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PRELIMINARY EVALUATION OF THE EFFECTS OF ALKALINE PLUME MIGRATION ON THE NEAR-FIELD ENVIRONMENT OF A HIGH-LEVEL WASTE GEOLOGIC REPOSITORY

The proposed U.S. Department of Energy (DOE) repository design in the past year for the Yucca Mountain (YM), Nevada, indicates that the use of cementitious materials in the form of concrete inverts and linings is being considered for the estimated 179 km of emplacement drifts. The use of these materials is in addition to the already planned use of cement in roadways for construction and emplacement ramps and service mains discussed in the Advanced Conceptual Design report (TRW Environmental Safety Systems, Inc., 1996). Although cement is used primarily for its structural (e.g., high compressive strength) and physical (e.g., low permeability) properties, its effect on the near-field chemical environment of a repository could be pronounced. Cements are extremely fine-grained, high-surface area materials containing somewhat soluble and thermodynamically metastable phases (e.g., a gel-like phase designated CSH because it contains Ca, Si, and H_2O) that are unstable with respect to crystalline cement phases. These properties and the partially interconnected pore network of the solids make these materials potentially reactive with the near-field environment and the engineered barrier system (EBS).

The chemistry of pore fluids in contact with hydrated cement phases is characterized by persistent alkaline pH (>10). Early in the evolution of cement pore fluids, the preferential partitioning of Na^+ and K^+ into the aqueous phase results in pH values of 13.5 or higher (Atkins and Glasser, 1992; Berner, 1992; Reardon, 1992). Subsequent cement degradation processes could dilute the concentration of alkalis resulting in a lower cement pore fluid pH, buffered at about 12.5 by dissolution of portlandite. Depletion of portlandite would cause the pH to decrease to approximately 11, controlled by dissolution of CSH, particularly the Ca/Si ratio of the gel (Berner, 1992). When dissolution of CSH is complete, the pH of the cement pore fluid would approach that of the groundwater pH.

Hyperalkaline cement pore water is chemically incompatible with silica, a major component of the proposed YM repository host rock unit Topopah Spring Tuff, which is comprised predominantly of alkali-feldspar, quartz, cristobalite, and tridymite (Bish et al., 1996). Thus, migration of the high pH cement pore water into the host rock is likely to result in strong alteration of the tuff. Because of the low silica concentration of the cement pore water, the host rock would begin to dissolve on contact with the hyperalkaline fluid (Lichtner and Eikenberg, 1995). As the host rock dissolved and the silica concentration increased, CSH and other calcium-silicate-hydrate phases would precipitate and clog the pore spaces. Precipitation of calcite would also occur as the low CO_2-high Ca cement pore fluid mixes with the ambient groundwater containing high CO_2 concentrations (Lichtner and Eikenberg, 1995; Steefel and Lichtner, 1994).

A troublesome scenario is the flow of a hyperalkaline fluid along fractures in the tuffaceous host rock of the proposed repository. Dissolution of the tuff could lead to widening of the fractures and enhancement of groundwater flow through the repository. Alternatively, precipitation of calcite and calcium-silicate-hydrates along the fracture/matrix interface could seal the fractures from the matrix producing isolated channels through which radionuclides could be

NOTE: Due To The relatively few number of pages, regular binding of This notebook is not possible; it is being bound with staples. BSon 7/28/97

transported relatively unimpeded by matrix diffusion. However, if sufficient amounts of calcite, CSH, and other calcium-silicate-hydrate phases are precipitated along fracture walls, reduction in fracture porosity/permeability or fracture plugging could result in diminished groundwater flow through the repository.

The relative importance of the above processes to repository performance is not known. No previous studies have been conducted regarding the effects of alkaline plume migration on the near-field environment of a geologic repository similar to YM. However, a study has been published regarding the spatial propagation of a hyperalkaline plume into a marl host rock, comprised predominantly of calcite, clays, and quartz, of a low-level radioactive waste repository (Lichtner and Eikenberg, 1995). The study, which used the geochemical transport model MPATH (Lichtner, 1992) indicated that interaction between a hyperalkaline plume released from a cement-based radioactive waste repository and a marl host rock could result in a rapid decrease in porosity of the host rock several meters from the repository due to precipitation of secondary phases, whereas porosity could increase at the interface of the marl host rock and the cement due to mineral dissolution.

OBJECTIVE:

To provide preliminary information regarding the potential effects of alkaline plume migration on the near-field environment of the proposed YM repository, calculations will be carried out simulating interactions between cement and tuff.

TECHNICAL APPROACH:

Calculations will be carried out describing cement-tuff interaction with pure diffusive transport of solute species. Three different cases will be considered. First, a hyperalkaline plume emanating from a cementitious body is allowed to react with a tuffaceous host rock such as found at YM. Second, the reverse situation of tuff pore water diffusing into the cement is analyzed. And third, interaction between cement and tuff is described by counter-diffusion across the cement-tuff contact. The reactive transport submodule GEM associated with the computer code MULTIFLO (Lichtner and Seth, 1997) is used to perform the calculations. Thermodynamic data for cement-related phases are taken from Atkins et al. (1994) and from Glasser[1]. pH-dependent kinetic rate laws for mineral reactions are used where data are available. The computer program, CEMCHEM, will be used to calculate the initial equilibrium phase assemblage in the cement material.

The GEM calculations will be done by Peter Lichtner and will not be documented in this laboratory notebook. Only the cement chemistry calculations will be documented here.

CEMENT CHEMISTRY CALCULATIONS

Anhydrous cement material contains many different phases, including alite (C_3S)[2], belite (C_2S), calcium aluminate (C_3A), calcium aluminum ferrite (C_4AF), and periclase (MgO) as the

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[1]Glasser, F.P. (Aberdeen University) July 29, 1996, Personal Communication.

