# Modelling the synthesis and growth of inorganic nanoparticles

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**Abstract**

In this paper we investigate a new stochastic particle method (SPM) for solving an extended sintering-coagulation equation and model two particle systems: the production of silicon dioxide and titanium dioxide. A model, which includes both, a particle source and an area dependent surface growth term as well as coagulation and sintering is presented. A new mass-flow stochastic algorithm to solve the model is stated. The stochastic method is able to simulate the evolution the bivariate particle size distribution function (PSDF) and is computationally very efficient when compared to traditional finite element methods. The SPM is compared to a bivariate sectional method for a system with coagulation and sintering as the only mechanisms. Despite using a different form of coagulation kernel to the sectional investigation, the results obtained agree closely to those in the literature and were obtained in a small fraction of the time quoted. The full model with particle inception and surface growth was then used to model the $TiCl_4 \rightarrow TiO_2$ system under various conditions. At low precursor concentration we investigate the effect of changing temperature, whilst at high precursor concentration we investigate the effect of surface growth on the system. The results agree with many of the conclusions reached in the literature.