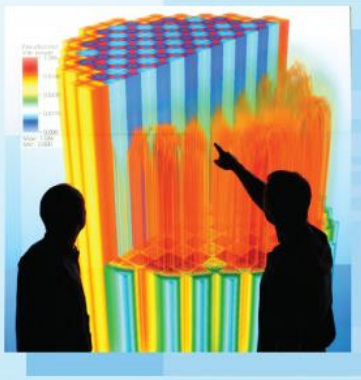
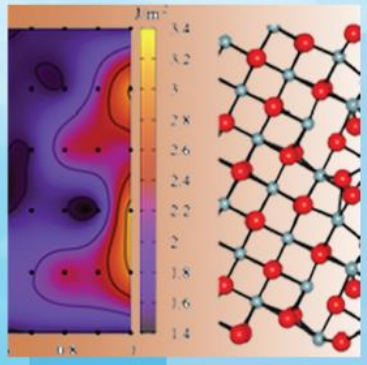
CASL-U-2013-0121-000

Power uprates
and plant life extension



Engineering design
and analysis

Science-enabling
high performance
computing



Fundamental science

Plant operational data

Consortium for Advanced Simulation of LWRs

L3:MPO.CRUD.P7.02

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ORNL

Completed: June 28, 2013

U.S. DEPARTMENT OF ENERGY | Nuclear Energy

Milestone L3:MPO.CRUD.P7.02

Implementation of More Complete Thermochemical Database in MAMBA

Milestone Description: Add Zn to the current spinel model and extend the previously computed solubility data as a function of temperature to a wider range of input parameters of $B(OH)_3$, LiOH, H_2, O_2, Ni, Fe concentrations as specified by the needs of the MAMBA code development and provide data file. Document data file generation and results in a report.

Introduction:

A major phase in CRUD is the complex spinel containing steel corrosion product metals Fe, Cr, Ni, Co, and Mn. Also found in the phase is Zn, which is purposely added to PWR coolant to suppress corrosion. Previous efforts produced a compound energy formalism (CEF) solution model [1] for the Fe-Cr-Ni spinel phase based on Kjellqvist et al. [2]. In the current effort this was expanded to include Zn. A borate phase that is rare in nature, but commonly observed in CRUD is Bonaccordite, Ni_2FeBO_5. While there are no thermochemical assessments of this phase, first principles calculations were used to develop a free energy relation for Bonaccordite [3]. The thermodynamic values for Bonaccordite were used in equilibrium calculations to determine its general stability conditions within CRUD/PWR coolant. Thermochemical relations were used in equilibrium calculations with Ni and Fe under prototypical CRUD/PWR coolant conditions to generate a data table of solubilities for use with MAMBA.

Addition of Zn to Spinel Model:

This work focuses on adding zinc into an existing thermodynamic model for the spinel phase in the Fe-Cr-Ni-O system within the framework of the CEF [1] to predict phase stabilities of CRUD phases in the aqueous system. Fe-Zn-O ternary system has the most available experimental data among three Zn containing ternary oxide systems and current effort has been mainly focused on evaluating model parameters to self-consistently reproduce phase equilibrium data in the sublattice model given below.

$$(Zn^{+2},Cr^{+2},Cr^{+3},Fe^{+2},Fe^{+3},Ni^{+2})_1(Zn^{+2},Cr^{+3},Fe^{+2},Fe^{+3},Ni^{+2},Va)_2(Cr^{+2},Fe^{+2},Va)_2(O^{-2})_4$$

A reciprocal relationship, consistent with the approach of Kjellqvist et al. [2], has been used to reduce the number of independent adjustable parameters for Zn^{2+} containing CEF end-members. A self-consistent thermodynamic model for the spinel phase has been obtained to reproduce phase stabilities of the spinel phase in the isothermal section (Figure 1) and Fe_2O_3-ZnO pseudo-binary phase diagram (Figure 2).

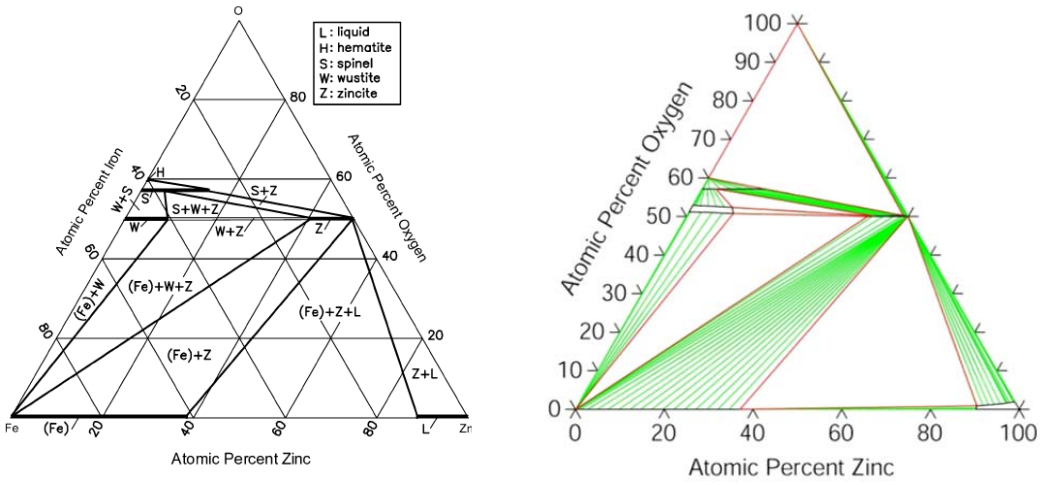

Figure 1. Calculated isothermal section of Fe-Zn-O at 1100K from the current work in comparison with experiments. Phase stabilities of spinel, wustite, and zincite with Zn^{+2} incorporated sublattice model are in good agreement.

