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Investigating Multi-Component Evaporation Effects on Nanoparticle Synthesis in the SpraySyn Burner Using Direct Numerical Simulations

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The synthesis of nanoparticles via spray flames is a complex phenomenon involving multiple physical and chemical interactions. A critical challenge in this process is selecting a suitable fuel to mix with the precursor in order to produce nanoparticles with the desired properties. The evaporation of the spray fuel and precursor directly affects the resulting nanoparticles. One direct application of such a system is the SpraySyn burner configuration [1]. In the present work, a configuration similar to the SpraySyn burner is considered. Direct Numerical Simulations (DNS) are performed to investigate the impact of the evaporation model in this setup for the production of titanium dioxide nanoparticles through spray combustion of a liquid mixture involving ethanol (as the primary fuel) and titanium tetraisopropoxide (TTIP, as the precursor). The in-house code (DINO) [2] is employed for these simulations. The computational domain measures $20\ \mathrm{mm} \times 10\ \mathrm{mm} \times 2.5\ \mathrm{mm}$ and is discretized over 67 million grid points, maintaining a grid resolution of $19\ \mu\mathrm{m}$. The spray is injected with variable droplet diameters following a Rosin–Rammler distribution. Two main aspects are examined concerning the effect of a multi-component evaporation model on (1) spray evaporation rates and flame structure, and (2) on nanoparticle formation. Most published simulation studies of the SpraySyn burner have adopted a single-component evaporation model [3]. First results indicate that using a multi-component evaporation model significantly alters the flame structure. In particular, the single-component model noticeably overestimates ethanol evaporation rates, resulting in different TTIP concentrations in the gas phase. These effects are expected to affect nanoparticle formation, the details of which will be presented at the conference.

References

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