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A Mathematical Investigation of the Turkevich Organizer Theory in the Citrate Method for the Synthesis of Gold Nanoparticles

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Abstract : Gold nanoparticles are commonly synthesized by reducing chloroauric acid with sodium citrate. This method, referred to as the citrate method, can produce spherical gold nanoparticles (NPs) in the size range 10-150 nm. Gold NPs of this size are useful in many applications. However, the NPs are usually polydisperse and irreproducible. A better understanding of the synthesis mechanisms is thus required. This work thoroughly investigated the only model that describes the synthesis. This model combines mass and population balance equations, describing the NPs synthesis through a sequence of chemical reactions. Chloroauric acid reacts with sodium citrate to form aurous chloride and dicarboxy acetone. The latter organizes aurous chloride in a nucleation step and concurrently degrades into acetone. The unconsumed precursor then grows the formed nuclei. However, depending on the pH, both the precursor and the reducing agent react differently thus affecting the synthesis. In this work, we investigated the model for different conditions of pH, temperature and initial reactant concentrations. To solve the model, we used Parsival, a commercial numerical code, whilst to test it, we considered various conditions studied experimentally by different researchers, for which results are available in the literature. The model poorly predicted the experimental data. We believe that this is because the model does not account for the acid-base properties of both chloroauric acid and sodium citrate.

Keywords : citrate method, gold nanoparticles, Parsival, population balance equations, Turkevich organizer theory
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