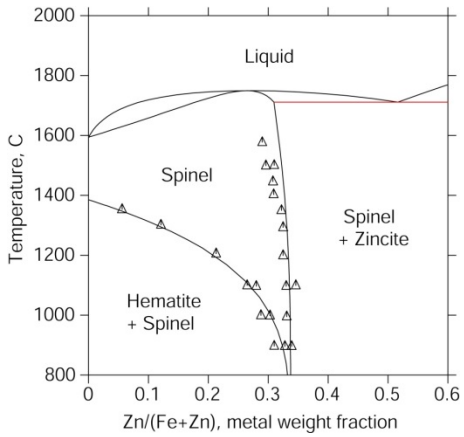

Figure 2. Calculated phase diagram of Fe_2O_3-ZnO from the current model with experimental phase boundary measurement of the spinel phase, which are in good agreement.

Thermodynamic descriptions for additional 21 Zn-containing end-members other than the ones in Fe-Zn-O have been estimated from the reciprocal relationship used in the model of Kjellqvist et al. [2] in a similar manner. Formation Gibbs energy for $ZnCr_2O_4$ has been obtained from experimental work by Ziemniak et al. [4] and incorporated in the current model.

Spinel and Lithium Tetraborate Precipitation:

The spinel model described above together with other relevant phases were used in equilibrium calculations to determine conditions under which they would precipitate under prototypical PWR coolant conditions and compositions. The coolant concentrations were assumed to be fixed at those listed in Table 1.

Table 1. PWR coolant concentrations assumed for solubility calculations.

Element	Molarity (mols/kg H_2O)
Cr	1.92E-08
Ni	8.52E-08
Zn	3.06E-07
B	0.147997
H_2	0.002

An aqueous phase using the Helgeson-Kirkham-Flowers representation within the SUPCRT [5] database was implemented in the FactSage [6] equilibrium calculational software. The FactSage [6] compound database was used for gaseous and additional condensed phases. Computed solubility for the spinel phase described above can be seen in Fig. 3 plotted as a function of coolant temperature and Fe concentration. The total pressure was fixed at 153 bar and the pH was adjusted to ~7.2 using lithium additions.

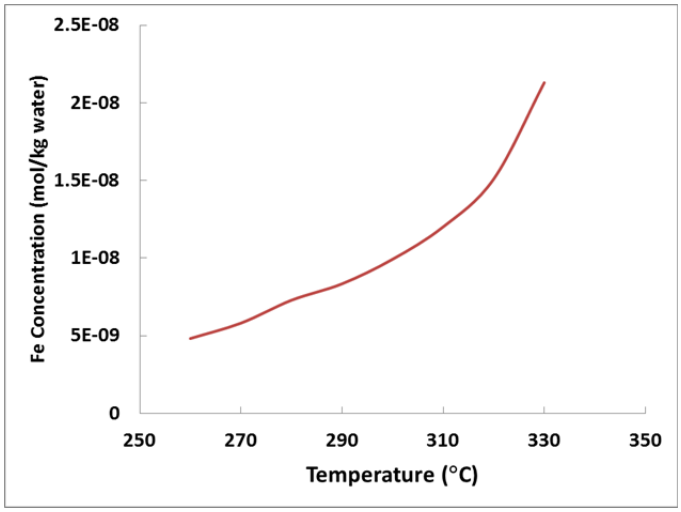

Figure 3. Solubility of Fe-Cr-Ni spinel in PWR coolant as a function of Fe concentration and temperature.

Lithium tetraborate solubility under PWR conditions was computed as a function of boron concentration, again at 153 bar with the pH adjusted to ~7.2 using lithium additions. The characteristic retrograde solubility curve is seen in Fig. 4.

