, model

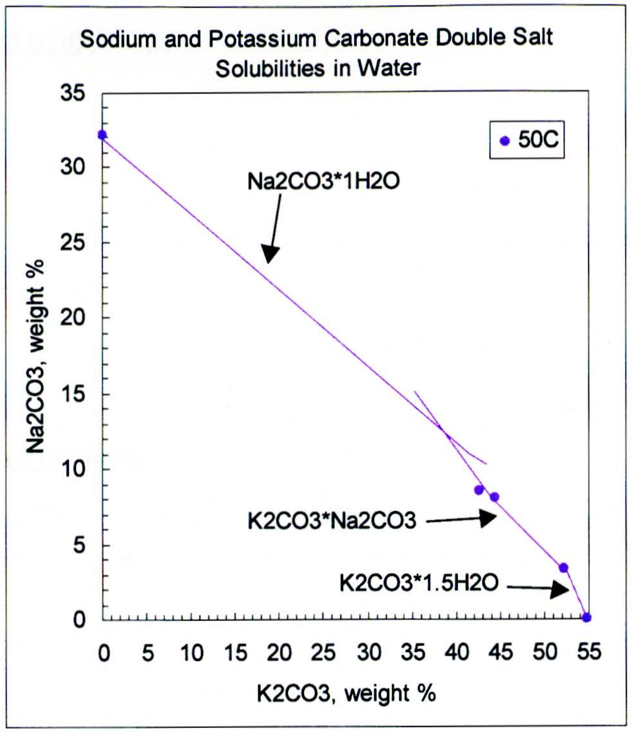

pCO2 = 0.01 atm; Calcium Carbonate Solubility in NaCl(aq)
CaCO3, molal
NaCl, molal
10 C
25 C
60 C
10 C, model
25 C, model
60 C, model

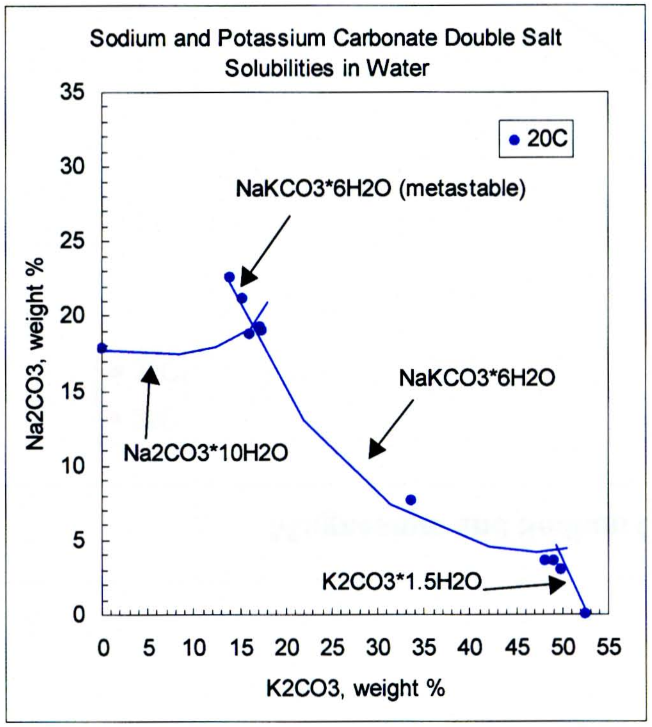

25 C, Calcium Carbonate Solubility in NaCl(aq)
CaCO3, molal
NaCl, molal
pCO2 = 0.01 atm
pCO2 = 0.1 atm
pCO2 = 1 atm
0.01 atm, model
0.1 atm, model
1 atm, model

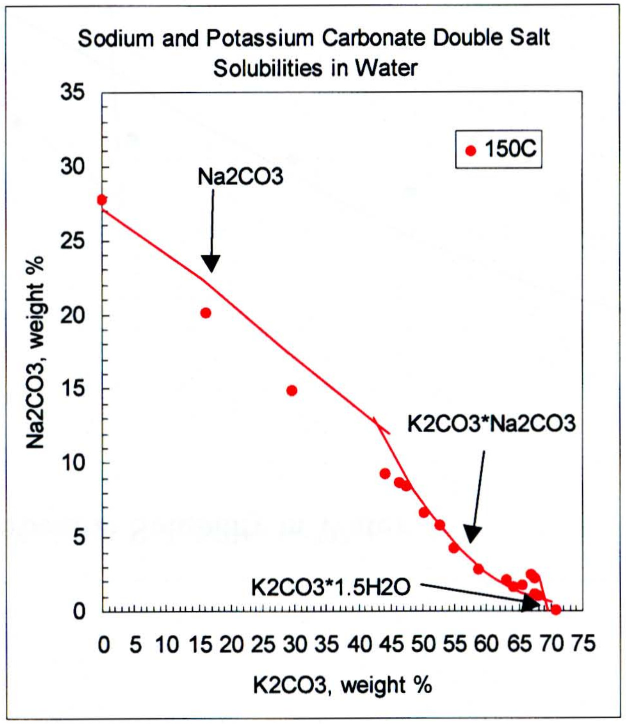

Calcium Carbonate Solubility in CaCl2(aq); pCO2 = 0.01 atm
CaCO3, molal
CaCl2, molal
10 C
25 C
60 C
10 C, model
25 C, model
60 C, model
0.0009
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0.0000
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5

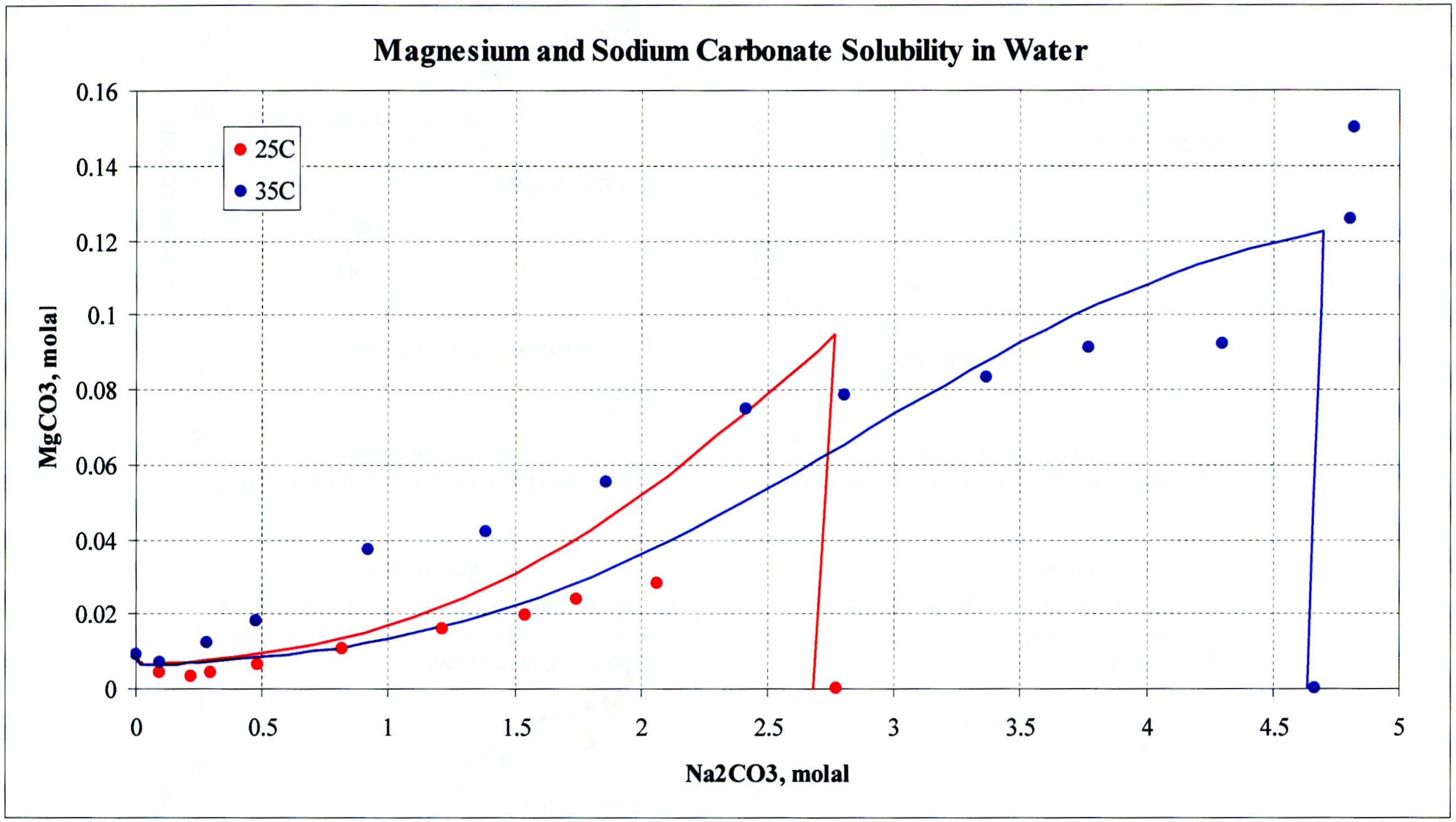

25 C, Calcium Carbonate Solubility in CaCl2(aq)
CaCO3, molal
pCO2/atm
0.1 mCaCl2
0.25 mCaCl2
0.50 mCaCl2
1.00 mCaCl2
1.90 mCaCl2
0.1 mCaCl2, model
0.25 mCaCl2, model
0.50 mCaCl2, model
1.00 mCaCl2, model
1.90 mCaCl2, model
0.0045
0.0040
0.0035
0.0030
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0.40
0.45
0.50