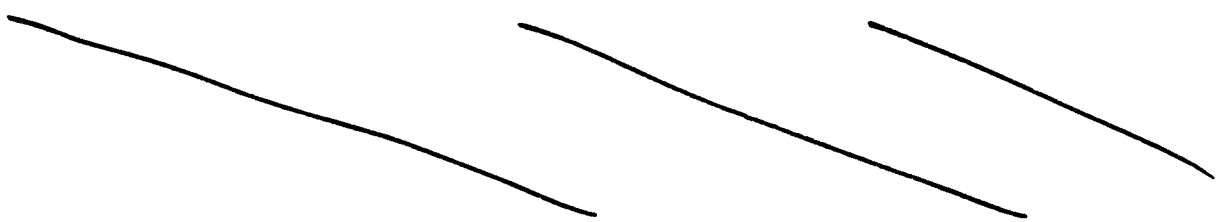
[2]Cement chemistry nomenclature: C — CaO, S — SiO_2, A — Al_2O_3, $\bar{S}$ — SO_3, H — H_2O, F — Fe_2O_3, M—MgO. CSH is a special case of this nomenclature and refers to a gel of variable Ca/Si ratio.

principal phases, and free lime (CaO), anhydrite ($CaSO_4$; $CaSO_4 \cdot 2H_2O$ is also present as a cement additive) and potassium and sodium sulfates (K_2SO_4 and Na_2SO_4) as minor phases. Upon addition of water, the soluble constituents—free lime, alkali sulfates, and anhydrite—dissolve and reprecipitate portlandite and gypsum. The bulk of sodium and potassium contributed from soluble alkali sulfates partition into the solution phase except for a portion, that is associated with CSH. The major phases—C_3S, C_2S, C_3A, C_4AF, and MgO—react more slowly but are transformed into hydrated cement phases, which include CSH, portlandite, hydrogarnet, ettringite, and monoaluminosulfate (Reardon, 1992). A typical cement paste with a water/cement ratio of 0.4 becomes about 40 percent hydrated within 1 day, 70 percent within 1 mo, and 80 percent after about 6 mo (Parrot and Killoh, 1984). Within 12 mo, 95-98 percent of a typical modern cement will have hydrated at ~15 to 25 °C, assuming that the moisture content of the system is conserved (Atkins and Glasser, 1992).

The composition of cement pore fluids, as well as the solid phase assemblage arising from hydration of cement, depend on the chemical composition of the initial anhydrous cement material. The exact composition of the cement mixture to be used at YM is not known at this time. However, it is expected that Portland cement will comprise one end-member of the mixture. Several variants of Portland cement are commercially available. Type II Portland cement has been used in constructing the concrete inverts for the Exploratory Shaft Facility. Recent DOE presentations indicate that Type V Portland cement, a formulation designed to be more resistant to attack by sulphate-bearing groundwaters, and possibly modified by addition of silica fume, may be used in making concrete ground supports for the repository emplacement drifts. However, for the purposes of this study, the cement material to be used in the calculations will be assumed to be Type II Portland cement with a typical composition listed in table 1.

Although Na and K concentrations in the Portland cement material are low (table 1), these are dominant cations in the pore fluid due to the absence of solid phase controls on these elements in a mature cement. Due to charge balance constraints, Na^+ and K^+ concentrations must be balanced by an equivalent concentration of anions, predominantly OH^-, giving rise to high pH. Most commercial cements have pore fluid pHs in the range 12.8-13.5; cements with high alkali contents may have pH up to 14, especially if formulated with low water/cement ratios (Atkins and Glasser, 1992). As pointed out earlier, the alkali content of the cement material determines the pH of cement porewater at early stages of cement hydration; thus, it also influences the solubility of other phases in the cement mixture. However, the alkalis are not firmly held and their concentration is reduced through cement degradation processes resulting in a decrease in pH.

Presently, there is no accurate model for predicting the influence of alkalis on cement chemistry (Atkins et al., 1992); alkali effect on the evolution of cement chemistry is a subject of current research.[3] Thus, for this study, alkali concentrations in the cement material will be set to zero. The Portland cement composition listed in column two of table 1 was normalized to zero alkali content to yield the values listed in column 3.



[3]Glasser, F.P. (Aberdeen University) May 8, 1997, Personal Communication.

Table 1. Composition of Type II Portland cement (taken from Clifton et al., 1991). Values in column 3 are normalized to an alkali-free composition.

Oxide Component	Weight Percent	Adjusted Weight Percent (Alkali-free)
SiO_2	21.0	22.0
Al_2O_3	4.4	4.6
Fe_2O_3	3.1	0.0
CaO	63.5	66.7
MgO	3.4	3.6
SO_3	2.94	3.1
Na_2O	0.26	0
K_2O	0.50	0
Loss on Ignition	1.00	0
TOTAL	100.1	100.0

A computer model, CEMCHEM (Atkins et al., 1992), will be used to calculate the equilibrium phase assemblage that results from hydration of alkali-free Portland cement composition given in table 1. CEMCHEM was developed by Aberdeen University researchers to predict the solid phase assemblage in a mature cement based on thermodynamic considerations and on results of phase equilibrium experiments (Atkins et al., 1992). The model converts the chemical composition of Portland cement and a blending agent, such as silica fume, fly ash, or blast furnace slag, into mole percent of constituent hydrated phases as a function of blending proportions. Calculations in this initial study will use 100 percent alkali-free Portland cement, but future analyses could include evaluation of the potential effect of silica fume or other additives on cement chemistry and alkaline plume migration.

