Numerical Simulation of Titanium(IV) Isopropoxide/p-Xylene Precursor Solution Spray Flames in the Counterflow Configuration for Use in Flame Spray Pyrolysis

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Abstract: Sprays of precursor solutions are used to produce functional nanoparticles with specific properties using flame spray pyrolysis (FSP). The present study concerns the precursor titanium(IV) isopropoxide (TTIP) in p-xylene. A dilute monodisperse spray carried by an air stream is directed against an air stream to establish a counterflowing laminar spray flame. The complex thermo-physical properties of the bi-component droplets are considered as well as the chemical reactions of the system with 213 chemical reactions among 52 species. For the TTIP, thermal decomposition is considered and for p-xylene, a reduced chemical reaction system is used. The droplets are modeled using a multi-component evaporation model where the distillation-limit model is used for droplet heating and the diffusion model describes the vaporization. Drag and gravity forces are considered in the equation of droplet motion. Thus, the liquid and gas equations are described in an Lagrangian-Eulerian framework. The spray flame structures are presented where the effect of changing the precursor mass loading, the gas strain rate, the droplet size as well as the equivalence ratio are considered. Multiple spray flame structures occur and their effect on the nanoparticle synthesis is discussed.

Keywords: TTIP/p-xylene precursor solution, laminar spray flames, counterflow configuration, detailed chemistry, bi-component sprays

Conference Title: ICFMHTT 2024: International Conference on Fluid Mechanics, Heat Transfer and Thermodynamics

Conference Location: Dubai, United Arab Emirates

Conference Dates: January 28-29, 2024