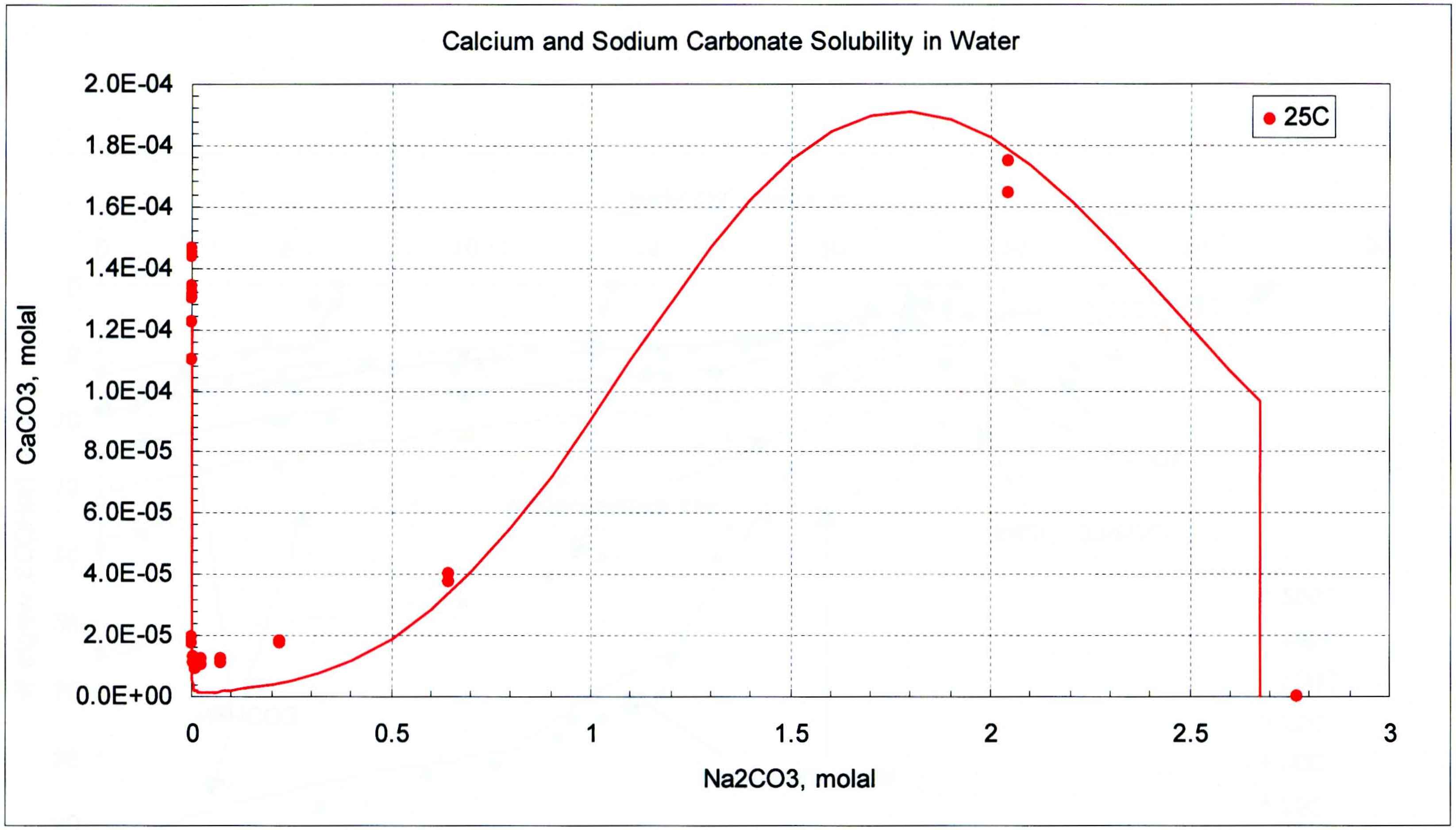

Sodium and Potassium Carbonate Double Salt Solubilities in Water
25C
30C
Na2CO3*10H2O
Na2CO3*7H2O
Na2CO3*1H2O
Na2CO3*7H2O
NaKCO3*6H2O
K2CO3*Na2CO3
K2CO3*1.5H2O
Na2CO3, weight %
K2CO3, weight %
0
5
10
15
20
25
30
35
40
45
50
55

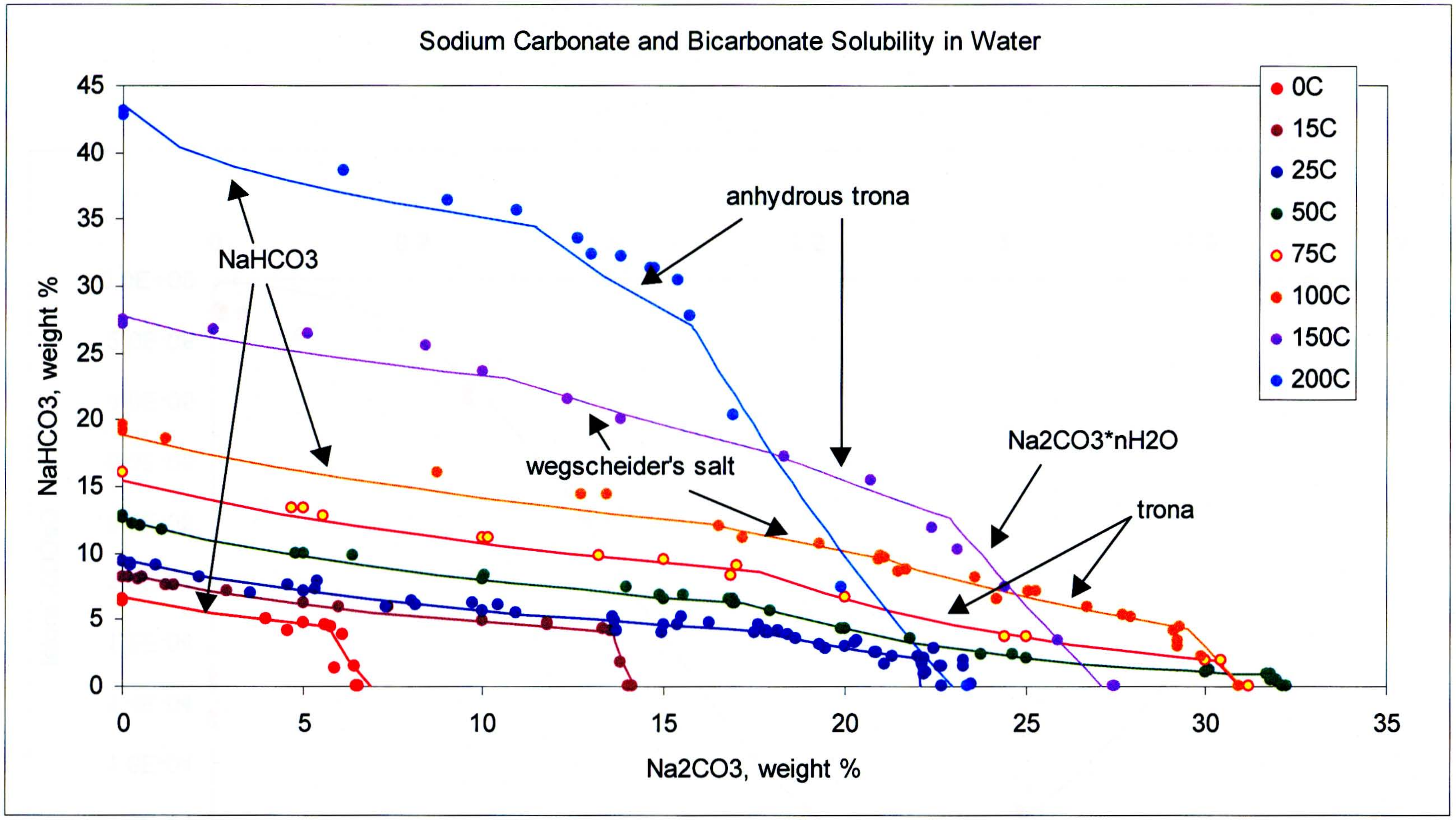

Sodium and Potassium Carbonate Double Salt Solubilities in Water
50C
Na2CO3*1H2O
K2CO3*Na2CO3
K2CO3*1.5H2O
Na2CO3, weight %
K2CO3, weight %
0
5
10
15
20
25
30
35
40
45
50
55

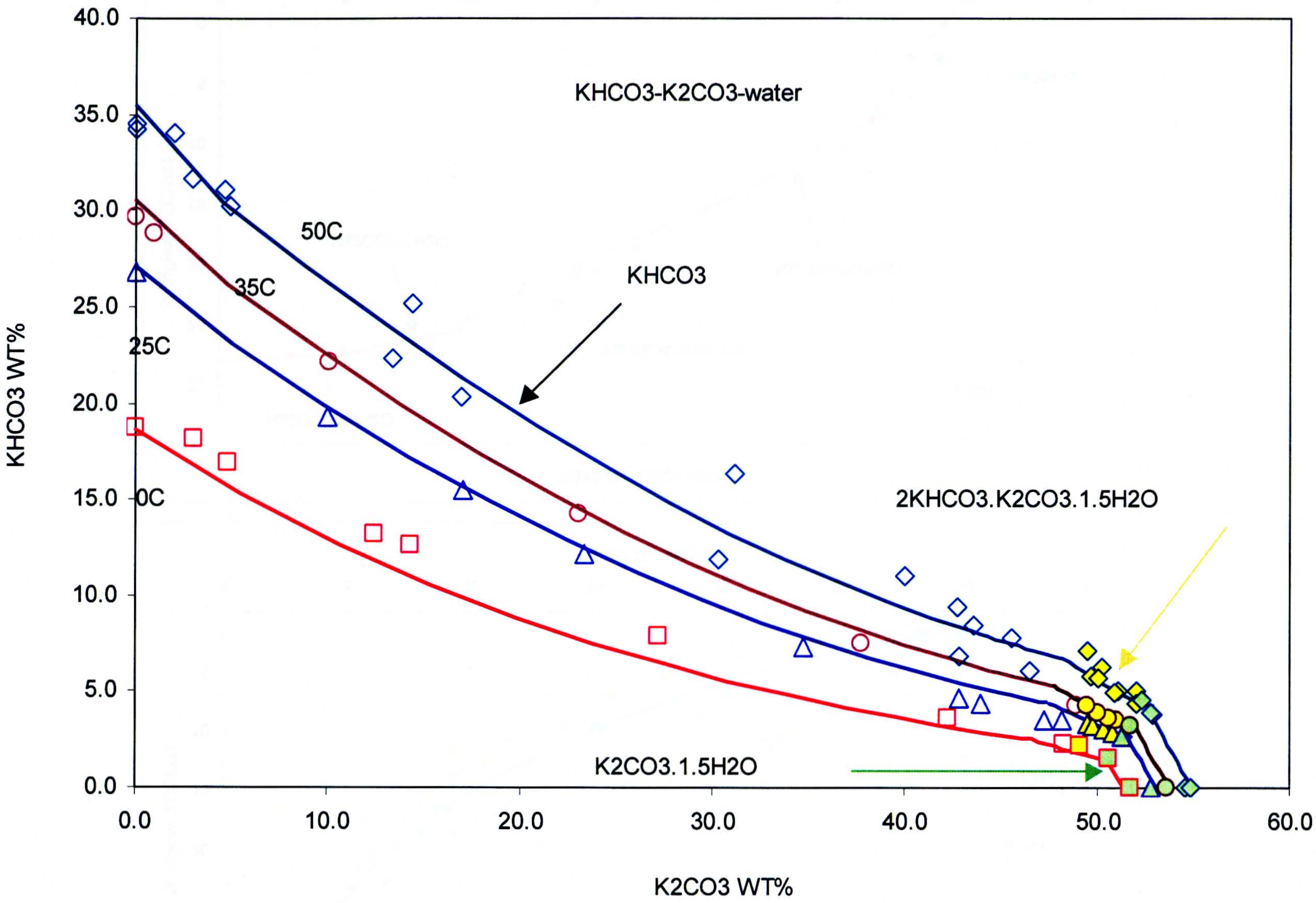

Sodium and Potassium Carbonate Double Salt Solubilities in Water
20C
NaKCO3*6H2O (metastable)
NaKCO3*6H2O
Na2CO3*10H2O
K2CO3*1.5H2O
Na2CO3, weight %
K2CO3, weight %
0
5
10
15
20
25
30
35
40
45
50
55


Sodium and Potassium Carbonate Double Salt Solubilities in Water
150C
Na2CO3
K2CO3*Na2CO3
K2CO3*1.5H2O
Na2CO3, weight %
K2CO3, weight %
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75


Magnesium and Sodium Carbonate Solubility in Water
25C
35C
MgCO3, molal
Na2CO3, molal
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0
0.5
1
1.5
2
2.5
3
3.5
4
4.5
5


Calcium and Sodium Carbonate Solubility in Water
25C
CaCO3, molal
2.0E-04
1.8E-04
1.6E-04
1.4E-04
1.2E-04
1.0E-04
8.0E-05
6.0E-05
4.0E-05
2.0E-05
0.0E+00
0
0.5
1
1.5
2
2.5
3
Na2CO3, molal


Sodium Carbonate and Bicarbonate Solubility in Water
NaHCO3, weight %
Na2CO3, weight %
0C
15C
25C
50C
75C
100C
150C
200C
anhydrous trona
NaHCO3
wegscheider's salt
Na2CO3*nH2O
trona
45
40
35
30
25
20
15
10
5
0
0
5
10
15
20
25
30
35