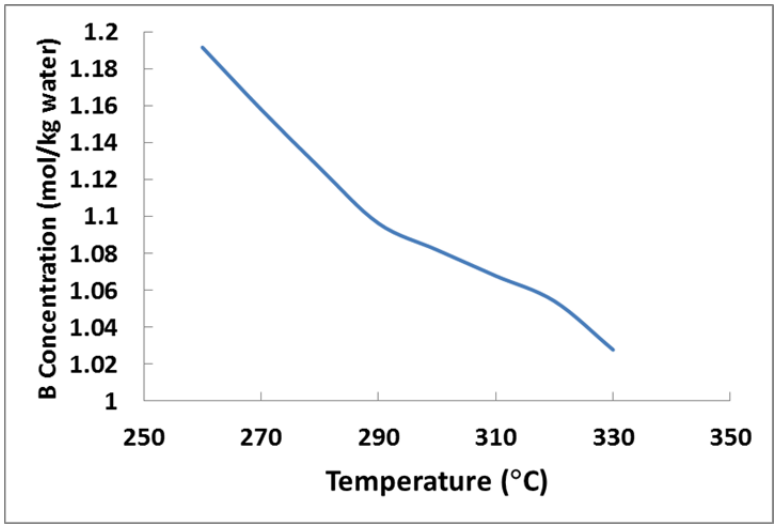

Figure 4. Solubility of $Li_2B_4O_7$ in PWR coolant as a function of B concentration and temperature.

Computed Bonaccordite Stability under PWR Conditions:

A thermochemical analysis of selected constituents of CRUD was used to predict formation of Bonaccordite. Thermodynamic values for the gas and independent compounds were also taken from databases within FactSage [6]. A thermochemical representation of the Ni-Fe spinel phase was generated from the approach of Kjellquist, et al. [2] and used in the calculations, which as noted above was the basis for the more complex spinel. Besides the spinel phase, elemental boron and lithium and their relevant phases and aqueous and gaseous species were included, again from the FactSage [6] databases as noted in the previous section.

Calculations were performed to determine conditions for the formation of Bonaccordite. It was computed that under typical PWR coolant conditions with a pH adjusted to ~7.2 using lithium additions, it is the oxygen partial pressure that governs whether the phase is stable, i.e., whether it will precipitate from the coolant, provided of course sufficient concentration of metal species. The log of the oxygen pressure as a function of reciprocal absolute temperature (Ellingham diagram) is plotted in Fig. 5 for phases under PWR conditions indicating typical oxygen pressures based on equilibrium calculations. The injection of hydrogen into the coolant maintains the calculated low oxygen pressure. The line for a reaction with NiO, the spinel and a boron hydroxide species delineates the boundary above which (at the higher oxygen pressures) where Bonaccordite can precipitate assuming sufficient concentration of constituent species. This is a result of global equilibrium calculations, with the reaction indicated in the figure being simply illustrative. The phase is seen in equilibrium with the Ni-Fe spinel and Ni or NiO. For comparison similar plots are shown for NiO formation simply from the equilibrium with oxygen and Ni, and also within the PWR coolant system in the presence of the spinel.

From Fig. 3 the spinel and Ni are present at the low oxygen pressure assumed for the coolant, with neither NiO nor Bonaccordite stable. However, observations of CRUD compositions

contradict this observation, with both NiO and Bonaccordite present within layers in CRUD.[7, 8] The formation of these phases in CRUD must therefore be the result of higher oxygen pressure conditions within CRUD layers. The less reducing conditions within the CRUD layer can be speculatively attributed to radiolysis of water releasing oxygen. The more reducing coolant (containing injected hydrogen) likely does not fully dilute the higher oxygen content fluid in the CRUD, thus allowing the oxide phases to form.

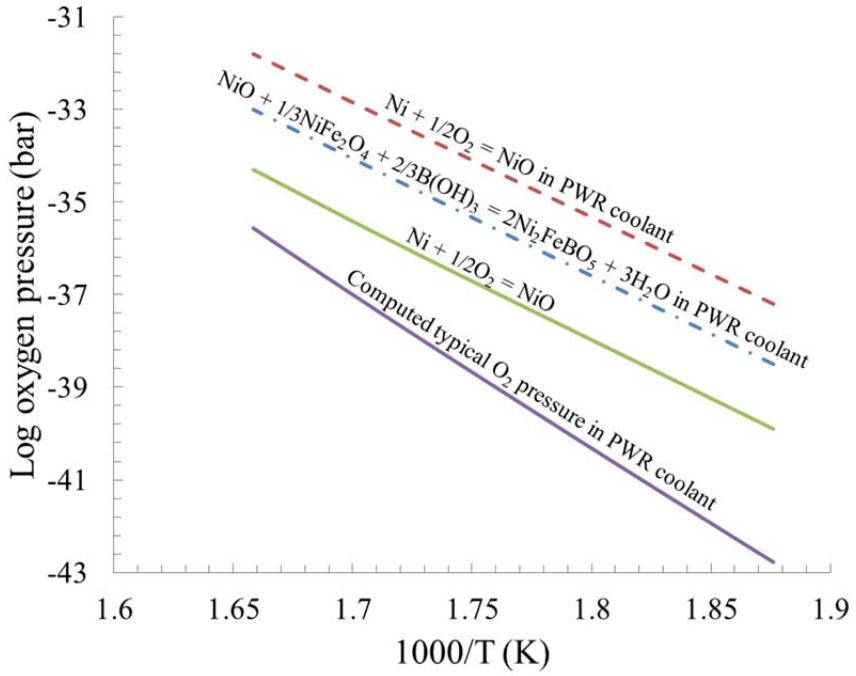

Figure 3. Ellingham diagram of the stability of Bonaccordite and NiO in PWR coolant in equilibrium with Ni-Fe spinel, and also for Ni only in the presence of O_2 and Ni.

