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Development of an empirical equation to calculate nucleation and growth processes in cement systems

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The paper focusses on the calculation of rate of nucleation and growth of cement systems .The research is focused on the idea of comparing the process of phase change of cement system to nucleation kinetics. Cahn's and Avrami's equations are presently popular with the same idea but fail with complex systems and at some temperature and experimental conditions. The main reason for this is that though rate kinetics of cement hydration is similar to the reaction kinetics of nucleation and growth models but **the Avrami's and Cahn's equations do not model the process**. We simulated the cement processes using software, Mic and with the results present formulated tables with different growth rates and initial densities of nucleation. The idea in the new equation proposed to assume **the grain boundaries to be spherical in nature** (overcoming the limitation of Cahn's equation pf parallel and perpendicular grain boundaries). On these, spherical boundaries, with a constant initial density of nucleation and fixed rate of growth, the transformed volume at any particular time were calculated. For the same assumptions, the simulated and mathematical results were compared and an empirical equation with a better fit and more accuracy was derived for that particular case. This equation format was generalized which was calibrated for different experimental conditions and results were again observed. The overall efficiency of the results obtained from the empirical equation were about (96-99) %.

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