5/14/97

INSTALLATION TESTING OF CEMCHEM, Version 1.0

The source code for a computer model, CEMCHEM Version 1.0, was taken from a report by Atkins et al., 1992 (Appendix 1) and retyped into a new electronic file. CEMCHEM 1.0 was developed by Aberdeen University researchers to predict the solid phase assemblage in a mature cement based on thermodynamic considerations and on results of phase equilibrium experiments (Atkins et al., 1992). The model converts the chemical composition of Portland cement and a blending agent, such as silica fume, fly ash, or blast furnace slag, into mole percent of constituent hydrated phases as a function of blending proportions. Input to the program is in the form of a

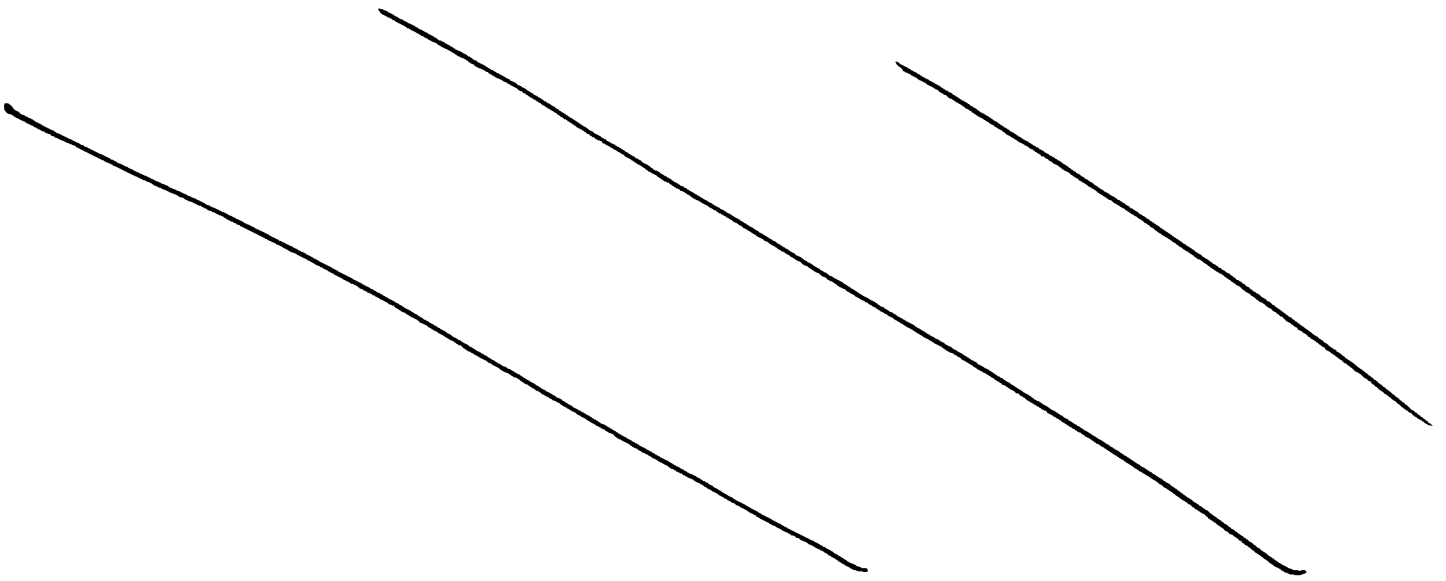
simple ASCII text file on which is specified the desired output filename (A8), followed by a line of comments and then the chemical compositions of the OPC and the blending agent in terms of weight percent of the oxides CaO, MgO, SiO_2, Al_2O_3, and SO_3 (five lines of 10X,2E10.3). The program generates two output files. The first (namefile.tab) tabulates the calculated phase proportions and compositions as a function of the proportion of OPC in the blend. This file is suitable for use with proprietary spreadsheet/graphics software. The second output file (namefile.lst) lists the results in a more readable form, documenting the blend compositions as well as the predicted phase assemblage for each calculation made, as the program varies the blend proportions.

The source code was compiled and linked using Lahey Fortran-77. The code was tested using a sample input file that came with the source code. The input file is as follows:

```
TRY1.OUT
        OPC       BFS
CAO      70.000    40.000
MGO       2.000    10.000
SIO2     20.000    40.000
AL2O3     5.000    10.000
SO3       3.000     0.000
```

On the following two pages is a tabulation of the calculated phase proportion and composition as a function of the OPC in the blend.

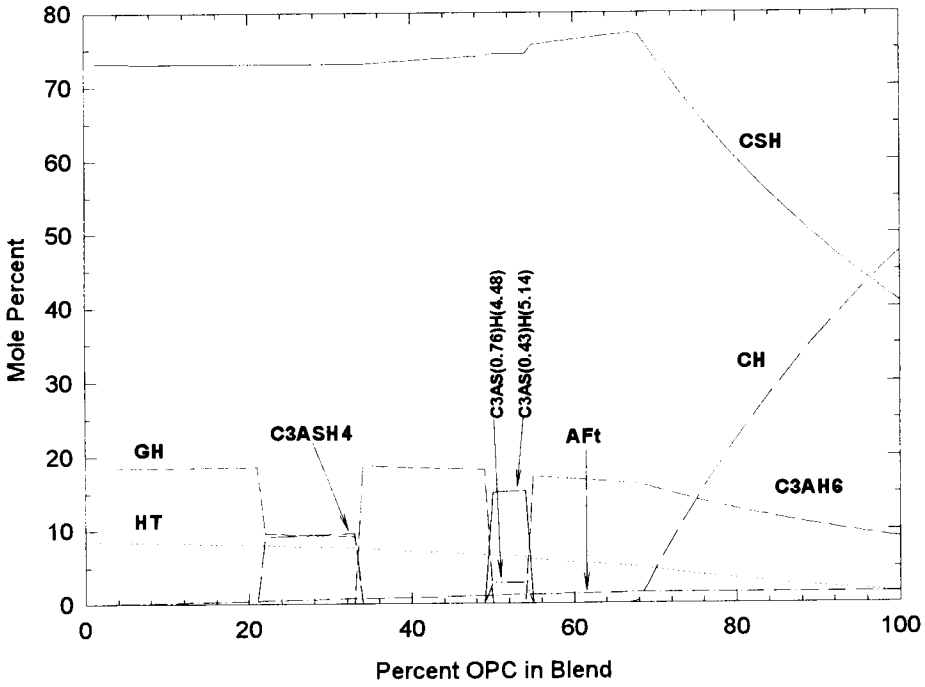
Following the table is a plot of the phase proportions of an OPC-BFS blend predicted by CEMCHEM (listed in the previous table). For comparison, a copy of the figure taken from Atkins et al. (1992) is pasted below it.