Solubility Database for PWR Coolant Containing Fe and Ni:

A preliminary set of data tables were generated from equilibrium calculations performed using FactSage [6] for use with MAMBA, with compositions provided by MAMBA developers. The calculations included all Fe and Ni phases, including the spinel and the aqueous phase. $B(OH)_3$ and LiOH were included in prototypical amounts, with the LiOH used to control pH. Hydrogen concentrations were also introduced as it is procedure to maintain soluble hydrogen in PWR coolant to suppress oxygen levels. These are limited solubility calculations and do not include nickel borate or the Bonaccordite phase. Results are seen in the data tables provided in the Appendix.

References:

[1] M. Hillert, B. Jansson, B. Sundman, *Z. Metallk.*, 79(2): 81-7, 1988.

[2] L. Kjellqvist, M. Selleby, B. Sundman, *CALPHAD*, 32(3): 577-92, 2008.

[3] C.J. O'Brien, A.D. Andersson, C.L. Stanek, D.W. Brenner, T.M. Besmann, Conditions for forming Bonaccordite in CRUD from First-Principles-Informed Thermodynamics., to be submitted to *J. Nucl. Mater.*

[4] S. E. Ziemniak, L. M. Anovitz, R. A. Castelli, W. D. Porter, *J. Chem. Thermodyn.*, 39(11): 1474-92, 2007.

[5] J.W. Johnson, E.H. Oelkers, H.C. Helgeson, SUPCRT92: A software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5000 bar and 0 to 1000°C, *Computers & Geosciences*. 18 (1992) 899–947.

[6] C.W. Bale, P. Chartrand, S.A. Degterov, K. Eriksson, K. Hack, R.B. Mahfoud, J. Melancon, A.D. Pelton and S. Petersen, *Computer Coupling of Phase Diagrams and Thermochemistry*, 26 (2002) 89-228.

[7] J.A. Sawicki, *J. Nucl. Mater*. 374 (2008) 248–269.

[8] J.-W. Yeon, I.-K. Choi, K.-K. Park, H.-M. Kwon, K. Song, *J. Nucl. Mater*. 404 (2010) 160-164.

Appendix:

	Conditions						
	1 mol H2O						
	1.5e-3 mol B(OH)3						
	6.636e-6 mol LiOH						
	3.535e-5 mol H2						
	2.25e-6 mol O2						
	1.4e-10 mol Ni						
	P=153 atm						
T(C)	Input mol Fe	Mol-H[+](AQDD)	Mol-(NiO)(Fe2O3)(s)	Mol-O4Fe3(s)	Mol-Ni(s)	Mol-ONi(s)	pH
260	5.00E-09	9.93E-09	0	0	2.52E-11	0	-6.41604
260	6.00E-09	9.93E-09	5.34E-11	0	0	0	-6.41602
260	7.00E-09	9.93E-09	7.54E-11	0	0	0	-6.41601
260	8.00E-09	9.93E-09	8.22E-11	1.95E-10	0	0	-6.416
260	9.00E-09	9.93E-09	8.22E-11	5.29E-10	0	0	-6.416
260	1.00E-08	9.93E-09	8.22E-11	8.62E-10	0	0	-6.416
270	5.00E-09	9.37E-09	3.68E-11	0	0	0	-6.44844
270	6.00E-09	9.37E-09	6.75E-11	0	0	0	-6.44842
270	7.00E-09	9.37E-09	8.64E-11	0	0	0	-6.44839
270	8.00E-09	9.37E-09	9.69E-11	4.25E-11	0	0	-6.44837
270	9.00E-09	9.37E-09	9.79E-11	3.76E-10	0	0	-6.44837
270	1.00E-08	9.37E-09	9.78E-11	7.09E-10	0	0	-6.44837
280	5.00E-09	8.82E-09	4.96E-11	0	0	0	-6.48262
280	6.00E-09	8.82E-09	7.62E-11	0	0	0	-6.48258
280	7.00E-09	8.82E-09	9.30E-11	0	0	0	-6.48255
280	8.00E-09	8.82E-09	1.04E-10	0	0	0	-6.48252
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290	8.00E-09	8.31E-09	1.08E-10	0	0	0	-6.51681
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	Conditions						
	1 mol H2O						
	1.5e-3 mol B(OH)3						
	6.636e-6 mol LiOH						
	3.535e-5 mol H2						
	2.25e-6 mol O2						
	2.8e-10 mol Ni						
	P=153 atm						
T(C)	Input mol Fe	Mol-H[+](AQDD)	Mol-(NiO)(Fe2O3)(s)	Mol-O4Fe3(s)	Mol-Ni(s)	Mol-ONi(s)	pH
260	5.00E-09	9.93E-09	0	0	1.65E-10	0	-6.41604

