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Analysis on premixed combustion of H_2–CH_4 mixed fuels for SiO_2 particle preparation

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HIGHLIGHTS

- The SiO_2 nanoparticle synthesis by H_2-CH_4 combustion was analyzed numerically.
- The profiles of velocity, temperature, species concentrations etc. were calculated.
- Increase of CH_4 concentration affects the properties of SiO_2 particles.
- The trajectories and temperature histories of SiO_2 particles were calculated.

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ABSTRACT

The combustion of premixed H_2 and CH_4 fuels to prepare SiO_2 nanoparticles was analyzed numerically. The commercial CFD-code Fluent was used to calculate the profiles of gas velocities, temperature, species concentrations and reaction rates for various process conditions in the premixed flame reactor. To understand the effect of CH_4 addition to H_2 fuel, the CH_4 mole fraction was changed from 0% to 10%, while keeping the H_2 concentration constant. With the increase of CH_4 concentration, flame temperature increases, which will affect the properties of SiO_2 particles prepared in premixed flame reactor. Using the data of gas temperatures and velocities extracted from Fluent, the trajectories and temperature histories of SiO_2 particles were calculated inside the premixed flame reactor. This study shows that particles starting at different initial positions move inside the reactor with different particle trajectories and have different temperature histories, and the properties of SiO_2 nanoparticles prepared in the premixed flame reactor will depend on those process variables significantly.

1. Introduction

There are dry processes (plasma processes, flame synthesis, etc.) [1,2] and wet processes [3,4] which are being used for the synthesis of silica-related nanoparticle. Flame aerosol synthesis has been widely utilized for the manufacture of nanoparticles in large scale because they are generally cleaner, more energy-effective, environmentally safer, and easier to produce preferred nanoparticles than the traditional wet chemistry routes [5–11]. Because the nanoparticles are synthesized in the flame reactor at the extremely high temperature and in a very short residence time, it is quite difficult to control the properties of particles precisely. It is necessary to understand the physical and chemical phenomena in flame processes to improve the particle properties and also to develop the better flame reactor.

Several numerical investigations have been performed for premixed and non-premixed combustion [10–13] and also for nanoparticle synthesis by flame reactor [14–19]. Lee et al. [16] simulated the growth of nonspherical silica nanoparticles in a premixed flat flame, including the effects of convection, diffusion, thermophoresis, chemical reactions, coagulation, and coalescence. The effect of Brownian diffusion of nanoparticles was also investigated and found to be significant only near the burner exit. Yu et al. [7,15] applied the computational model combining the fluid dynamics with the particle kinetics to study TiO_2 nanoparticle synthesis in a diffusion flame reactor. They reached excellent agreements between the model predictions and experimental data in terms of flame temperature distribution and particle kinetics, also they obtained some key factors influencing the nanoparticle characteristics by taking the particle size and surface area as independent variables. A simulation of particle formation and deposition during lightguide preform fabrication by modified chemical vapor deposition at non-isothermal conditions was presented by Kim and Pratsinis [20,21]. They solved the Navier–Stokes equation including continuity, momentum, energy and mass balance equations

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