Kinetic and mechanistic aspects of the CaSO₄-H₂O solid-gas transformations: Gypsum dehydration reactions

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Gypsum is the mineralogical term used to describe materials that are mainly constituted of calcium sulfate dihydrate (CaSO₄·2H₂O). The calcination of gypsum to produce plaster is a large-scale industrial process with paramount importance for the modern construction materials industry. During this process, two main dehydration reactions usually occur during calcination depending on temperature and humidity conditions: CaSO₄·2H₂O dehydrates to hemihydrate (CaSO₄·0.5H₂O) and the latter can also dehydrate forming soluble anhydrite (CaSO₄).[1,2]

Despite the fact that the literature in gypsum dehydration is considerably extensive, there is a substantial lack in accordance about several aspects of the aforementioned dehydration reactions. For instance, there is no accordance if the type of kinetic model to be used to describe the reaction needs to take account of both nucleation and growth or only one of these processes. Furthermore, when the nucleation and growth processes are considered, the JMAEK model is generally used, which lacks in physical meaning for solid-gas reactions. In addition, as there is no accordance concerning the employed kinetic models, published reaction mechanisms and apparent activation energy values also differ. Hence, the lack in accordance about several aspects of these reactions makes it necessary to investigate in detail the intrinsic chemical reactivity of this system. [3,4]

In this context, one of the objectives of the present work is to describe and analyze with precision the different solid-gas transformations within the chemical system $CaSO_4$ - H_2O and clarify remaining questions on reaction kinetics still present in the literature. In order to perform this, the dehydration of a highly pure calcium sulfate dihydrate powder was monitored using thermogravimetric analysis under isotherm and isobaric conditions to obtain kinetic curves. Temperature ranging from $30^{\circ}C$ to $250^{\circ}C$ and water vapor partial pressure ranging from of 5 hPa to 60 hPa were investigated. Morphological and textural characterizations of the solids were also employed to understand the way of transformation. Based on this knowledge, a kinetic nucleation-growth model was then proposed and applied to the experimental data in order to obtain kinetic parameters for nucleation and growth. A growth mechanism was written and the change of kinetic parameters with temperature and water vapor partial pressure was explained. [5,6]

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