BLEND	HT	AFT	Ca/Si(CSH)	CSH	CH	GH	C3AH6	Si	H	C3AS(0.43)H(5.14)	C3A(0.76)H(4.48)	C3(1.0)H(4.0)	TOTAL
100	1.52	1.52	1.7	40.62	47.43	0	8.9	0	6	0	0	0	100.0
99	1.6	1.52	1.7	41.42	46.4	0	9.06	0	6	0	0	0	100.0
98	1.68	1.52	1.7	42.23	45.34	0	9.22	0	6	0	0	0	100.0
97	1.76	1.52	1.7	43.06	44.27	0	9.39	0	6	0	0	0	100.0
96	1.84	1.52	1.7	43.91	43.17	0	9.56	0	6	0	0	0	100.0
95	1.92	1.52	1.7	44.77	42.06	0	9.73	0	6	0	0	0	100.0
94	2	1.52	1.7	45.65	40.92	0	9.91	0	6	0	0	0	100.0
93	2.09	1.52	1.7	46.55	39.76	0	10.09	0	6	0	0	0	100.0
92	2.18	1.52	1.7	47.47	38.57	0	10.27	0	6	0	0	0	100.0
91	2.26	1.52	1.7	48.41	37.36	0	10.46	0	6	0	0	0	100.0
90	2.36	1.51	1.7	49.36	36.12	0	10.65	0	6	0	0	0	100.0
89	2.45	1.51	1.7	50.34	34.86	0	10.84	0	6	0	0	0	100.0
88	2.54	1.51	1.7	51.33	33.57	0	11.04	0	6	0	0	0	100.0
87	2.64	1.51	1.7	52.35	32.25	0	11.25	0	6	0	0	0	100.0
86	2.74	1.51	1.7	53.39	30.9	0	11.45	0	6	0	0	0	100.0
85	2.84	1.51	1.7	54.46	29.53	0	11.67	0	6	0	0	0	100.0
84	2.94	1.51	1.7	55.54	28.12	0	11.88	0	6	0	0	0	100.0
83	3.05	1.51	1.7	56.65	26.68	0	12.11	0	6	0	0	0	100.0
82	3.16	1.51	1.7	57.79	25.21	0	12.33	0	6	0	0	0	100.0
81	3.27	1.5	1.7	58.95	23.71	0	12.56	0	6	0	0	0	100.0
80	3.38	1.5	1.7	60.14	22.17	0	12.8	0	6	0	0	0	100.0
79	3.5	1.5	1.7	61.36	20.59	0	13.05	0	6	0	0	0	100.0
78	3.62	1.5	1.7	62.61	18.97	0	13.3	0	6	0	0	0	100.0
77	3.74	1.5	1.7	63.89	17.32	0	13.55	0	6	0	0	0	100.0
76	3.86	1.5	1.7	65.2	15.63	0	13.81	0	6	0	0	0	100.0
75	3.99	1.5	1.7	66.54	13.89	0	14.08	0	6	0	0	0	100.0
74	4.12	1.5	1.7	67.92	12.11	0	14.36	0	6	0	0	0	100.0
73	4.26	1.49	1.7	69.33	10.28	0	14.64	0	6	0	0	0	100.0
72	4.4	1.49	1.7	70.77	8.41	0	14.93	0	6	0	0	0	100.0
71	4.54	1.49	1.7	72.26	6.49	0	15.22	0	6	0	0	0	100.0
70	4.68	1.49	1.7	73.78	4.51	0	15.53	0	6	0	0	0	100.0
69	4.83	1.49	1.7	75.35	2.49	0	15.84	0	6	0	0	0	100.0
68	4.98	1.49	1.7	76.96	0.41	0	16.16	0	6	0	0	0	100.0
67	5.08	1.47	1.69	77.17	0	0	16.28	0.03	5.95	0	0	0	100.0
66	5.15	1.44	1.67	77.05	0	0	16.35	0.06	5.88	0	0	0	100.0
65	5.23	1.42	1.66	76.93	0	0	16.42	0.09	5.82	0	0	0	100.0
64	5.31	1.39	1.64	76.81	0	0	16.5	0.12	5.75	0	0	0	100.0
63	5.38	1.37	1.63	76.68	0	0	16.57	0.16	5.69	0	0	0	100.0
62	5.46	1.34	1.61	76.55	0	0	16.64	0.19	5.62	0	0	0	100.0
61	5.54	1.32	1.6	76.43	0	0	16.72	0.22	5.55	0	0	0	100.0
60	5.61	1.3	1.58	76.3	0	0	16.8	0.26	5.49	0	0	0	100.0
59	5.69	1.27	1.57	76.16	0	0	16.87	0.29	5.42	0	0	0	100.0
58	5.77	1.25	1.55	76.03	0	0	16.95	0.32	5.35	0	0	0	100.0
57	5.85	1.23	1.54	75.89	0	0	17.04	0.36	5.29	0	0	0	100.0
56	5.93	1.2	1.53	75.75	0	0	17.12	0.39	5.22	0	0	0	100.0
55	6	1.18	1.51	75.61	0	0	17.2	0.42	5.15	0	0	0	100.0
54	6.36	1.21	1.5	74.37	0	0	0	0	6	2.85	15.22	0	100.0
53	6.4	1.18	1.5	74.37	0	0	0	0	6	2.87	15.18	0	100.0
52	6.45	1.15	1.5	74.37	0	0	0	0	6	2.88	15.15	0	100.0
51	6.49	1.12	1.5	74.38	0	0	0	0	6	2.9	15.11	0	100.0
50	6.53	1.09	1.5	74.38	0	0	0	0	6	2.92	15.07	0	100.0
49	6.65	1.07	1.48	74.09	0	0	18.18	0.77	4.46	0	0	0	100.0

