Original Research Article

An empirical technique for prediction of nucleation mechanism and interfacial tension of potassium chloride nanoparticles

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ABSTRACT

Prediction of the nucleation mechanism is one of the most critical factors in the design of a crystallization system. Information about the nucleation mechanism helps to control the size, shape, size distribution, and purity of the produced crystals. When the crystallization method is used for producing nanoparticles, the nucleation mechanism should be predicted. In this study, an empirical correlation based on the induction time, classical nucleation theory, and Kashchive model is used to determine the nucleation mechanism. Nanoparticles are produced in the presence of Cetyl Trimethyl Ammonium Bromide (CTAB) and the effect of CTAB on the induction time and the interfacial tensions of potassium chloride nanoparticles have been investigated. The obtained results demonstrated that the nucleation mechanism of potassium chloride nanoparticles is heterogeneous. This method is simple and can be applied at ambient

conditions for synthesis other mineral nanoparticles. It can also be applied to study the induction time with high accuracy.

Keywords: Nucleation mechanism, Potassium chloride, Nanoparticles, Induction time, Interfacial tension

Introduction

Among the numerous ways of producing nanoparticles, one of the important methods is the precipitation from the liquid phase, which is based on crystallization. This method is very common due to the easier control of the size and the morphology of the produced nanoparticles [1]. The induced crystallization is a well-established precipitation method, which has been known for decades. In this process, a solute precipitates from a primary solvent, by adding a second solvent (anti-solvent), in which the solute is relatively insoluble. The anti-solvent is miscible with the primary solvent and decreases the solubility of the solute in the binary mixture, which ultimately leads to precipitation [2].

In crystallization processes, the induction time is an empirical approach to study the nucleation kinetics. It can be defined as the time between the achievement of supersaturation and the appearance of detectable changes in the physical properties of the solution due to the formation of the new nucleus. This change can occur in the colour, conductivity, or viscosity of the solution [3].

The induction time consists of three parts as follows: 1. The relaxation time (tr), which is the required time to achieve a quasi-steady-state distribution of molecular clusters; 2. The time needed for the formation of stable nuclei (t_n); 3. The time required for the growth of the nuclei (tg) and appearance of detectable changes in the system. In a low-viscous aqueous solution, the relaxation time is very short [4] and therefore, the induction time is expressed as below:

$$t_{ind} = t_n + t_g \tag{1}$$