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Evaluation of TiO_2 particle size distribution and crystallinity in burner-stabilised stagnation flames using sectional models

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Using flames as heat sources for producing high-quality nanoparticles has gained significant attention due to their one-step, high-throughput nature and the absence of liquid by-products compared to traditional wet chemistry methods. Titanium nanoparticles, such as, Titanium Dioxide (TiO_2), have been widely used as photocatalysts for solar fuels and semiconductors for gas sensors. Macroscopic properties of the produced TiO_2 are directly influenced by nanoscale characteristics of particles, such as, Particle Size Distributions (PSDs) and crystalline phase composition. Accurate modelling characteristics of nanoparticles is vital for the production of high-quality nanomaterial in the industrial applications. A mass and number density preserving sectional method, originally developed to predict soot PSDs [1], is here extended to compute titanium dioxide nanoparticle size distributions and crystallinity phase fractions. The gas phase chemistry combines a detailed C/H/N/O mechanism [2] with a Ti reaction mechanism featuring 25 species and 65 reactions for Titanium Tetra-Iso-Propoxide (TTIP) decomposition to $Ti(OH)_4$ [3]. The mechanism features inception of TiO_2 particles through barrierless dissociation of $Ti(OH)_4$. Coagulation and aggregation using fixed and varying collision efficiencies are explored and surface growth is assumed via condensation of $Ti(OH)_4$ molecules on the particle surface. Crystalline phase transport equations are proposed and integrated with the sectional model with two distinct phase identification models. The methodology is applied to the formation of TiO_2 in three sets of laminar, premixed, ethylene-oxygen-argon stagnation flame experimentally studied by Tolmachoff et al. [4] and Manuputty et al. [5, 6]. Results are compared with experimental data of TiO_2 PSDs and phase composition with TTIP loading in the range of 306 ppm to 1454 ppm. Satisfactory results are obtained for all data sets in both fuel lean and rich conditions supporting the applicability of the augmented sectional model in representing both PSDs and crystalline phases.

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