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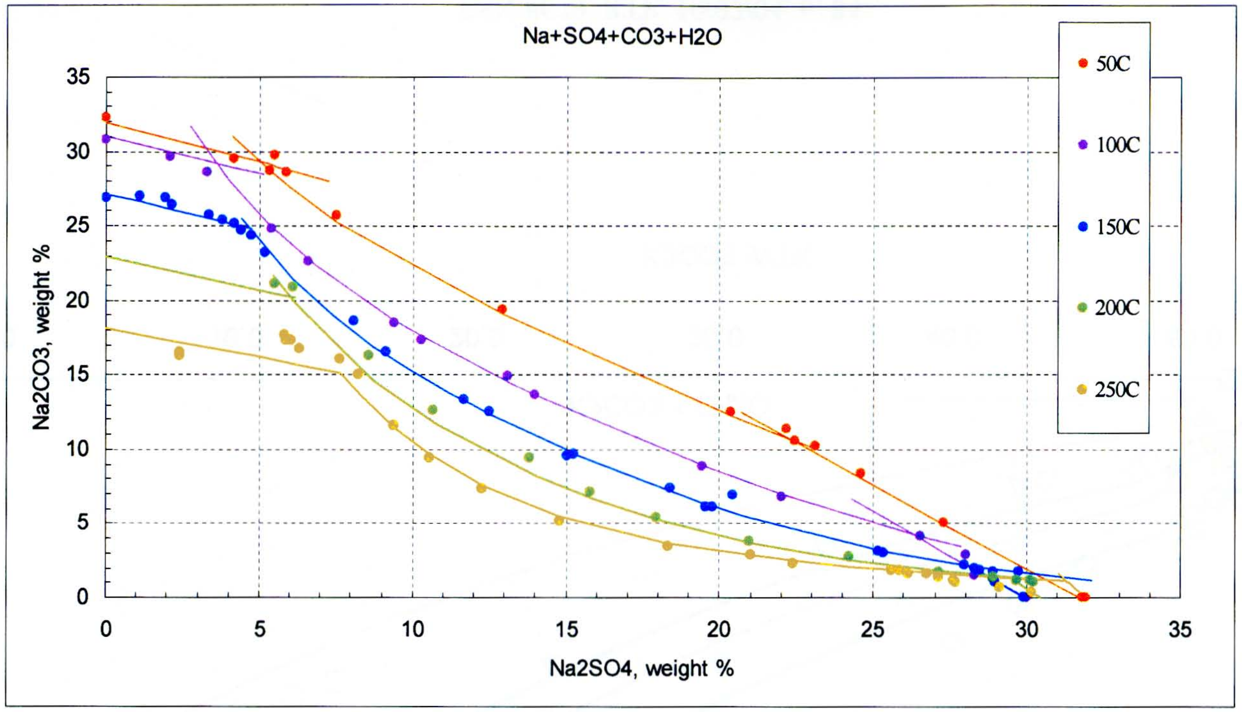
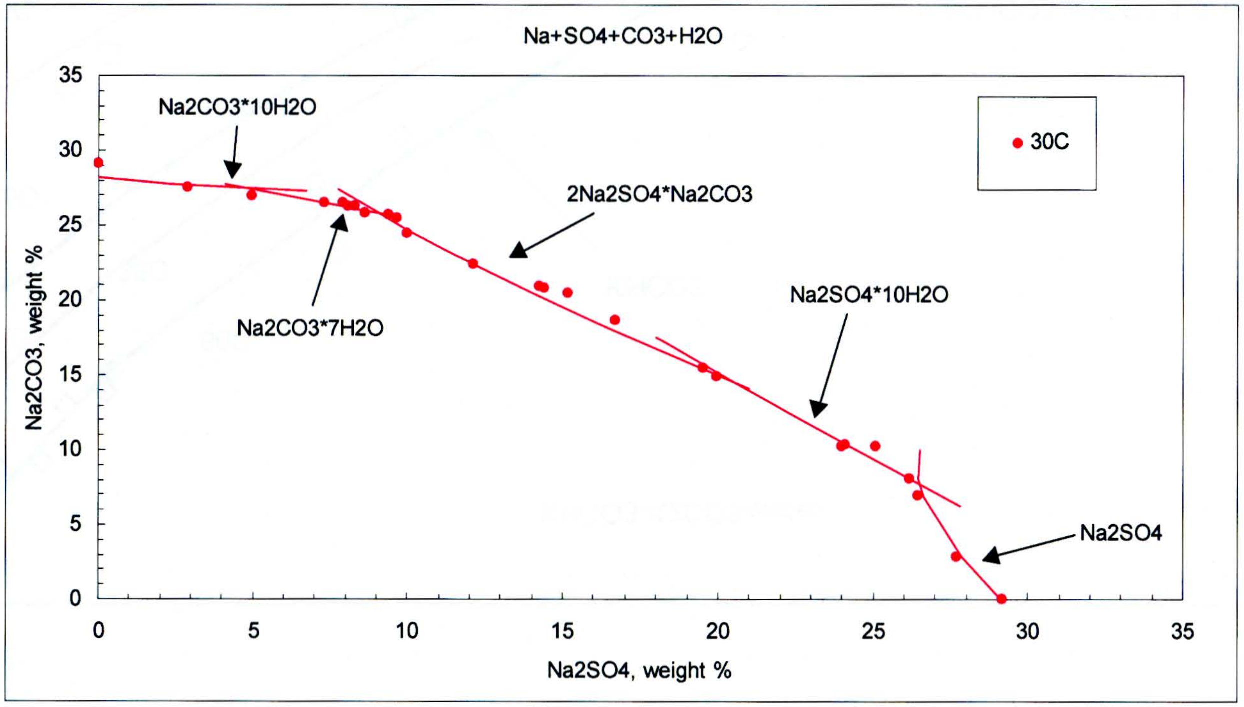
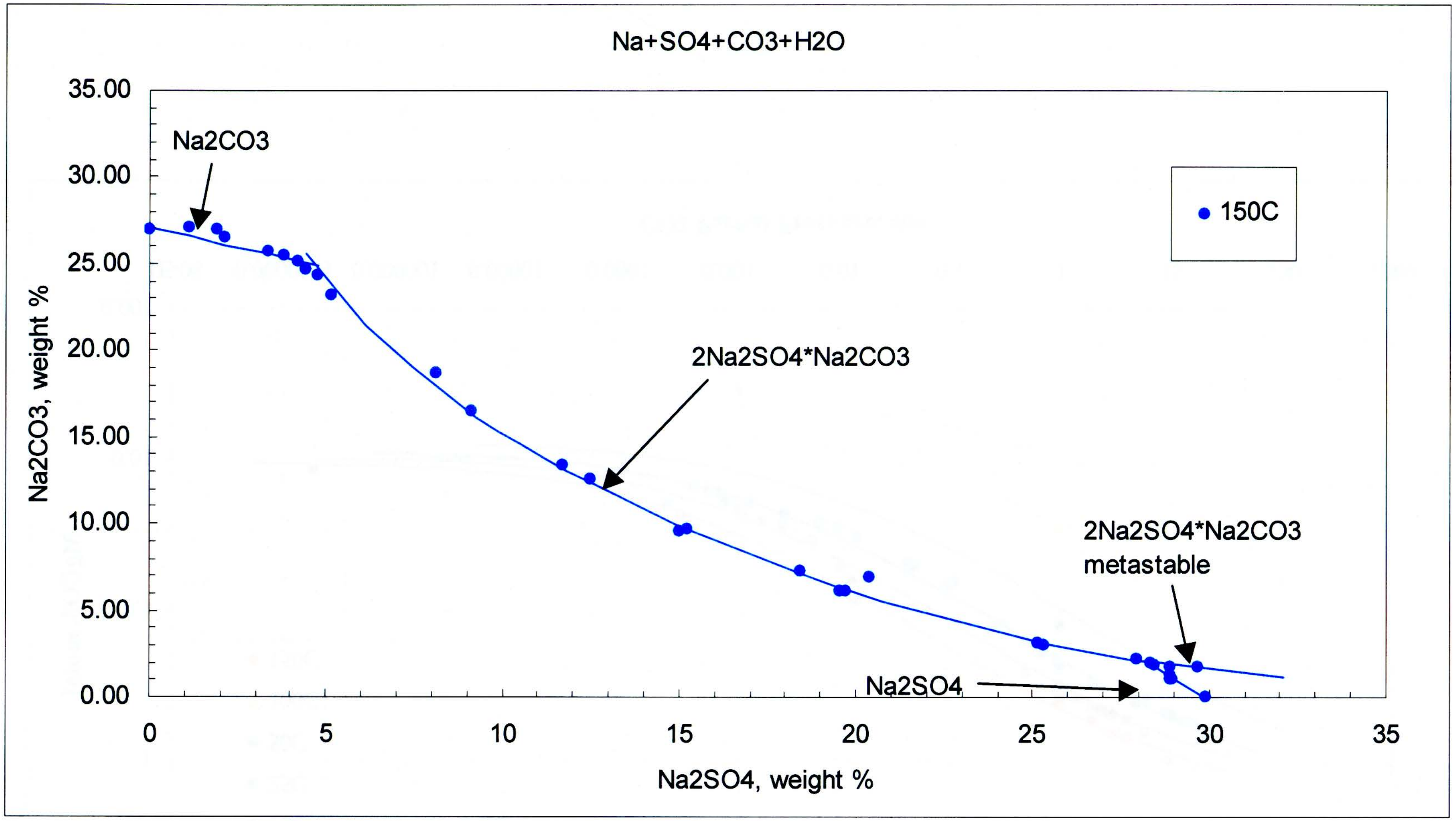
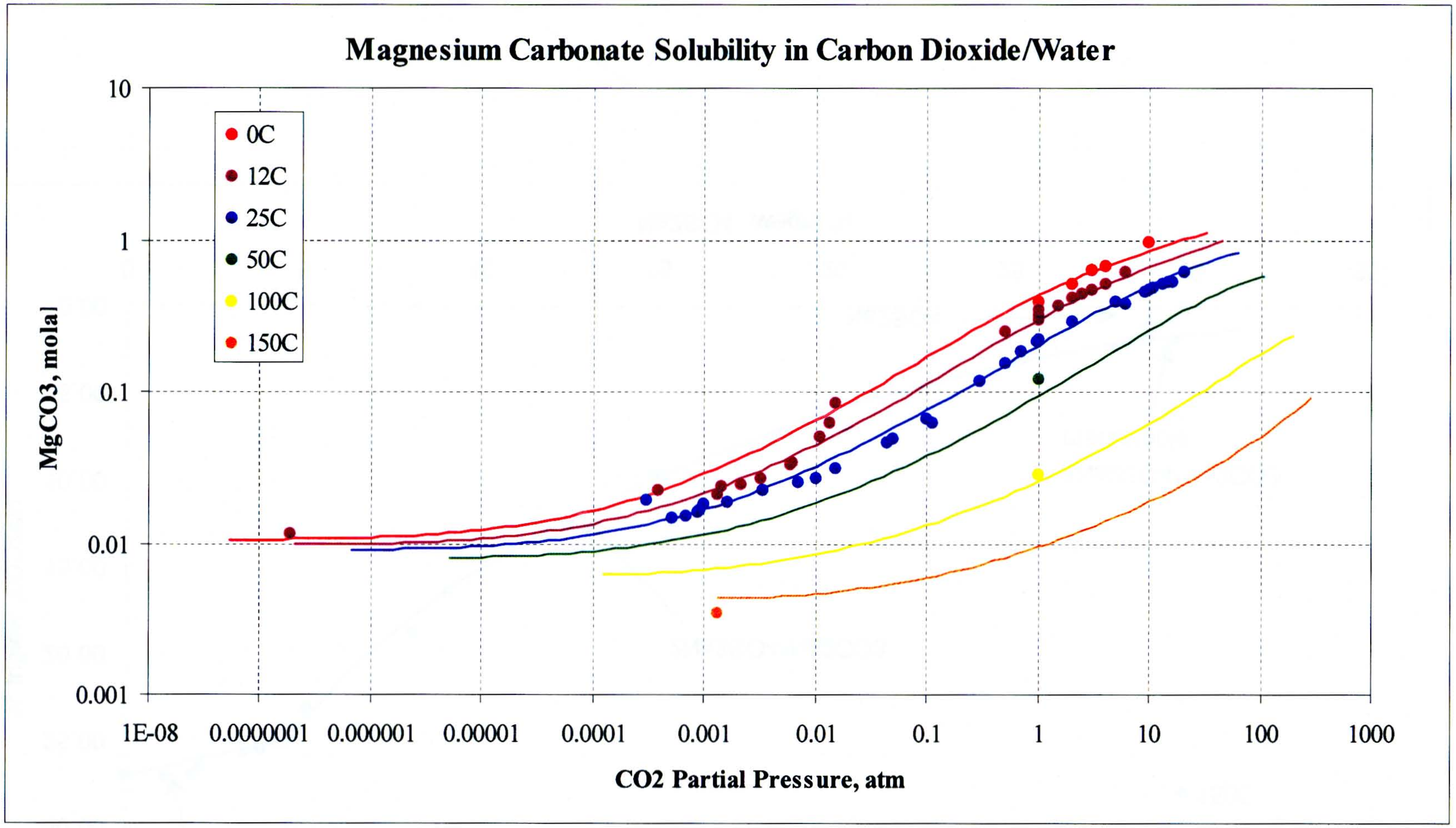
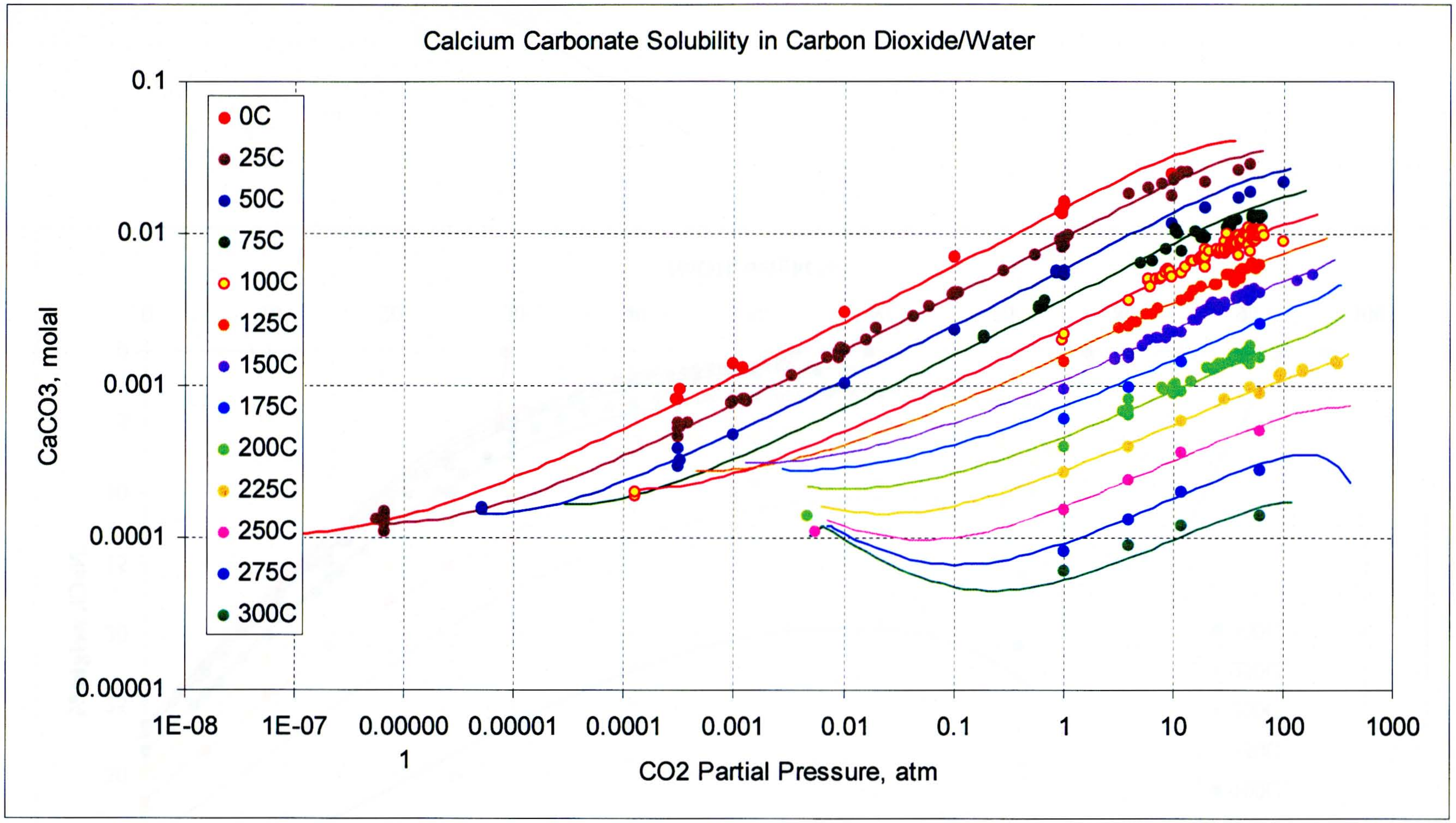
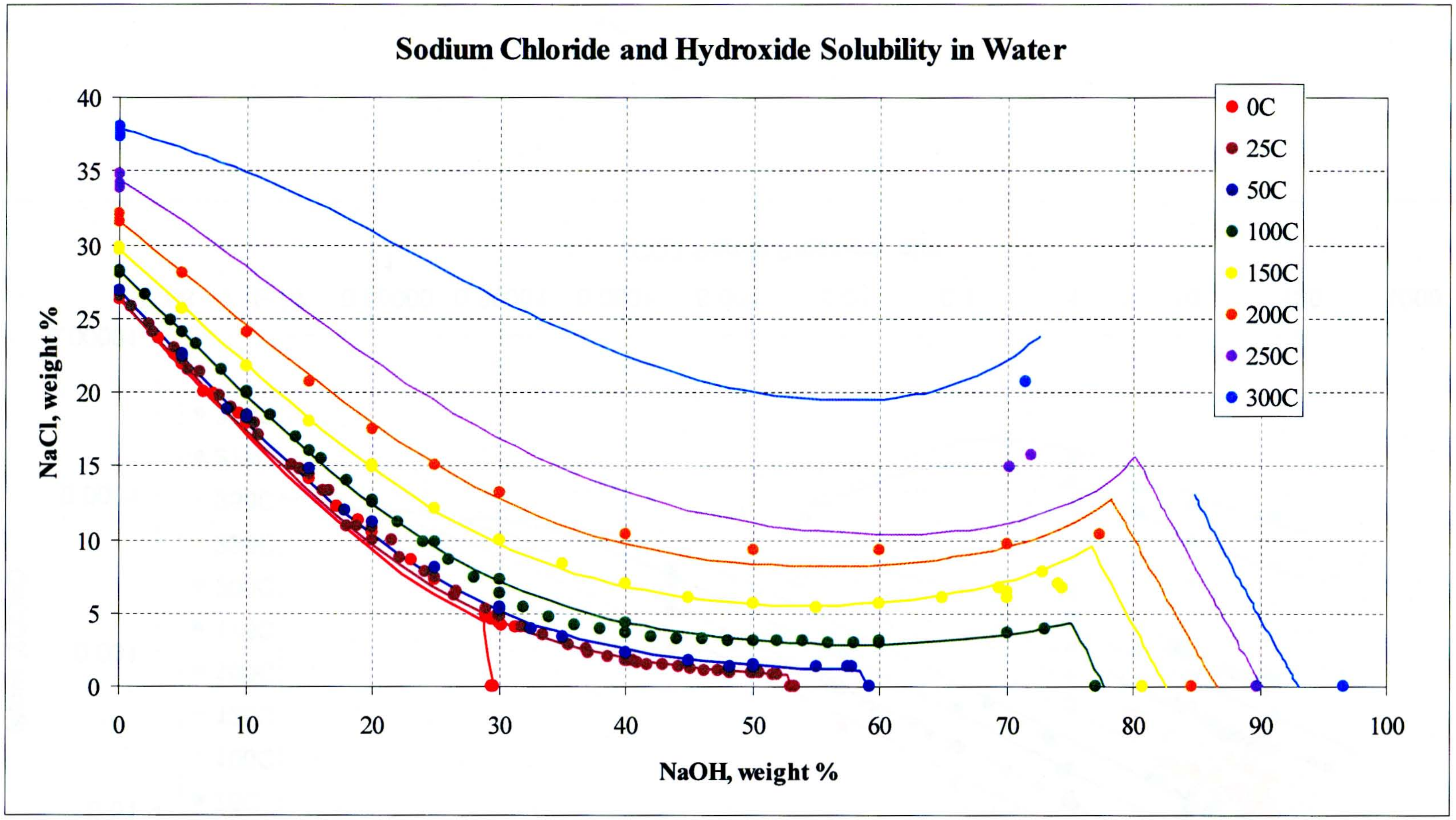