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340	1.00E-08	1.39E-08	2.38E-10	0	0	0	-6.37402
	Conditions						
	1 mol H2O						
	5e-4 mol B(OH)3						
	6.636e-6 mol LiOH						
	3.535e-5 mol H2						
	2.25e-6 mol O2						
	1.4e-10 mol Ni						
	P=153 atm						
T(C)	Input mol Fe	Mol-H[+](AQDD)	Mol-(NiO)(Fe2O3)(s)	Mol-O4Fe3(s)	Mol-Ni(s)	Mol-ONi(s)	pH
260	5.00E-09	3.37E-09	0	0	1.09E-10	0	-6.83164
260	6.00E-09	3.37E-09	0	0	1.09E-10	0	-6.8316
260	7.00E-09	3.37E-09	0	0	1.09E-10	0	-6.83156
260	8.00E-09	3.37E-09	1.07E-10	0	1.47E-12	0	-6.83152
260	9.00E-09	3.37E-09	1.15E-10	0	0	0	-6.83148
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270	6.00E-09	3.21E-09	0	0	1.08E-10	0	-6.85764
270	7.00E-09	3.21E-09	0	0	1.08E-10	0	-6.85759
270	8.00E-09	3.21E-09	1.09E-10	0	0	0	-6.85756
270	9.00E-09	3.21E-09	1.15E-10	0	0	0	-6.85751
270	1.00E-08	3.21E-09	1.20E-10	0	0	0	-6.85746
280	5.00E-09	3.05E-09	0	0	1.05E-10	0	-6.88532
280	6.00E-09	3.05E-09	0	0	1.05E-10	0	-6.88527
280	7.00E-09	3.05E-09	0	0	1.05E-10	0	-6.88522

280	8.00E-09	3.05E-09	1.08E-10	0	0	0	-6.88518
280	9.00E-09	3.05E-09	1.14E-10	0	0	0	-6.88513
280	1.00E-08	3.05E-09	1.19E-10	0	0	0	-6.88508
290	5.00E-09	2.90E-09	0	0	1.02E-10	0	-6.91293
290	6.00E-09	2.90E-09	0	0	1.02E-10	0	-6.91288
290	7.00E-09	2.90E-09	0	0	1.02E-10	0	-6.91282
290	8.00E-09	2.90E-09	1.06E-10	0	0	0	-6.91278
290	9.00E-09	2.90E-09	1.13E-10	0	0	0	-6.91273
290	1.00E-08	2.90E-09	1.18E-10	0	0	0	-6.91268
300	5.00E-09	2.78E-09	0	0	9.76E-11	0	-6.93741
300	6.00E-09	2.78E-09	0	0	9.76E-11	0	-6.93735
300	7.00E-09	2.78E-09	0	0	9.76E-11	0	-6.9373
300	8.00E-09	2.78E-09	1.03E-10	0	0	0	-6.93725
300	9.00E-09	2.78E-09	1.11E-10	0	0	0	-6.9372
300	1.00E-08	2.78E-09	1.16E-10	0	0	0	-6.93714
310	5.00E-09	2.73E-09	0	0	8.96E-11	0	-6.95281
310	6.00E-09	2.73E-09	0	0	8.96E-11	0	-6.95276
310	7.00E-09	2.73E-09	0	0	8.96E-11	0	-6.9527
310	8.00E-09	2.74E-09	9.86E-11	0	0	0	-6.95266
310	9.00E-09	2.74E-09	1.07E-10	0	0	0	-6.9526
310	1.00E-08	2.74E-09	1.14E-10	0	0	0	-6.95254
320	5.00E-09	2.83E-09	0	0	7.46E-11	0	-6.94745
320	6.00E-09	2.83E-09	0	0	7.46E-11	0	-6.94739
320	7.00E-09	2.83E-09	7.60E-11	0	0	0	-6.94734
320	8.00E-09	2.83E-09	9.18E-11	0	0	0	-6.94728
320	9.00E-09	2.83E-09	1.02E-10	0	0	0	-6.94723
320	1.00E-08	2.83E-09	1.09E-10	0	0	0	-6.94717
330	5.00E-09	3.28E-09	0	0	0	4.89E-11	-6.89623
330	6.00E-09	3.28E-09	0	0	0	4.89E-11	-6.89617
330	7.00E-09	3.28E-09	6.02E-11	0	0	0	-6.89612
330	8.00E-09	3.28E-09	7.88E-11	0	0	0	-6.89606
330	9.00E-09	3.28E-09	9.17E-11	0	0	0	-6.89601
330	1.00E-08	3.28E-09	1.01E-10	0	0	0	-6.89595
340	5.00E-09	4.94E-09	0	0	0	0	-6.7354
340	6.00E-09	4.94E-09	0	0	0	0	-6.73534
340	7.00E-09	4.94E-09	7.92E-12	0	0	0	-6.73528
340	8.00E-09	4.94E-09	3.75E-11	0	0	0	-6.73523
340	9.00E-09	4.94E-09	5.88E-11	0	0	0	-6.73517
340	1.00E-08	4.94E-09	7.37E-11	0	0	0	-6.73511

