o.m6.p1 Modelling of Alite: an industrial challenge.
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Unhydrated cement is essentially made of a synthetic compound, designated as clinker, obtained by firing a mixture of limestone (~80%) and clay (~20%) at high temperature (~1450°C) in a cement plant kiln. The combined effects of various fuels, the mineralogy of the raw meal extracted from quarries and the thermal conditions inside the kiln and during the cooling process, play an important role in the crystalline form of each of the phases.

Among the four main compounds which constitute clinker, alite, in a concentration ranging from 40 to 70%, is a tricalcic silicate Ca_3SiO_5which has trapped various impurities: MgO, Fe_2O_3, Na_2O, K_2O, SO_3,… Depending on the nature of these impurities together with the thermal conditions, one can find various high temperature phases of pure tricalcic silicate. Among the seven known polymorphic forms of alite, those most frequently ones found in clinker are the so-called M1 and M3 phases. While the structure of the M3 form has been understood since the 80's thanks to single crystal studies, the structure of the M1 form remained unknown until recent work[1].

The elementary analysis of clinker is traditionally obtained by X-ray fluorescence. Thereby, using Bogue's stoechiometric calculation, one can obtain the relative concentration of the various oxides, among which the rate of non-combined CaO is an important parameter for the monitoring of the kiln. But this elementary analysis produces only a rough estimation of the concentrations of the species and no information at all on the very nature of their polymorphic form.

Based on a proper modelling of silicate phases and taking into account all the other phases present in the clinker, X-ray powder diffraction, combined with the exploitation of diffractograms by the Rietveld method, makes it possible to carry out quantification and thereby to monitor the clinker variability. The accurate structural information obtained from the processing of the diffractograms may contribute to the building of data bases which, if correctly used, would provide the elements leading to a better understanding of the reactivity of clinkers and ultimately lead to improvement of the final product: cement. Data processing capacities and the use of appropriate refinement software now make it possible to carry out a strict control over clinker and cement production at the factory level.

[1] This issue : M.N. de Noirfontaine et al.