Na+SO4+CO3+H2O
50C
100C
150C
200C
250C
Na2CO3, weight %
Na2SO4, weight %
0
5
10
15
20
25
30
35

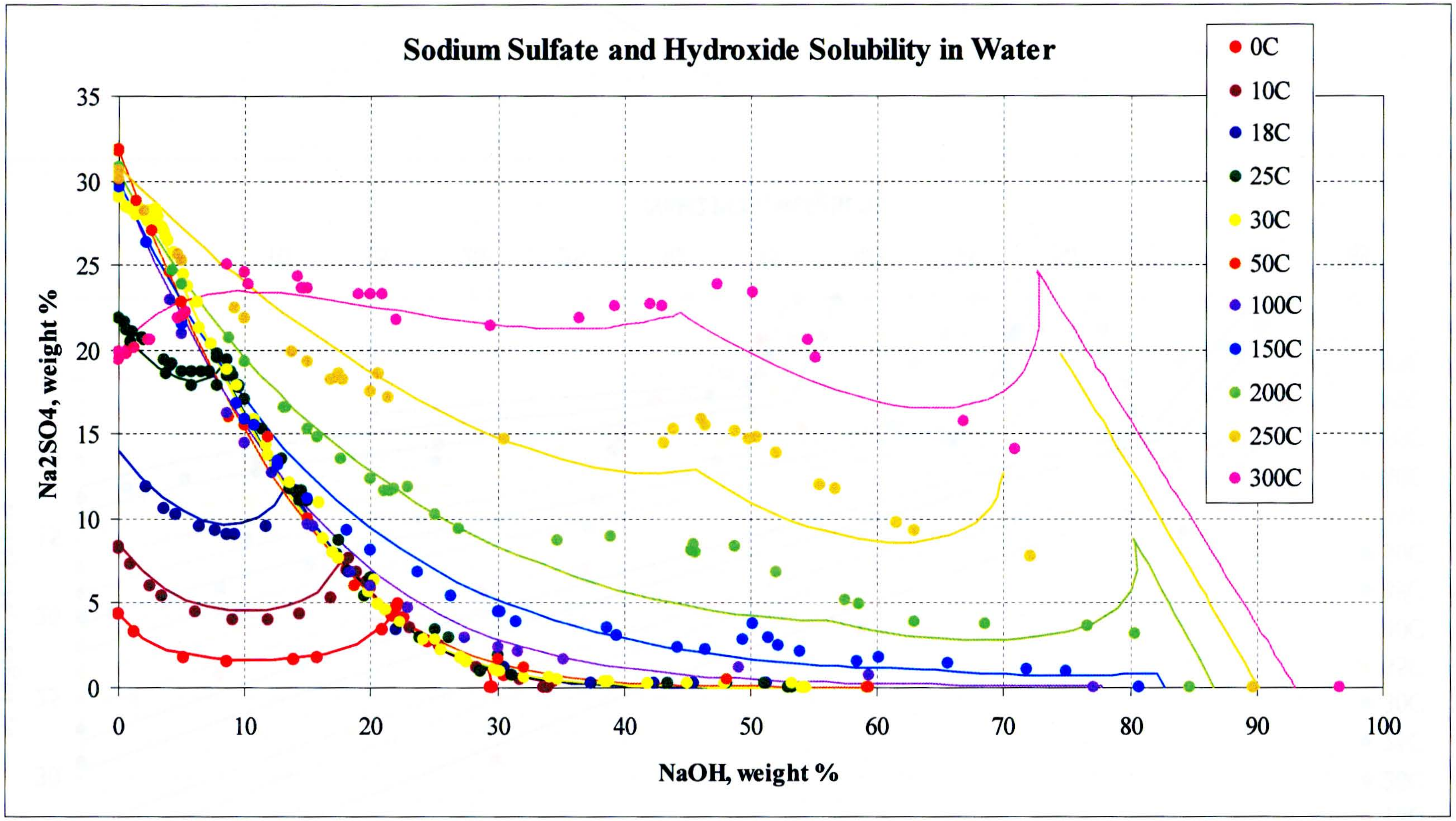

Na+SO4+CO3+H2O
30C
Na2CO3*10H2O
Na2CO3*7H2O
2Na2SO4*Na2CO3
Na2SO4*10H2O
Na2SO4
Na2CO3, weight %
Na2SO4, weight %
0
5
10
15
20
25
30
35