48	6.71	1.05	1.46	74.03	0	0	18.21	0.78	4.43	0	0	0	100.0
47	6.77	1.02	1.44	73.97	0	0	18.24	0.8	4.41	0	0	0	100.0
46	6.83	0.99	1.42	73.91	0	0	18.27	0.81	4.38	0	0	0	100.0
45	6.88	0.97	1.4	73.84	0	0	18.3	0.82	4.35	0	0	0	100.0
44	6.94	0.94	1.39	73.78	0	0	18.33	0.84	4.32	0	0	0	100.0
43	7	0.92	1.37	73.71	0	0	18.37	0.85	4.29	0	0	0	100.0
42	7.06	0.89	1.35	73.64	0	0	18.4	0.87	4.26	0	0	0	100.0
41	7.12	0.87	1.33	73.58	0	0	18.44	0.88	4.24	0	0	0	100.0
40	7.18	0.84	1.31	73.5	0	0	18.47	0.9	4.2	0	0	0	100.0
39	7.24	0.82	1.29	73.43	0	0	18.51	0.91	4.17	0	0	0	100.0
38	7.3	0.8	1.28	73.36	0	0	18.55	0.93	4.14	0	0	0	100.0
37	7.36	0.77	1.26	73.28	0	0	18.59	0.94	4.11	0	0	0	100.0
36	7.42	0.75	1.24	73.21	0	0	18.63	0.96	4.08	0	0	0	100.0
35	7.48	0.73	1.22	73.13	0	0	18.67	0.98	4.05	0	0	0	100.0
34	7.54	0.7	1.21	73.05	0	0	18.71	0.99	4.01	0	0	0	100.0
33	7.58	0.68	1.2	73.02	0	9.1	0	0	6	0	0	9.57	100.0
32	7.62	0.66	1.2	73.02	0	9.2	0	0	6	0	0	9.52	100.0
31	7.65	0.63	1.2	73.02	0	9.2	0	0	6	0	0	9.47	100.0
30	7.69	0.61	1.2	73.03	0	9.3	0	0	6	0	0	9.42	100.1
29	7.72	0.58	1.2	73.03	0	9.3	0	0	6	0	0	9.37	100.0
28	7.76	0.56	1.2	73.03	0	9.3	0	0	6	0	0	9.33	100.0
27	7.79	0.54	1.2	73.04	0	9.4	0	0	6	0	0	9.28	100.1
26	7.82	0.51	1.2	73.04	0	9.4	0	0	6	0	0	9.23	100.0
25	7.86	0.49	1.2	73.04	0	9.4	0	0	6	0	0	9.19	100.0
24	7.89	0.47	1.2	73.05	0	9.5	0	0	6	0	0	9.15	100.1
23	7.92	0.45	1.2	73.05	0	9.5	0	0	6	0	0	9.1	100.0
22	7.95	0.42	1.2	73.05	0	9.5	0	0	6	0	0	9.06	100.0
21	7.98	0.4	1.2	73.06	0	18.6	0	0	6	0	0	0	100.0
20	8.02	0.38	1.18	73.06	0	18.5	0	0	6	0	0	0	100.0
19	8.05	0.36	1.16	73.06	0	18.5	0	0	6	0	0	0	100.0
18	8.08	0.34	1.14	73.06	0	18.5	0	0	6	0	0	0	100.0
17	8.11	0.32	1.12	73.07	0	18.5	0	0	6	0	0	0	100.0
16	8.14	0.3	1.1	73.07	0	18.5	0	0	6	0	0	0	100.0
15	8.17	0.28	1.09	73.07	0	18.5	0	0	6	0	0	0	100.0
14	8.19	0.26	1.07	73.07	0	18.5	0	0	6	0	0	0	100.0
13	8.22	0.24	1.05	73.08	0	18.5	0	0	6	0	0	0	100.0
12	8.25	0.22	1.03	73.08	0	18.4	0	0	6	0	0	0	100.0
11	8.28	0.2	1.02	73.08	0	18.4	0	0	6	0	0	0	100.0
10	8.31	0.18	1	73.08	0	18.4	0	0	6	0	0	0	100.0
9	8.34	0.16	0.98	73.09	0	18.4	0	0	6	0	0	0	100.0
8	8.36	0.14	0.97	73.09	0	18.4	0	0	6	0	0	0	100.0
7	8.39	0.12	0.95	73.09	0	18.4	0	0	6	0	0	0	100.0
6	8.42	0.11	0.93	73.09	0	18.4	0	0	6	0	0	0	100.0
5	8.44	0.09	0.92	73.1	0	18.4	0	0	6	0	0	0	100.0
4	8.47	0.07	0.9	73.1	0	18.4	0	0	6	0	0	0	100.0
3	8.5	0.05	0.89	73.1	0	18.4	0	0	6	0	0	0	100.1
2	8.52	0.03	0.87	73.1	0	18.3	0	0	6	0	0	0	100.0
1	8.55	0.02	0.85	73.11	0	18.3	0	0	6	0	0	0	100.0

