The structural equilibria in heterogeneous silicate systems: On the hypothesis to practice

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The structural disproportionation equilibria are known in the simple silicate systems and glasses [1]. So, very likely, the simulation of phase equilibria in heterogeneous silicate systems should also include the structural melt equilibria modelling. This idea starts from the concept that increasing of some sort of structural units promotes the crystallization of corresponding crystalline phase, while the structural equilibrium guaranties rheological melt stability.

Some heterogeneous and structural equilibria, occurring in known reaction points [2], [3], are shown (Table 1).

These equilibria are sensitive to pressure. Its may be used for modeling the system behaviour in dynamics, including mineral dilution process and the fluid-melt interaction. The heterogeneous equilibria can be used for determination of the melt species thermodynamic properties

T°C	Heterogeneous and structural equilibria	ΔrH kJ	ΔrG kJ	K
1558	Fo + SiO_2 = En $Q^0 + Q^4 = 2Q^2$	-8.94	-9.85	1.91
1270	An + Ol = Di + + $MgAl_2O_4$ + SiO_2 $4Q^4 + Q^0 = 2Q^2 + 2Q^4 + Q^4$	269	0.21	0.98
1317	An + Ol = Sp + + $CaMgSi2O6$ + $SiO2$ $Q^0 + Q^4 = 2Q^2$ (abr.)	149	28.5	0.12
1232	3An+2Geh+4Ol= =5Di+2CaTsch.Px+3Sp $Q^4 + 2Q^1 + 2Q^0 = 7Q^2$ (abr.)	-102	-2.27	1.20
	An + $Na_2Si_2O_5$ + $3SiO_2$ = 2Ab + $CaSiO_3$ $2Q^3 = Q^4 + Q^2$ (abr.)			

Table 1: The enthalpy change ΔrH, Gibbs function change ΔrG and constants K of equilibria are calculated using thermodynamic data [4]. The melt species are italicized.

[1] Mysen (1995) *GCA* **59**, 455–474. [2] O'Xara&Biggar (1969) *Am. J. Sci*. **S.V. 267-A**, 364–390. [3] Osborn&Tait (1952) *Am. J. Sci*. **B.V.** 413–433. [4] Holland&Powell (1998) *J. metamorphic Geol*.**16**, 309–343.

Cr-rich smectite from a natural analogue of Suweileh cementitious repository, Jordan

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A green smectite from the new cementitious natural analogue of Suweileh area, Jordan acts as a sink for heavy metals. The Cr-rich smectite is found along bedding planes in sedimentary phosphatic limestone and marl of upper Cretaceous age at a distance of a marble zone (cement zone). The mineralogy of the marble is comparable to that of cement clinker and the hydrated cement products. The original rocks were highly bituminous and similar to their stratigraphic equivalent in central Jordan that was formed by spontaneous combustion of the bituminous precursor. Most of the metamorphic rocks are massive marbles similar in composition to Portland cement. The structural formula of Suweileh smectite is calculated as follows:

$(Ca_{0.30} Na_{0.23}) (Al_{0.47} Cr_{0.63} Fe_{0.13} Mg_{0.66} Zn_{0.06} Ti_{0.03}) (Si_{3.88} Al_{0.12}) O_{10} (OH)_2$
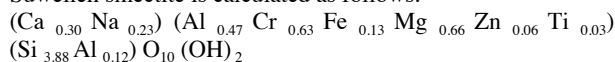
The scanning electron micrographs have indicated continuous and uninterrupted smectite crystal growth. Cr-smectite was precipitated as a secondary phase in voids and fissures after the metamorphic event. The infiltration of highly alkaline water through the combusted zone has led to the leaching of Cr^{3+} ion and the precipitation of Cr-rich smectite in the marly beds of the Phosphorite Unit.

The presence of Cr-rich smectites may suggest the use of Suweileh outcrops as analogues with the repository disturbed zone. Cr-Smectite is expected to be a sink for the alteration products as radionuclides and heavy metals in the late stage evolution of a high pH plume.