Na+SO4+CO3+H2O
35.00
30.00
25.00
20.00
15.00
10.00
5.00
0.00
Na2CO3, weight %
0
5
10
15
20
25
30
35
Na2SO4, weight %
150C
Na2CO3
2Na2SO4*Na2CO3
2Na2SO4*Na2CO3
metastable
Na2SO4

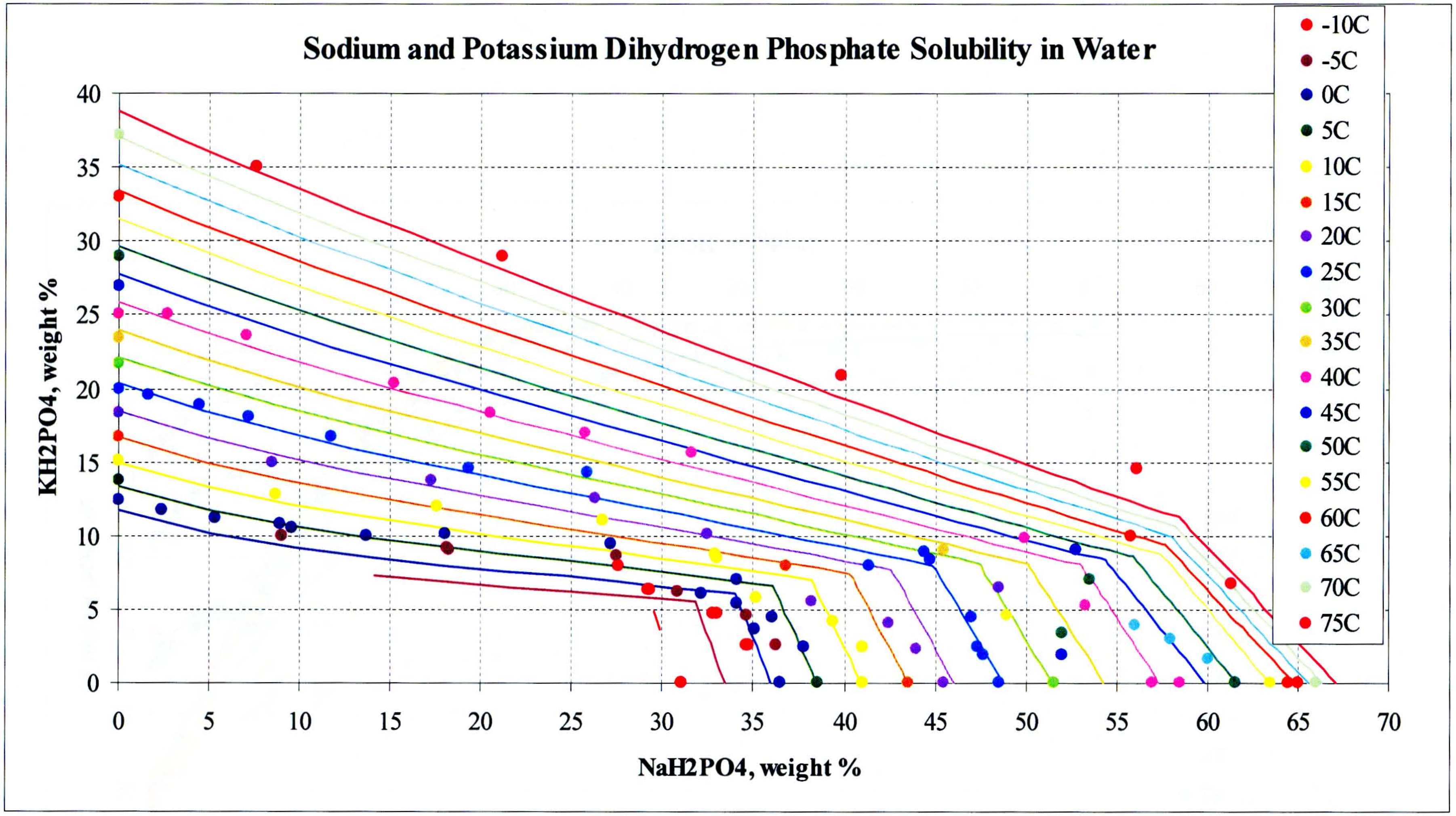

Magnesium Carbonate Solubility in Carbon Dioxide/Water
MgCO3, molal
CO2 Partial Pressure, atm
0C
12C
25C
50C
100C
150C
10
1
0.1
0.01
0.001
1E-08
0.0000001
0.000001
0.00001
0.0001
0.001
0.01
0.1
1
10
100
1000

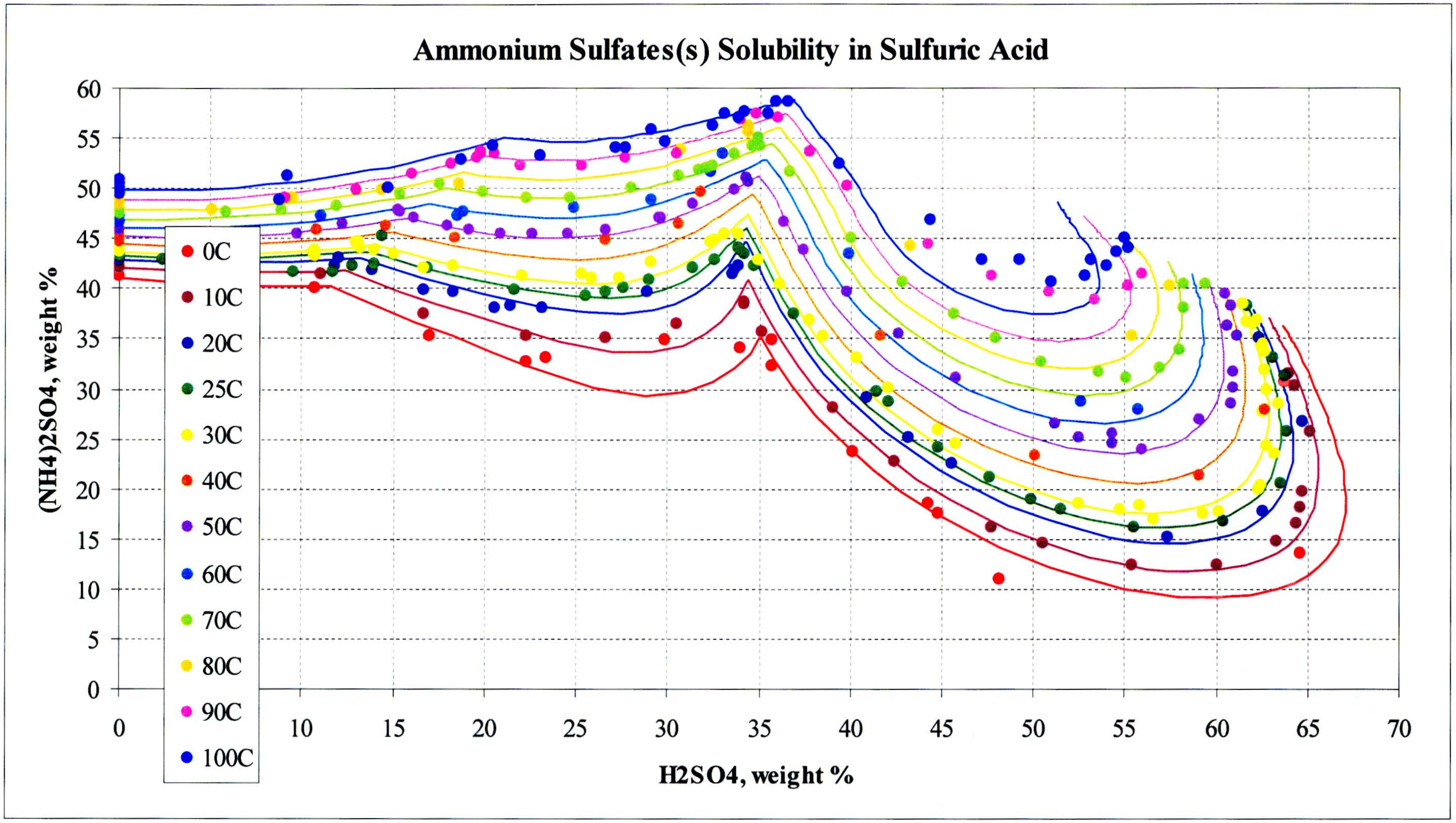

Calcium Carbonate Solubility in Carbon Dioxide/Water
CaCO3, molal
0.1
0.01
0.001
0.0001
0.00001
0C
25C
50C
75C
100C
125C
150C
175C
200C
225C
250C
275C
300C
1E-08
1E-07
0.000001
0.00001
0.0001
0.001
0.01
0.1
1
10
100
1000
CO2 Partial Pressure, atm