CEMCHEM model of OPC-BFS blend



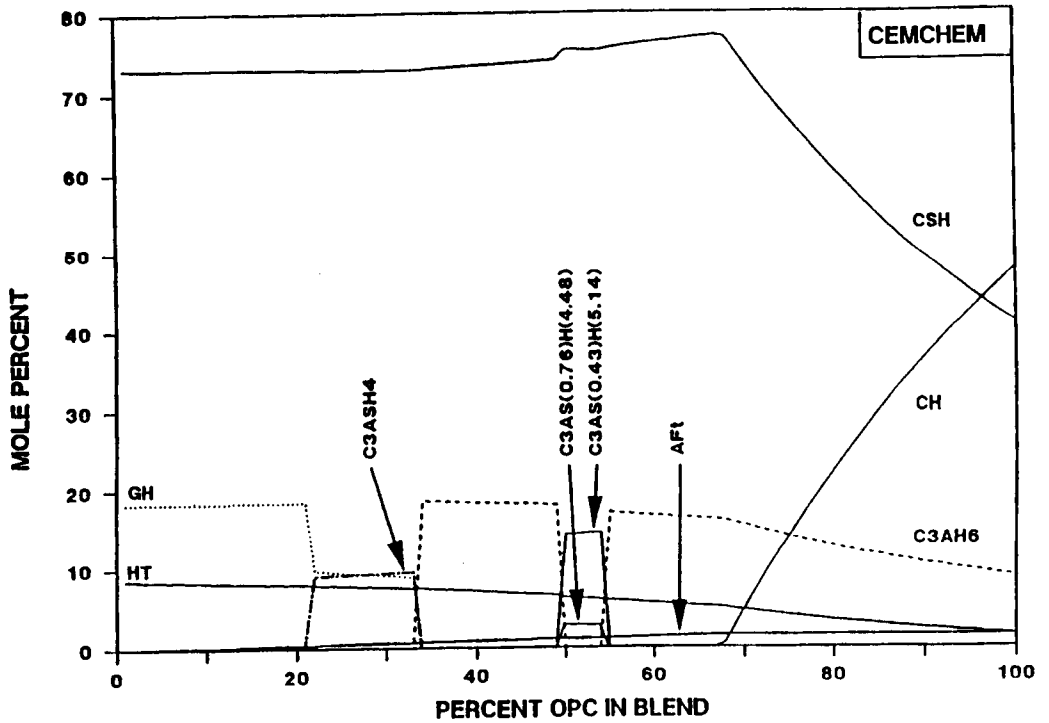


Figure 5.2a Predicted phase proportions from the CEMCHEM model of an OPC-BFS blend.

5/19/97

CALCULATION OF EQUILIBRIUM PHASE ASSEMBLAGE FOR ALKALI-FREE OPC

Using CEMCHEM, Version 1.0, the equilibrium phase assemblage for a cement blend of alkali-free portland cement (with oxide composition listed in column 3 of table 1) and blast furnace slag (BFS) was calculated as a function of the blend composition. BFS was assumed to be 40.0% SiO_2, 40.0% CaO, 10.0% Al_2O_3, and 10.0% MgO (Atkins et al., 1992).

INPUT FILE for CEMCHEM:

```
Clifton OPC
        OPC       BFS
CAO      66.700    40.000
MGO       3.600    10.000
SIO2     22.000    40.000
AL2O3     4.600    10.000
SO3       3.100     0.000
```

OUTPUT FILE for CEMCHEM:

```
*********************************************
*                                           *
*       CEMCHEM version :  1.0          *
*                                           *
*       Input datafile  :Clifton        *
*                                           *
*********************************************
```

BLEND	HT	AFT	Ca/Si(CSH)	CSH	CH	GH	C3AH6	Si	H	C3AS(0.43)H(5.14)	C3A(0.76)H(4.48)	C3(1.0)H(4.0)
100.00	2.87	1.65	1.70	46.84	41.63	0.0	7.00	0.00	6.00	0.00	0.00	0.00
99.00	2.95	1.65	1.70	47.68	40.55	0.0	7.17	0.00	6.00	0.00	0.00	0.00
98.00	3.03	1.65	1.70	48.53	39.45	0.0	7.34	0.00	6.00	0.00	0.00	0.00
97.00	3.12	1.65	1.70	49.39	38.33	0.0	7.51	0.00	6.00	0.00	0.00	0.00
96.00	3.20	1.65	1.70	50.28	37.19	0.0	7.69	0.00	6.00	0.00	0.00	0.00
95.00	3.29	1.65	1.70	51.18	36.02	0.0	7.87	0.00	6.00	0.00	0.00	0.00
94.00	3.37	1.64	1.70	52.10	34.83	0.0	8.06	0.00	6.00	0.00	0.00	0.00
93.00	3.46	1.64	1.70	53.03	33.61	0.0	8.25	0.00	6.00	0.00	0.00	0.00
92.00	3.55	1.64	1.70	53.99	32.37	0.0	8.44	0.00	6.00	0.00	0.00	0.00
91.00	3.64	1.64	1.70	54.97	31.11	0.0	8.64	0.00	6.00	0.00	0.00	0.00
90.00	3.74	1.64	1.70	55.96	29.82	0.0	8.84	0.00	6.00	0.00	0.00	0.00
89.00	3.84	1.64	1.70	56.98	28.50	0.0	9.05	0.00	6.00	0.00	0.00	0.00
88.00	3.93	1.64	1.70	58.02	27.15	0.0	9.26	0.00	6.00	0.00	0.00	0.00
87.00	4.03	1.64	1.70	59.08	25.77	0.0	9.47	0.00	6.00	0.00	0.00	0.00
86.00	4.14	1.64	1.70	60.17	24.37	0.0	9.69	0.00	6.00	0.00	0.00	0.00
85.00	4.24	1.63	1.70	61.28	22.93	0.0	9.91	0.00	6.00	0.00	0.00	0.00
84.00	4.35	1.63	1.70	62.41	21.46	0.0	10.14	0.00	6.00	0.00	0.00	0.00
83.00	4.46	1.63	1.70	63.57	19.96	0.0	10.38	0.00	6.00	0.00	0.00	0.00
82.00	4.57	1.63	1.70	64.76	18.42	0.0	10.62	0.00	6.00	0.00	0.00	0.00