	Conditions						
	1 mol H2O						
	5e-4 mol B(OH)3						
	6.636e-6 mol LiOH						
	3.535e-5 mol H2						
	2.25e-6 mol O2						
	2.8e-10 mol Ni						
	P=153 atm						
T(C)	Input mol Fe	Mol-H[+](AQDD)	Mol-(NiO)(Fe2O3)(s)	Mol-O4Fe3(s)	Mol-Ni(s)	Mol-ONi(s)	pH
260	5.00E-09	3.37E-09	0	0	2.49E-10	0	-6.83164
260	6.00E-09	3.37E-09	0	0	2.49E-10	0	-6.8316
260	7.00E-09	3.37E-09	0	0	2.49E-10	0	-6.83156
260	8.00E-09	3.37E-09	1.08E-10	0	1.41E-10	0	-6.83152
260	9.00E-09	3.37E-09	2.54E-10	0	0	0	-6.83149
260	1.00E-08	3.37E-09	2.59E-10	0	0	0	-6.83145
270	5.00E-09	3.21E-09	0	0	2.48E-10	0	-6.85769
270	6.00E-09	3.21E-09	0	0	2.48E-10	0	-6.85764
270	7.00E-09	3.21E-09	0	0	2.48E-10	0	-6.85759
270	8.00E-09	3.21E-09	1.68E-10	0	7.97E-11	0	-6.85756
270	9.00E-09	3.21E-09	2.54E-10	0	0	0	-6.85752
270	1.00E-08	3.21E-09	2.59E-10	0	0	0	-6.85747
280	5.00E-09	3.05E-09	0	0	2.45E-10	0	-6.88532
280	6.00E-09	3.05E-09	0	0	2.45E-10	0	-6.88527
280	7.00E-09	3.05E-09	0	0	2.45E-10	0	-6.88522
280	8.00E-09	3.05E-09	2.20E-10	0	2.58E-11	0	-6.88519
280	9.00E-09	3.05E-09	2.53E-10	0	0	0	-6.88514
280	1.00E-08	3.05E-09	2.58E-10	0	0	0	-6.88509
290	5.00E-09	2.90E-09	0	0	2.42E-10	0	-6.91293
290	6.00E-09	2.90E-09	0	0	2.42E-10	0	-6.91288
290	7.00E-09	2.90E-09	0	0	2.42E-10	0	-6.91282
290	8.00E-09	2.90E-09	2.43E-10	0	0	0	-6.9128
290	9.00E-09	2.90E-09	2.51E-10	0	0	0	-6.91274
290	1.00E-08	2.90E-09	2.57E-10	0	0	0	-6.91269
300	5.00E-09	2.78E-09	0	0	2.38E-10	0	-6.93741
300	6.00E-09	2.78E-09	0	0	2.38E-10	0	-6.93735
300	7.00E-09	2.78E-09	0	0	2.38E-10	0	-6.9373
300	8.00E-09	2.78E-09	2.40E-10	0	0	0	-6.93727

300	9.00E-09	2.78E-09	2.49E-10	0	0	0	-6.93721
300	1.00E-08	2.78E-09	2.55E-10	0	0	0	-6.93716
310	5.00E-09	2.73E-09	0	0	2.30E-10	0	-6.95281
310	6.00E-09	2.73E-09	0	0	2.30E-10	0	-6.95276
310	7.00E-09	2.73E-09	0	0	2.30E-10	0	-6.9527
310	8.00E-09	2.74E-09	2.35E-10	0	0	0	-6.95267
310	9.00E-09	2.74E-09	2.45E-10	0	0	0	-6.95262
310	1.00E-08	2.74E-09	2.52E-10	0	0	0	-6.95256
320	5.00E-09	2.83E-09	0	0	2.15E-10	0	-6.94745
320	6.00E-09	2.83E-09	0	0	2.15E-10	0	-6.94739
320	7.00E-09	2.83E-09	1.48E-10	0	6.78E-11	0	-6.94735
320	8.00E-09	2.83E-09	2.28E-10	0	0	0	-6.9473
320	9.00E-09	2.83E-09	2.40E-10	0	0	0	-6.94724
320	1.00E-08	2.83E-09	2.48E-10	0	0	0	-6.94719
330	5.00E-09	3.28E-09	0	0	0	1.89E-10	-6.89623
330	6.00E-09	3.28E-09	0	0	0	1.89E-10	-6.89617
330	7.00E-09	3.28E-09	1.94E-10	0	0	0	-6.89614
330	8.00E-09	3.28E-09	2.14E-10	0	0	0	-6.89608
330	9.00E-09	3.28E-09	2.28E-10	0	0	0	-6.89602
330	1.00E-08	3.28E-09	2.38E-10	0	0	0	-6.89597
340	5.00E-09	4.94E-09	0	0	0	1.20E-10	-6.7354
340	6.00E-09	4.94E-09	0	0	0	1.20E-10	-6.73534
340	7.00E-09	4.94E-09	1.38E-10	0	0	0	-6.7353
340	8.00E-09	4.94E-09	1.70E-10	0	0	0	-6.73524
340	9.00E-09	4.94E-09	1.93E-10	0	0	0	-6.73519
340	1.00E-08	4.94E-09	2.10E-10	0	0	0	-6.73513

