XRD based quantification methods of
CO$_2$-reduced building materials - Cements, Calcined Clay, Pozzolanes and Limestone

Herbert Pöllmann

herbert.poellmann@geo.uni-halle.de

New cementitious materials came into focus of manufacture of cement due to their probable effect on CO$_2$-reduction. As many industrial residues, like slags and ashes, are already used and their amount would not be sufficient for supplying the complete cement chain, other natural materials came into focus. As many of these supplementary cementitious materials influence and change the hydration behaviour of the classic cements it is necessary to characterize and determine their reactions behaviour. Primarily mainly interground or interblended cements came into focus, but also complete new cement clinkers are under investigation.

Mainly nowadays people are interested in calcined clay and typical pozzolanes from sedimentary and igneous origin. As these supplementary cementitious materials contain high amounts of amorphous materials the determination methods must be adapted. Sometimes it is even necessary to distinguish between reactive amorphous and unreactive amorphous contents.

As these SCM´s do not contain CO$_2$, they are of high importance in building chemistry due to their favourable effect of reducing CO$_2$ during manufacturing.

X-ray methods can be used to quantify these materials mineralogically. The following methods will be demonstrated for cements, calcined clay, pozzolanes and limestone additions using binary up to quaternary systems.

1. Quantification using Rietveld method, Rietveld method with internal standard for amorphous contents
2. Cluster analysis for summarizing potentially similar reaction behaviour of the complex mixtures
3. PCA, Principal component analysis for similar hydraulic reactions
4. PLSR (partial Least Squares Refinement) methodology for different mixtures
5. PONCS (Partial or not known crystal structure) method for special quantifications in addition to Rietveld methodology

Using the different methods, also including typical physical and chemical methods, it is possible to get excellent results on the complex mixtures and also to predict their properties similar as it is possible already for classical cement materials.

It is now possible to classify these large data sets using cluster analysis into clusters with similar properties and concentrate on more definite calculations with Rietveld and PONKCs for the more interesting and demanding samples. For long term studies it is also appropriate to use PLSR calculations and calibrations as these methods allow a very fast and reliable quantification on already known samples.

Literature

Galluccio S, Beirau T, Pöllmann H. Maximization of the reuse of industrial residues for the production of eco-friendly CSA-belite clinker. Construction and Building Materials 2019,, 208, 250-257

Galluccio, S.; Pöllmann, H.: „Quantifications of cements composed of OPC, Calcined Clay, Pozzolanes and Limestone." 3th International Conference on Calcined Clays for Sustainable Concrete. New Delhi, Volume II. S. 135 – 153. 2019