81.00	4.69	1.63	1.70	65.97	16.85	0.0	10.86	0.00	6.00	0.00	0.00	0.00
80.00	4.80	1.63	1.70	67.21	15.24	0.0	11.11	0.00	6.00	0.00	0.00	0.00
79.00	4.93	1.63	1.70	68.48	13.60	0.0	11.37	0.00	6.00	0.00	0.00	0.00
78.00	5.05	1.62	1.70	69.78	11.91	0.0	11.63	0.00	6.00	0.00	0.00	0.00
77.00	5.17	1.62	1.70	71.12	10.18	0.0	11.90	0.00	6.00	0.00	0.00	0.00
76.00	5.30	1.62	1.70	72.48	8.42	0.0	12.18	0.00	6.00	0.00	0.00	0.00
75.00	5.44	1.62	1.70	73.88	6.60	0.0	12.46	0.00	6.00	0.00	0.00	0.00
74.00	5.57	1.62	1.70	75.31	4.75	0.0	12.75	0.00	6.00	0.00	0.00	0.00
73.00	5.71	1.62	1.70	76.78	2.84	0.0	13.05	0.00	6.00	0.00	0.00	0.00
72.00	5.85	1.62	1.70	78.29	0.89	0.0	13.35	0.00	6.00	0.00	0.00	0.00
71.00	5.95	1.60	1.69	78.90	0.00	0.0	13.55	0.02	5.96	0.00	0.00	0.00
70.00	6.00	1.57	1.68	78.78	0.00	0.0	13.65	0.05	5.90	0.00	0.00	0.00
69.00	6.06	1.55	1.66	78.65	0.00	0.0	13.75	0.08	5.83	0.00	0.00	0.00
68.00	6.11	1.52	1.64	78.51	0.00	0.0	13.85	0.12	5.77	0.00	0.00	0.00
67.00	6.17	1.50	1.63	78.38	0.00	0.0	13.96	0.15	5.70	0.00	0.00	0.00
66.00	6.22	1.47	1.62	78.25	0.00	0.0	14.06	0.18	5.64	0.00	0.00	0.00
65.00	6.28	1.44	1.60	78.11	0.00	0.0	14.17	0.21	5.57	0.00	0.00	0.00
64.00	6.34	1.42	1.59	77.97	0.00	0.0	14.27	0.25	5.51	0.00	0.00	0.00
63.00	6.39	1.39	1.57	77.83	0.00	0.0	14.38	0.28	5.44	0.00	0.00	0.00
62.00	6.45	1.37	1.56	77.69	0.00	0.0	14.49	0.31	5.37	0.00	0.00	0.00
61.00	6.51	1.35	1.54	77.55	0.00	0.0	14.60	0.35	5.31	0.00	0.00	0.00
60.00	6.56	1.32	1.53	77.40	0.00	0.0	14.71	0.38	5.24	0.00	0.00	0.00
59.00	6.62	1.30	1.52	77.25	0.00	0.0	14.83	0.41	5.18	0.00	0.00	0.00
58.00	6.95	1.33	1.50	76.18	0.00	0.0	0.00	0.00	6.00	2.55	12.99	0.00
57.00	6.98	1.29	1.50	76.14	0.00	0.0	0.00	0.00	6.00	2.57	13.01	0.00
56.00	7.01	1.26	1.50	76.10	0.00	0.0	0.00	0.00	6.00	2.59	13.03	0.00
55.00	7.03	1.23	1.50	76.06	0.00	0.0	0.00	0.00	6.00	2.62	13.05	0.00
54.00	7.06	1.20	1.50	76.03	0.00	0.0	0.00	0.00	6.00	2.64	13.07	0.00
53.00	7.15	1.19	1.49	75.75	0.00	0.0	15.91	0.77	4.47	0.00	0.00	0.00
52.00	7.20	1.16	1.47	75.67	0.00	0.0	15.98	0.78	4.44	0.00	0.00	0.00
51.00	7.24	1.13	1.45	75.58	0.00	0.0	16.05	0.79	4.42	0.00	0.00	0.00
50.00	7.28	1.11	1.43	75.49	0.00	0.0	16.13	0.80	4.39	0.00	0.00	0.00
49.00	7.32	1.08	1.41	75.40	0.00	0.0	16.20	0.82	4.37	0.00	0.00	0.00
48.00	7.36	1.05	1.40	75.31	0.00	0.0	16.27	0.83	4.34	0.00	0.00	0.00
47.00	7.40	1.03	1.38	75.22	0.00	0.0	16.35	0.84	4.31	0.00	0.00	0.00
46.00	7.44	1.00	1.36	75.13	0.00	0.0	16.42	0.86	4.29	0.00	0.00	0.00
45.00	7.48	0.98	1.34	75.04	0.00	0.0	16.50	0.87	4.26	0.00	0.00	0.00
44.00	7.53	0.95	1.33	74.95	0.00	0.0	16.58	0.88	4.23	0.00	0.00	0.00
43.00	7.57	0.93	1.31	74.85	0.00	0.0	16.65	0.90	4.20	0.00	0.00	0.00
42.00	7.61	0.90	1.29	74.76	0.00	0.0	16.73	0.91	4.17	0.00	0.00	0.00
41.00	7.65	0.88	1.28	74.66	0.00	0.0	16.81	0.93	4.15	0.00	0.00	0.00
40.00	7.70	0.86	1.26	74.56	0.00	0.0	16.89	0.94	4.12	0.00	0.00	0.00
39.00	7.74	0.83	1.24	74.46	0.00	0.0	16.97	0.96	4.09	0.00	0.00	0.00
38.00	7.78	0.81	1.23	74.36	0.00	0.0	17.05	0.97	4.06	0.00	0.00	0.00
37.00	7.83	0.78	1.21	74.26	0.00	0.0	17.13	0.99	4.03	0.00	0.00	0.00
36.00	7.87	0.76	1.20	74.16	0.00	8.4	0.00	0.00	6.00	0.00	0.00	8.79
35.00	7.89	0.74	1.20	74.13	0.00	8.5	0.00	0.00	6.00	0.00	0.00	8.77
34.00	7.91	0.71	1.20	74.10	0.00	8.5	0.00	0.00	6.00	0.00	0.00	8.75
33.00	7.94	0.69	1.20	74.06	0.00	8.6	0.00	0.00	6.00	0.00	0.00	8.74
32.00	7.96	0.66	1.20	74.03	0.00	8.6	0.00	0.00	6.00	0.00	0.00	8.72
31.00	7.98	0.64	1.20	73.99	0.00	8.7	0.00	0.00	6.00	0.00	0.00	8.71
30.00	8.00	0.61	1.20	73.96	0.00	8.7	0.00	0.00	6.00	0.00	0.00	8.69
29.00	8.02	0.59	1.20	73.93	0.00	8.8	0.00	0.00	6.00	0.00	0.00	8.68
28.00	8.05	0.57	1.20	73.90	0.00	8.8	0.00	0.00	6.00	0.00	0.00	8.66
27.00	8.07	0.54	1.20	73.86	0.00	8.9	0.00	0.00	6.00	0.00	0.00	8.65
26.00	8.09	0.52	1.20	73.83	0.00	8.9	0.00	0.00	6.00	0.00	0.00	8.63
25.00	8.11	0.50	1.20	73.80	0.00	9.0	0.00	0.00	6.00	0.00	0.00	8.62
24.00	8.13	0.48	1.20	73.77	0.00	9.0	0.00	0.00	6.00	0.00	0.00	8.61