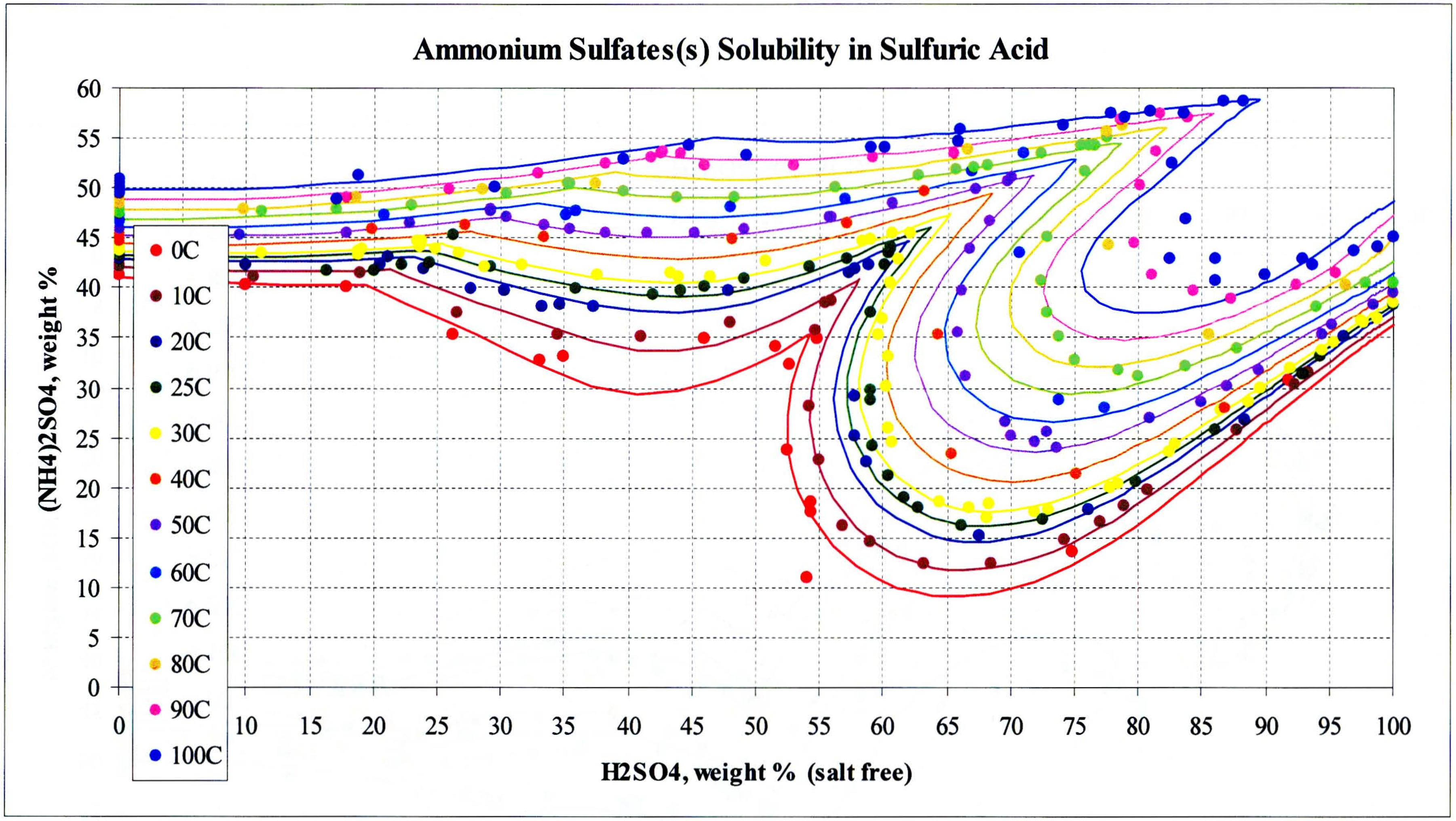

Sodium Chloride and Hydroxide Solubility in Water
NaCl, weight %
NaOH, weight %
0C
25C
50C
100C
150C
200C
250C
300C
0
5
10
15
20
25
30
35
40
0
10
20
30
40
50
60
70
80
90
100

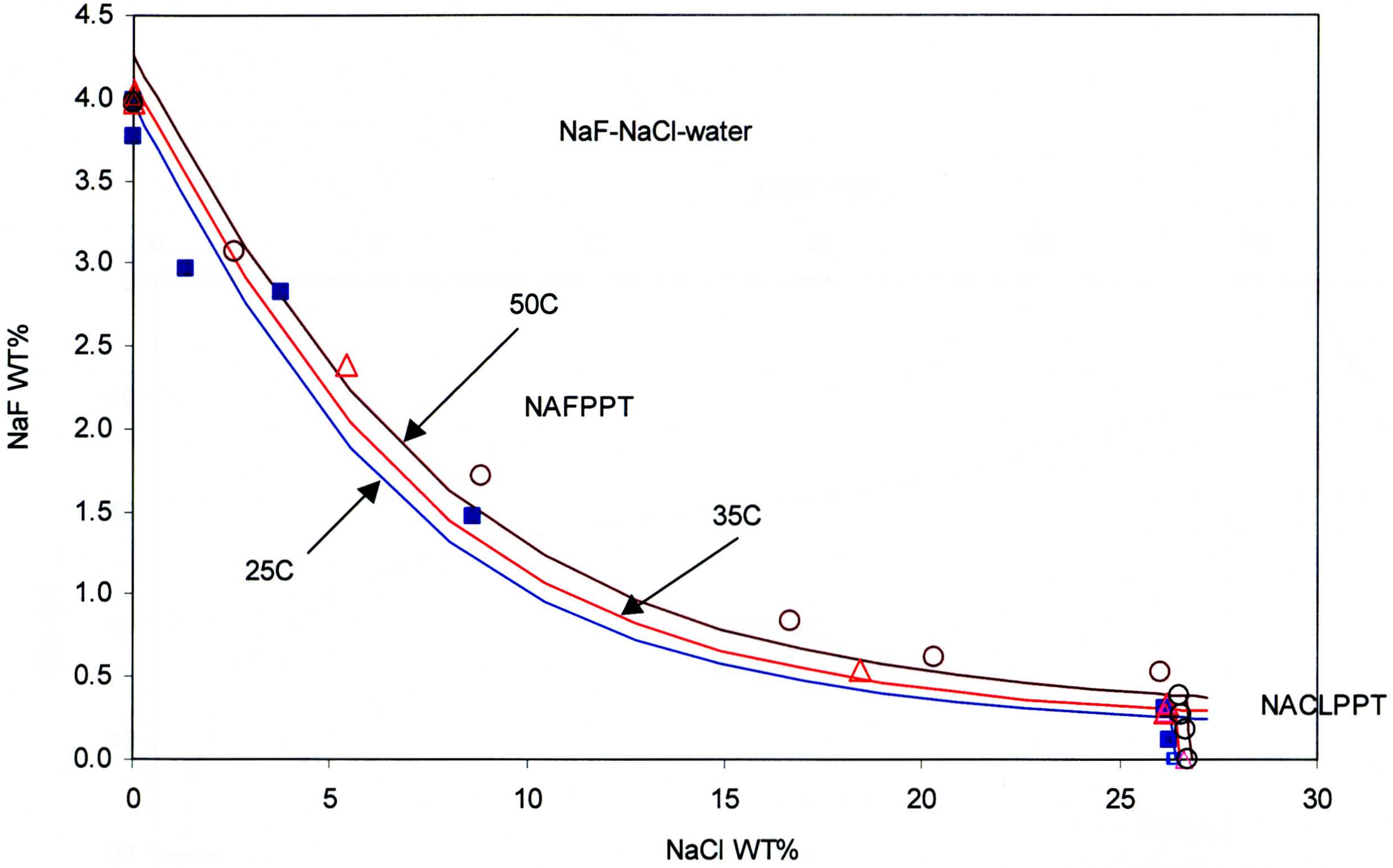


Sodium Sulfate and Hydroxide Solubility in Water
Na2SO4, weight %
NaOH, weight %
0C
10C
18C
25C
30C
50C
100C
150C
200C
250C
300C

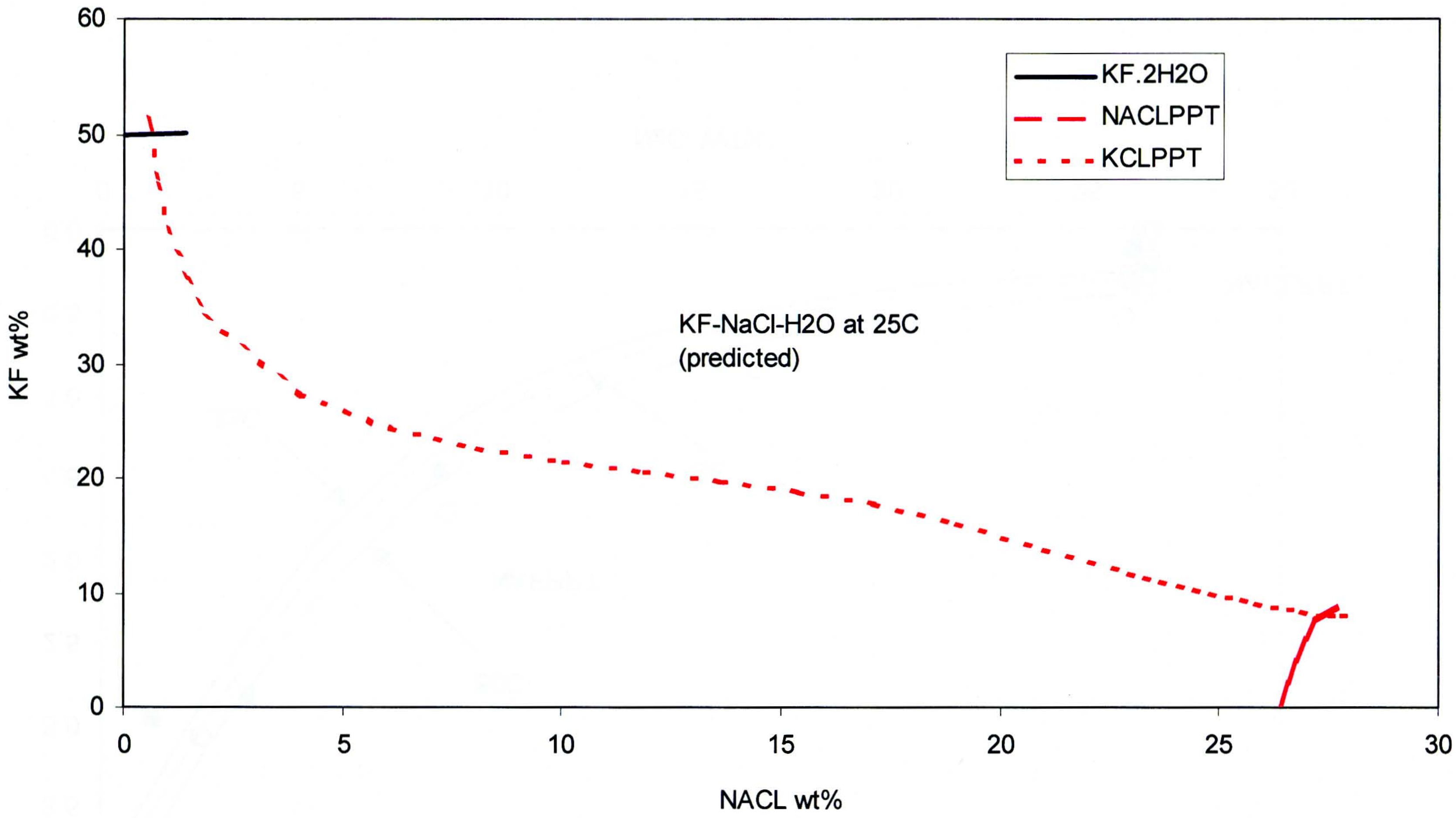

Sodium and Potassium Dihydrogen Phosphate Solubility in Water
KH2PO4, weight %
NaH2PO4, weight %
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
-10C
-5C
0C
5C
10C
15C
20C
25C
30C
35C
40C
45C
50C
55C
60C
65C
70C
75C

