Combustion of Individual Iron Microparticles With Resolved Boundary Layers II

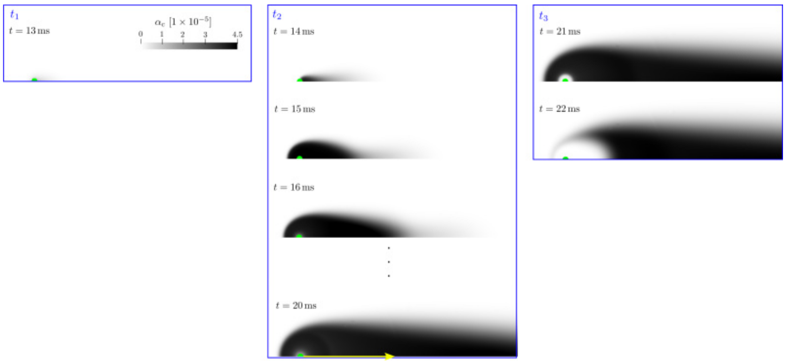

Figure 1: Distribution of the nanoparticle volume fraction during different phases. The parent particle is depicted in green.

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Clusters
Lichtenberg II Cluster Darmstadt

Additional Software
OpenFOAM, ULF, Cantera

Institute
Simulation of Reactive Thermo-Fluid Systems

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Introduction

Iron powder is emerging as a promising carbon-free energy carrier that can be used for a clean iron-based energy cycle. The powder can be combusted with air to generate heat and power. Thereafter, the iron oxide powder is collected and regenerated by means of a thermochemical reduction with green hydrogen closing the loop. During the combustion, the formation of nanoparticles poses challenges in terms of particulate emissions and material losses. Nanoparticles are difficult to separate from the exhaust gases and are respirable, which is why a comprehensive understanding of their formation and how to avoid them is necessary. In this study, a model for nanoparticle formation is introduced, which is based on the condensation of supersaturated iron / iron oxide vapor to liquid nanoparticles in the boundary layer of the burning iron microparticle. Resolved boundary layer simulations of single iron microparticles are compared with recent in-situ measurements to investigate the onset of nanoparticle formation and characteristics of the nanoparticle cloud that is formed close to the burning parent microparticle. Nanoparticle formation and nanoparticle cloud evolution are investigated, considering combustion and transport processes in the boundary layer.

Methods

A two-phase, compressible, reactive solver within the open-source code OpenFOAM-v2012 is chosen for this work. The two-phase solver was developed for this study to separate the nanoparticles from the gas phase, since nanoparticle transport is different from the transport of gas molecules. Compressibility is necessary since the temperature and density gradients change tremendously in the boundary layer of a burning particle. The ability to handle chemical reactions in the boundary layer is necessary, since gaseous iron species are released which further react with the oxygen in the gas. Since iron particles are micro-sized, it is assumed that heat and mass transfer inside a particle is infinitely fast and therefore, the solid particle phase is not resolved. Instead, the particle is represented by a combustion model at the particle-to-gas interface.

Results

The utilized particle model reproduces the peak temperature, but notable deviations still exist in the temperature profiles between simulation and experiment. Prescribing the measured particle temperature evolution in the simulation, the onset temperature of nanoparticle formation is predicted well. Further analysis identifies convection and thermophoresis as the primary transport processes for the nanoparticle cloud, while diffusiophoresis is negligible. Additionally, the sensitivity of nanoparticle formation to the evaporation model and reaction mechanism is evaluated. It was found that the evaporation model has a significant effect on the amount of produced nanoparticles while the gas phase reaction mechanism has a minor effect.

Discussion

It is shown that the particle temperature is the most important parameter for nanoparticle formation and a correct prediction of particle temperature evolution is crucial for nanoparticle prediction. The study highlights that further reference datasets of nanoparticle formation are crucially needed for a quantitative evaluation of the nanoparticle model.

Publications

Nguyen B.-D.; Braig, D.; Scholtissek, A.; Ferraro, F.; Hasse, C. Simulation of single iron microparticle combustion with resolved boundary layers, European Combustion Meeting, Rouen, France, April 26-28, (2023)

Nguyen B.-D.; Braig, D.; Mich, J.; Scholtissek, A.; Ferraro, F.; Nicolai, H.; Hasse, C. Simulation of single iron microparticle combustion with resolved boundary layers, 15th International Conference on Combustion Technologies for a Clean Environment, Lisbon, Portugal, June 25- 29 (2023)

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