	Conditions						
	1 mol H2O						
	1.5e-3 mol B(OH)3						
	6.636e-6 mol LiOH						
	3.535e-5 mol H2						
	2.25e-6 mol O2						
	7e-11 mol Ni						
	P=153 atm						
T(C)	Input mol Fe	Mol-H[+](AQDD)	Mol-(NiO)(Fe2O3)(s)	Mol-O4Fe3(s)	Mol-Ni(s)	Mol-ONi(s)	pH
260	5.00E-09	9.93E-09	0	0	0	0	-6.41604
260	6.00E-09	9.93E-09	0	0	0	0	-6.41602
260	7.00E-09	9.93E-09	7.76E-12	0	0	0	-6.416
260	8.00E-09	9.93E-09	1.22E-11	2.42E-10	0	0	-6.416
260	9.00E-09	9.93E-09	1.21E-11	5.75E-10	0	0	-6.416
260	1.00E-08	9.93E-09	1.22E-11	9.09E-10	0	0	-6.416
270	5.00E-09	9.37E-09	0	0	0	0	-6.44844
270	6.00E-09	9.37E-09	0	0	0	0	-6.44841
270	7.00E-09	9.37E-09	1.86E-11	0	0	0	-6.44839
270	8.00E-09	9.37E-09	2.77E-11	8.92E-11	0	0	-6.44837
270	9.00E-09	9.37E-09	2.76E-11	4.23E-10	0	0	-6.44837
270	1.00E-08	9.37E-09	2.65E-11	7.56E-10	0	0	-6.44837
280	5.00E-09	8.82E-09	0	0	0	0	-6.48261
280	6.00E-09	8.82E-09	9.14E-12	0	0	0	-6.48258
280	7.00E-09	8.82E-09	2.54E-11	0	0	0	-6.48254
280	8.00E-09	8.82E-09	3.62E-11	0	0	0	-6.48251
280	9.00E-09	8.82E-09	3.85E-11	2.06E-10	0	0	-6.4825
280	1.00E-08	8.82E-09	3.84E-11	5.39E-10	0	0	-6.4825
290	5.00E-09	8.31E-09	0	0	0	0	-6.51692
290	6.00E-09	8.31E-09	1.33E-11	0	0	0	-6.51689
290	7.00E-09	8.31E-09	2.93E-11	0	0	0	-6.51685
290	8.00E-09	8.31E-09	3.81E-11	0	0	0	-6.51681
290	9.00E-09	8.32E-09	4.48E-11	0	0	0	-6.51677
290	1.00E-08	8.32E-09	4.58E-11	2.64E-10	0	0	-6.51676
300	5.00E-09	7.92E-09	0	0	0	0	-6.54826
300	6.00E-09	7.92E-09	1.56E-11	0	0	0	-6.54821
300	7.00E-09	7.92E-09	3.05E-11	0	0	0	-6.54817
300	8.00E-09	7.92E-09	3.92E-11	0	0	0	-6.54813
300	9.00E-09	7.92E-09	4.57E-11	0	0	0	-6.54809

300	1.00E-08	7.92E-09	5.16E-11	0	0	0	-6.54804
310	5.00E-09	7.73E-09	0	0	0	0	-6.57066
310	6.00E-09	7.73E-09	1.56E-11	0	0	0	-6.57061
310	7.00E-09	7.73E-09	2.93E-11	0	0	0	-6.57056
310	8.00E-09	7.73E-09	3.95E-11	0	0	0	-6.57052
310	9.00E-09	7.73E-09	4.49E-11	0	0	0	-6.57047
310	1.00E-08	7.73E-09	5.03E-11	0	0	0	-6.57043
320	5.00E-09	7.96E-09	0	0	0	0	-6.57237
320	6.00E-09	7.96E-09	1.18E-11	0	0	0	-6.57232
320	7.00E-09	7.96E-09	2.73E-11	0	0	0	-6.57227
320	8.00E-09	7.96E-09	3.75E-11	0	0	0	-6.57223
320	9.00E-09	7.96E-09	4.39E-11	0	0	0	-6.57218
320	1.00E-08	7.97E-09	4.88E-11	0	0	0	-6.57213
330	5.00E-09	9.20E-09	0	0	0	0	-6.52823
330	6.00E-09	9.20E-09	0	0	0	0	-6.52818
330	7.00E-09	9.21E-09	1.88E-11	0	0	0	-6.52813
330	8.00E-09	9.21E-09	3.06E-11	0	0	0	-6.52808
330	9.00E-09	9.21E-09	4.00E-11	0	0	0	-6.52803
330	1.00E-08	9.21E-09	4.50E-11	0	0	0	-6.52798
340	5.00E-09	1.39E-08	0	0	0	0	-6.37424
340	6.00E-09	1.39E-08	0	0	0	0	-6.37419
340	7.00E-09	1.39E-08	0	0	0	0	-6.37414
340	8.00E-09	1.39E-08	1.03E-11	0	0	0	-6.37409
340	9.00E-09	1.39E-08	2.20E-11	0	0	0	-6.37405
340	1.00E-08	1.39E-08	3.16E-11	0	0	0	-6.374