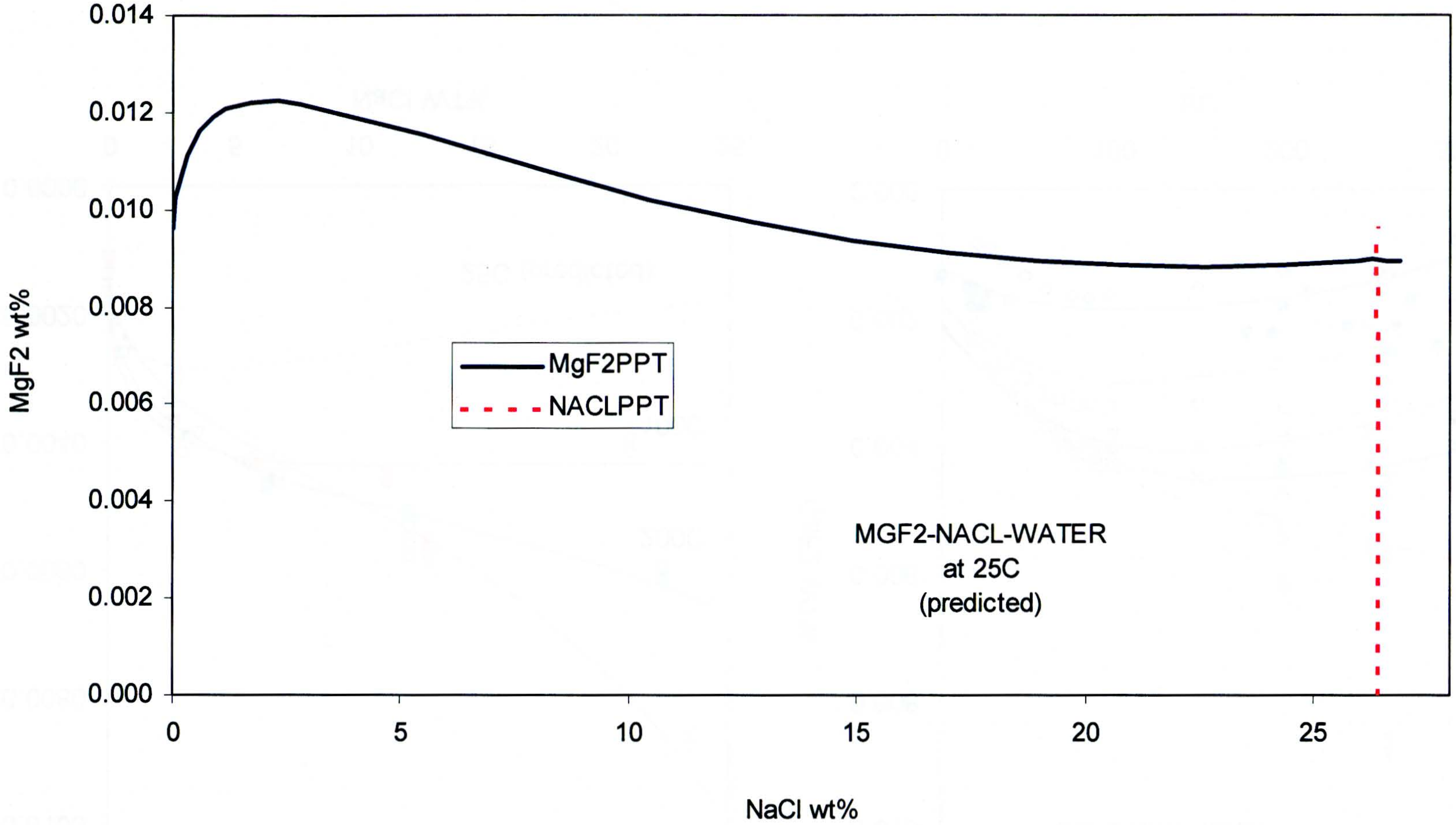

Ammonium Sulfates(s) Solubility in Sulfuric Acid
(NH4)2SO4, weight %
H2SO4, weight %
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
0C
10C
20C
25C
30C
40C
50C
60C
70C
80C
90C
100C

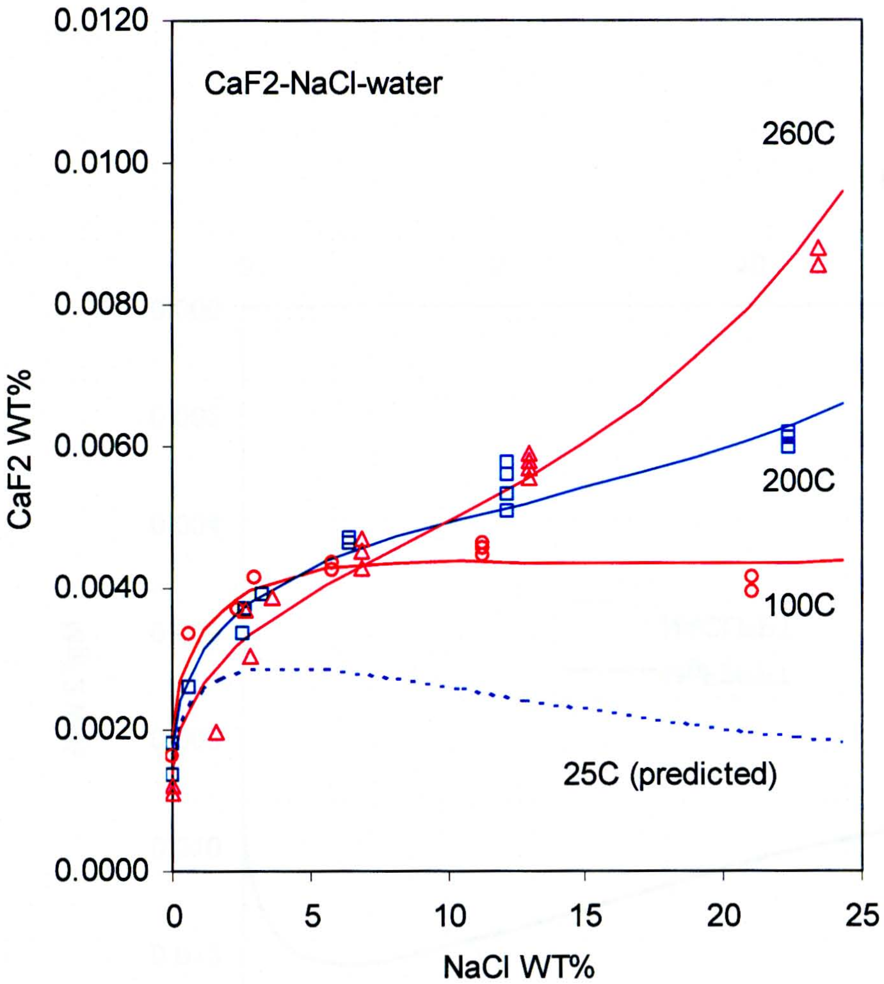

Ammonium Sulfates(s) Solubility in Sulfuric Acid
(NH4)2SO4, weight %
H2SO4, weight % (salt free)
0
5
10
15
20
25
30
35
40
45
50
55
60
65
70
75
80
85
90
95
100
0C
10C
20C
25C
30C
40C
50C
60C
70C
80C
90C
100C



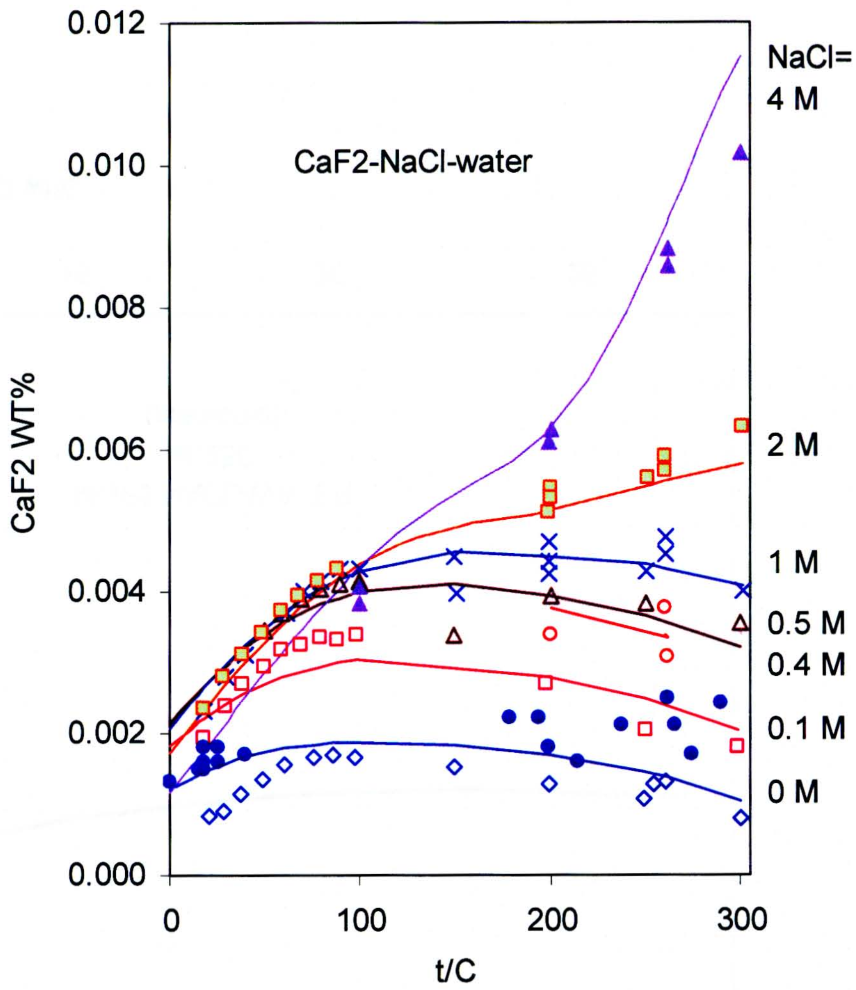
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
NaF WT%
NaF-NaCl-water
50C
NAFPPT
35C
25C
NACLPPT
0
5
10
15
20
25
30
NaCl WT%


KF.2H2O
NACLPPT
KCLPPT
KF-NaCl-H2O at 25C
(predicted)
KF wt%
NACL wt%
0
10
20
30
40
50
60
0
5
10
15
20
25
30

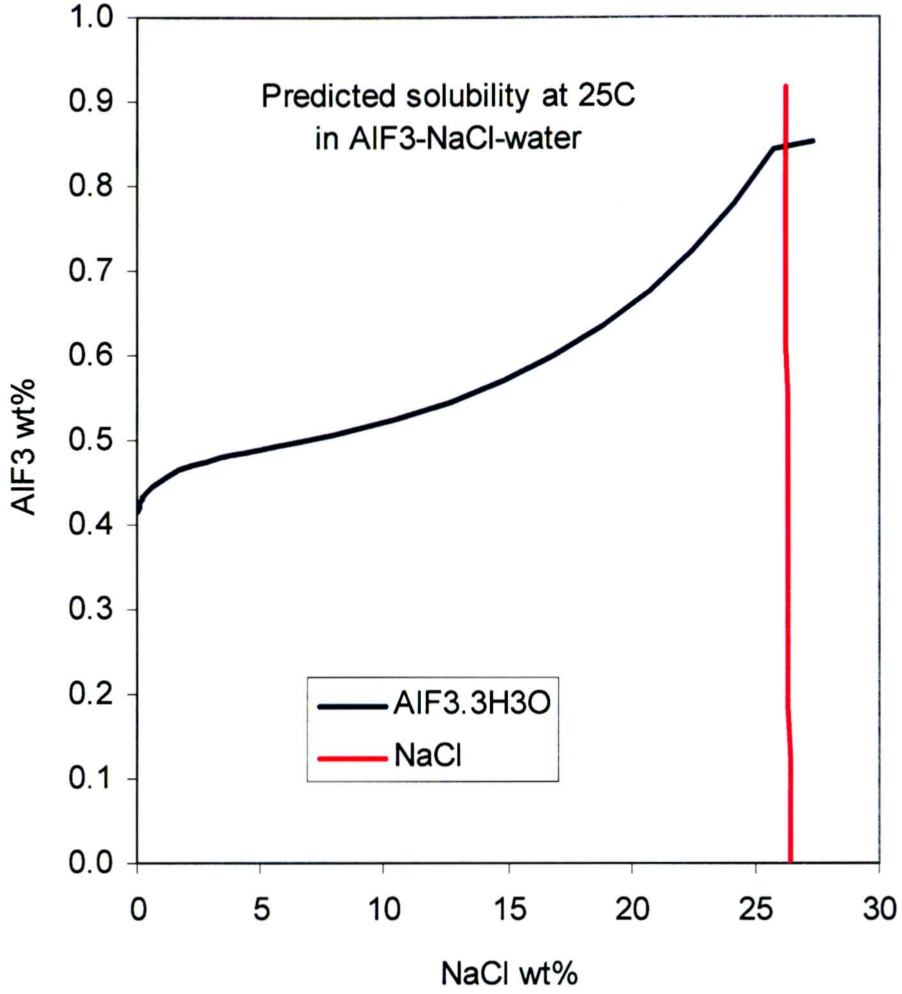

0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
MgF2 wt%
MgF2PPT
NACLPPT
MGF2-NACL-WATER
at 25C
(predicted)
0
5
10
15
20
25
NaCl wt%



