The Use of Calphad Thermodynamics in Building Materials Industry

ALEXANDER PISCH

LAFARGE CENTRE DE RECHERCHE, SAINT QUENTIN-FALLAVIER, FRANCE

ABSTRACT

Cement and Concrete are the most abundantly manufactured materials in the world. The annual amounts equal 3 Gt for cement and 7.5 km^3 for concrete.

Cement is produced by reaction of ground limestone, clay minerals, silica and iron oxide in a fuel fired rotary kiln at 1450°C followed by air quenching. The obtained material is called clinker and its constituents are hydraulically active calcium silicates and aluminates together with some minor compounds such as alkaline sulfates, lime and periclase. The exact mineralogical composition depends on the initial chemical composition and the burning conditions.

The chemistry is complex: classical cement clinker contains measureable amounts of at least 9 different components CaO-SiO_2-Al_2O_3-Fe_2O_3-MgO-K_2O-Na_2O-SO_3-P_2O_5. Optimum burning conditions imply the formation of a liquid phase whose total amount should not exceed 28 mass% to avoid sticking on the kiln refractories.

Thermodynamic calculations using the Calphad approach are therefore a very useful tool to optimize the chemical composition and process parameters such as the maximum burning temperature and gas composition. Optimization is interesting and important because the overall process is highly energy intensive with high CO_2 emissions.

However this is not the only field in which a thermodynamic Calphad type approach can be used. The produced cement is mixed with water, sand and aggregates to make concrete. The underlying chemical mechanism is the formation of hydrates which allows reaching the desired final properties such as compressive strength.

These properties depend on the nature and the amount of hydrates formed as well as on the final microstructure in the concrete. Thermodynamic calculations can help to better analyze and understand the observed reaction paths.

The purpose of this presentation is to give an overview of the current status of the use of Calphad thermodynamics for construction materials at high temperature but also in the field of aqueous chemistry.