23.00	8.15	0.45	1.19	73.74	0.00	17.7	0.00	0.00	6.00	0.00	0.00	0.00
22.00	8.17	0.43	1.18	73.71	0.00	17.7	0.00	0.00	6.00	0.00	0.00	0.00
21.00	8.19	0.41	1.16	73.68	0.00	17.7	0.00	0.00	6.00	0.00	0.00	0.00
20.00	8.21	0.39	1.14	73.65	0.00	17.8	0.00	0.00	6.00	0.00	0.00	0.00
19.00	8.23	0.37	1.13	73.62	0.00	17.8	0.00	0.00	6.00	0.00	0.00	0.00
18.00	8.25	0.35	1.11	73.59	0.00	17.8	0.00	0.00	6.00	0.00	0.00	0.00
17.00	8.27	0.33	1.09	73.56	0.00	17.8	0.00	0.00	6.00	0.00	0.00	0.00
16.00	8.29	0.31	1.08	73.53	0.00	17.9	0.00	0.00	6.00	0.00	0.00	0.00
15.00	8.31	0.28	1.06	73.50	0.00	17.9	0.00	0.00	6.00	0.00	0.00	0.00
14.00	8.33	0.26	1.05	73.48	0.00	17.9	0.00	0.00	6.00	0.00	0.00	0.00
13.00	8.34	0.24	1.03	73.45	0.00	18.0	0.00	0.00	6.00	0.00	0.00	0.00
12.00	8.36	0.22	1.01	73.42	0.00	18.0	0.00	0.00	6.00	0.00	0.00	0.00
11.00	8.38	0.20	1.00	73.39	0.00	18.0	0.00	0.00	6.00	0.00	0.00	0.00
10.00	8.40	0.19	0.98	73.37	0.00	18.0	0.00	0.00	6.00	0.00	0.00	0.00
9.00	8.42	0.17	0.97	73.34	0.00	18.1	0.00	0.00	6.00	0.00	0.00	0.00
8.00	8.44	0.15	0.95	73.31	0.00	18.1	0.00	0.00	6.00	0.00	0.00	0.00
7.00	8.45	0.13	0.94	73.29	0.00	18.1	0.00	0.00	6.00	0.00	0.00	0.00
6.00	8.47	0.11	0.92	73.26	0.00	18.2	0.00	0.00	6.00	0.00	0.00	0.00
5.00	8.49	0.09	0.91	73.23	0.00	18.2	0.00	0.00	6.00	0.00	0.00	0.00
4.00	8.50	0.07	0.90	73.21	0.00	18.2	0.00	0.00	6.00	0.00	0.00	0.00
3.00	8.52	0.05	0.88	73.18	0.00	18.2	0.00	0.00	6.00	0.00	0.00	0.00
2.00	8.54	0.04	0.87	73.16	0.00	18.3	0.00	0.00	6.00	0.00	0.00	0.00
1.00	8.55	0.02	0.85	73.13	0.00	18.3	0.00	0.00	6.00	0.00		

SUMMARY RESULT FOR TWO CEMENT BLEND COMPOSITIONS

Table 2. Equilibrium phase assemblage for a cement blend of ordinary portland cement (OPC) and blast furnace slag (BFS) calculated using the CEMCHEM code.*

CEMENT BLEND (%OPC)	Hydrotalcite	Ettringite	Ca/S (CSH)	C-S-H	Portlandite	Hydrogarnet
100	2.87	1.65	1.7	46.84	41.63	7
70	6	1.57	1.68	78.78	0	13.65

*OPC is assumed to have the following composition: 22.0% SiO_2, 66.7% CaO, 4.6% Al_2O_3, 3.6% MgO, and 3.1% SO_3. BFS is assumed to be 40.0% SiO_2, 40.0% CaO, 10.0% Al_2O_3, and 10.0% MgO.

The equilibrium phase assemblage calculated for the alkali-free Portland cement is as follows: 46.84 mole percent CSH, 41.63 mole percent portlandite, 7.0 mole percent hydrogarnet, 2.87 mole percent hydrotalcite, and 1.65 mole percent ettringite. The derived Ca/Si ratio for the CSH phase is 1.7.

7/23/97

The results of this preliminary study (particularly the GEM results) are reported in a report "Evaluation of Cement-Water Interactions Letter Report" (Intermediate Milestone 5708-561-750) submitted to NRC on July 23, 1997, under the title "Preliminary Evaluation of the Effects of

Alkaline Plume Migration on the Near-Field Environment of a HLW Geologic Repository." The authors of the report are P. Lichtner, R. Pabalan, and C. Steefel (consultant).

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