	Conditions						
	1 mol H2O						
	1e-3 mol B(OH)3						
	6.636e-6 mol LiOH						
	3.535e-5 mol H2						
	2.25e-6 mol O2						
	7e-11 mol Ni						
T(C)	Input mol Fe	Mol-H[+](AQDD)	Mol-(NiO)(Fe2O3)(s)	Mol-O4Fe3(s)	Mol-Ni(s)	Mol-ONi(s)	pH
260	5.00E-09	6.55E-09	0	0	2.75E-12	0	-6.5754
260	6.00E-09	6.55E-09	7.81E-12	0	0.00E+00	0	-6.57537
260	7.00E-09	6.55E-09	2.38E-11	0	0.00E+00	0	-6.57534

260	8.00E-09	6.55E-09	3.33E-11	2.48E-11	0.00E+00	0	-6.57531
260	9.00E-09	6.55E-09	3.38E-11	3.58E-10	0	0	-6.57531
260	1.00E-08	6.55E-09	3.38E-11	6.91E-10	0	0	-6.57531
270	5.00E-09	6.19E-09	0	0	2.22E-12	0	-6.60596
270	6.00E-09	6.19E-09	1.34E-11	0	0	0	-6.60592
270	7.00E-09	6.19E-09	2.85E-11	0	0	0	-6.60589
270	8.00E-09	6.19E-09	3.84E-11	0	0	0	-6.60585
270	9.00E-09	6.19E-09	4.22E-11	9.60E-11	0	0	-6.60583
270	1.00E-08	6.19E-09	4.29E-11	4.29E-10	0	0	-6.60583
280	5.00E-09	5.83E-09	0	0	5.55E-13	0	-6.63821
280	6.00E-09	5.83E-09	1.62E-11	0	0	0	-6.63817
280	7.00E-09	5.83E-09	2.93E-11	0	0	0	-6.63813
280	8.00E-09	5.83E-09	3.91E-11	0	0	0	-6.63809
280	9.00E-09	5.83E-09	4.61E-11	0	0	0	-6.63804
280	1.00E-08	5.83E-09	4.86E-11	1.05E-10	0	0	-6.63802
290	5.00E-09	5.51E-09	0	0	0	0	-6.67052
290	6.00E-09	5.51E-09	1.74E-11	0	0	0	-6.67047
290	7.00E-09	5.51E-09	3.06E-11	0	0	0	-6.67043
290	8.00E-09	5.51E-09	4.01E-11	0	0	0	-6.67038
290	9.00E-09	5.51E-09	4.61E-11	0	0	0	-6.67034
290	1.00E-08	5.51E-09	5.17E-11	0	0	0	-6.67029
300	5.00E-09	5.25E-09	0	0	0	0	-6.69977
300	6.00E-09	5.26E-09	1.65E-11	0	0	0	-6.69972
300	7.00E-09	5.26E-09	3.08E-11	0	0	0	-6.69967
300	8.00E-09	5.26E-09	4.00E-11	0	0	0	-6.69962
300	9.00E-09	5.26E-09	4.75E-11	0	0	0	-6.69958
300	1.00E-08	5.26E-09	5.04E-11	0	0	0	-6.69953
310	5.00E-09	5.14E-09	0	0	0	0	-6.72
310	6.00E-09	5.14E-09	1.49E-11	0	0	0	-6.71995
310	7.00E-09	5.14E-09	2.91E-11	0	0	0	-6.7199
310	8.00E-09	5.14E-09	3.92E-11	0	0	0	-6.71985
310	9.00E-09	5.14E-09	4.51E-11	0	0	0	-6.7198
310	1.00E-08	5.14E-09	4.99E-11	0	0	0	-6.71975
320	5.00E-09	5.29E-09	0	0	0	0	-6.71947
320	6.00E-09	5.29E-09	8.75E-12	0	0	0	-6.71942
320	7.00E-09	5.29E-09	2.49E-11	0	0	0	-6.71937
320	8.00E-09	5.30E-09	3.54E-11	0	0	0	-6.71931
320	9.00E-09	5.30E-09	4.25E-11	0	0	0	-6.71926
320	1.00E-08	5.30E-09	4.78E-11	0	0	0	-6.71921
330	5.00E-09	6.12E-09	0	0	0	0	-6.67302

330	6.00E-09	6.12E-09	0	0	0	0	-6.67296
330	7.00E-09	6.12E-09	1.53E-11	0	0	0	-6.67291
330	8.00E-09	6.12E-09	2.90E-11	0	0	0	-6.67286
330	9.00E-09	6.12E-09	3.68E-11	0	0	0	-6.6728
330	1.00E-08	6.12E-09	4.30E-11	0	0	0	-6.67275
340	5.00E-09	9.23E-09	0	0	0	0	-6.51669
340	6.00E-09	9.23E-09	0	0	0	0	-6.51663
340	7.00E-09	9.23E-09	0	0	0	0	-6.51658
340	8.00E-09	9.23E-09	5.44E-12	0	0	0	-6.51653
340	9.00E-09	9.23E-09	1.76E-11	0	0	0	-6.51647
340	1.00E-08	9.23E-09	2.84E-11	0	0	0	-6.51642