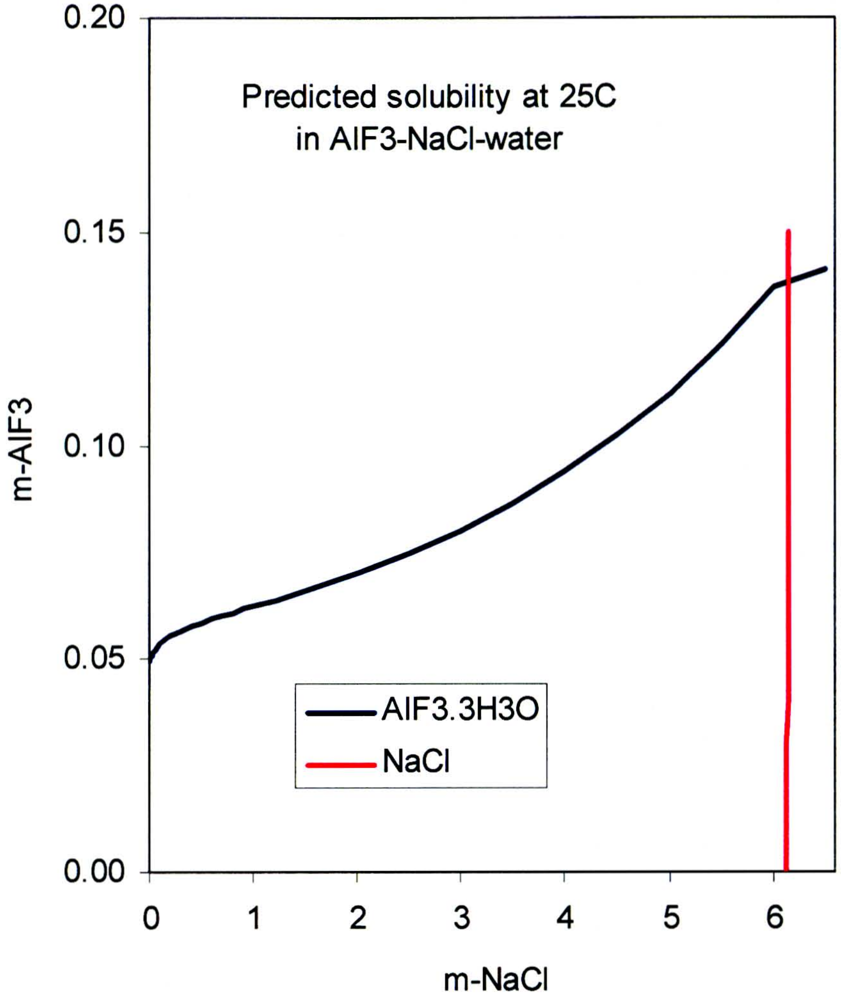
CaF2-NaCl-water
260C
200C
100C
25C (predicted)
CaF2 WT%
NaCl WT%
0.0000
0.0020
0.0040
0.0060
0.0080
0.0100
0.0120
0
5
10
15
20
25



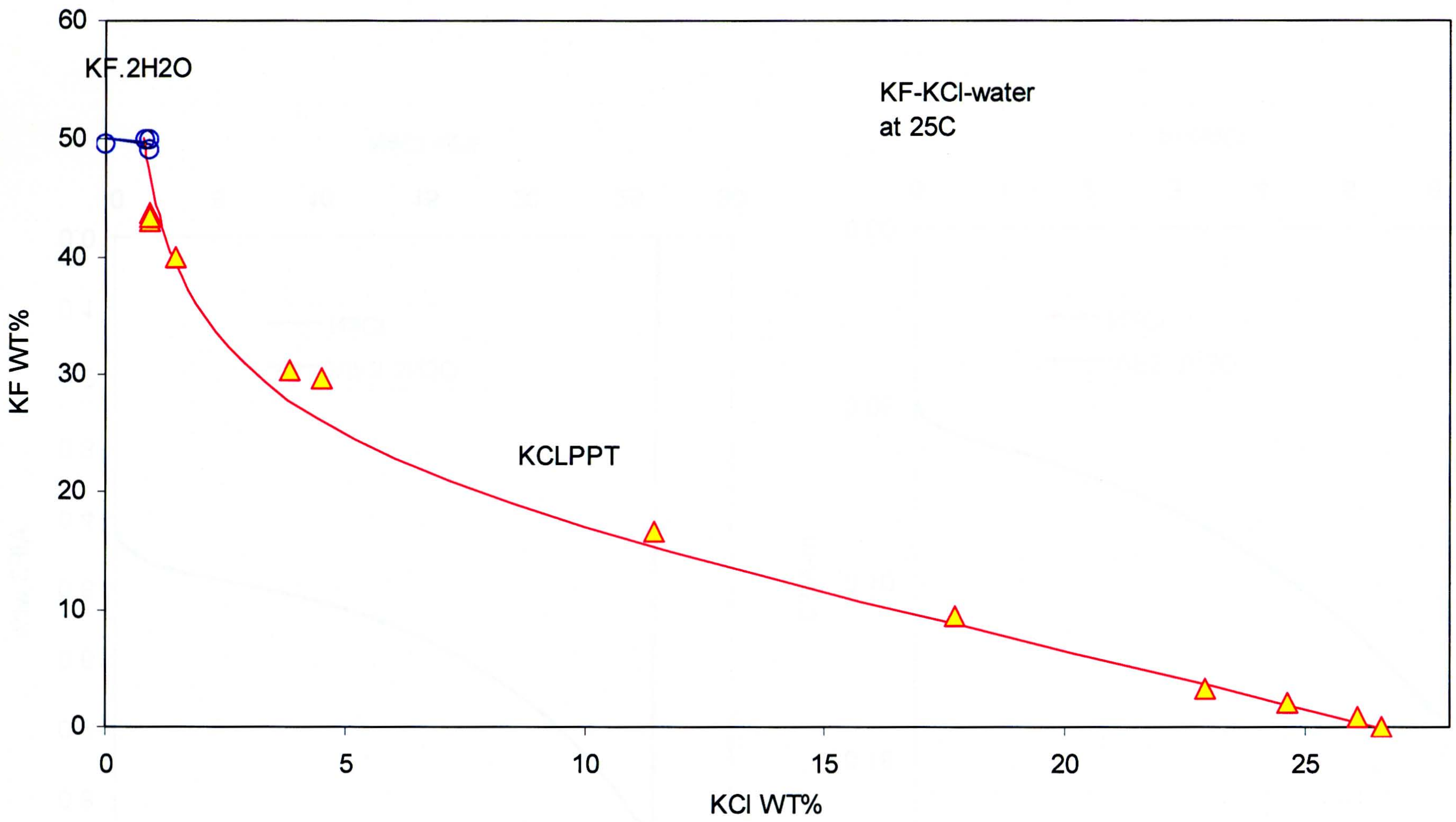
CaF2-NaCl-water
NaCl=
4 M
2 M
1 M
0.5 M
0.4 M
0.1 M
0 M
CaF2 WT%
t/C
0.000
0.002
0.004
0.006
0.008
0.010
0.012
0
100
200
300

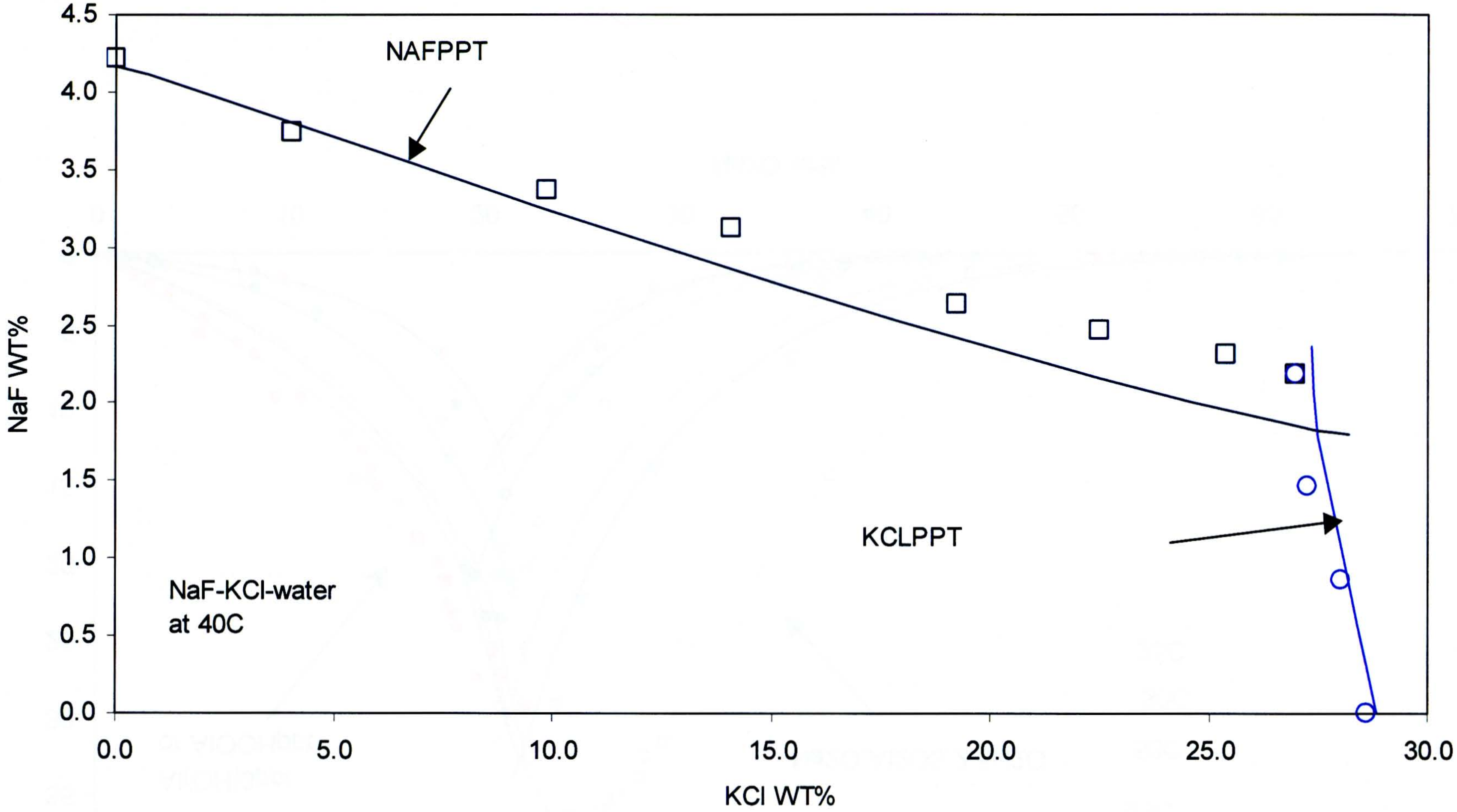


Predicted solubility at 25C
in AlF3-NaCl-water
AlF3 wt%
NaCl wt%
AlF3.3H3O
NaCl
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0
5
10
15
20
25
30



Predicted solubility at 25C
in AlF3-NaCl-water
m-AlF3
m-NaCl
AlF3.3H3O
NaCl
0.20
0.15
0.10
0.05
0.00
0
1
2
3
4
5
6


KF.2H2O
KF-KCl-water
at 25C
KCLPPT
KF WT%
KCl WT%
60
50
40
30
20
10
0
0
5
10
15
20
25



4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
NaF WT%
0.0
5.0
10.0
15.0
20.0
25.0
30.0
KCl WT%
NAFPPT
KCLPPT
NaF-KCl-water
at 40C