Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Numerical Analysis of Iron Dust/Air Combustion

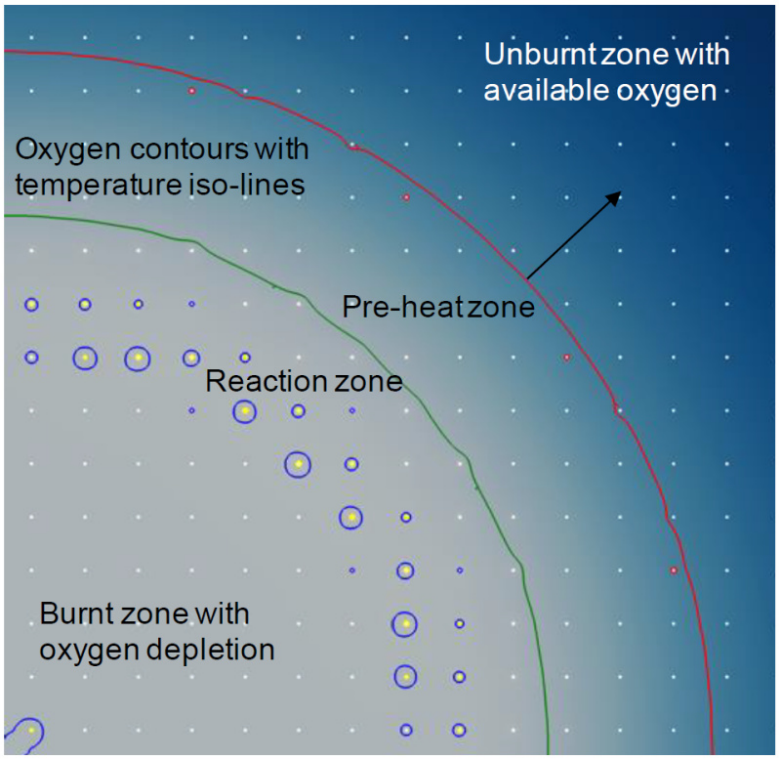


Figure 1: Contour plot of gas phase oxygen for a two-dimensional array of particles for stoichiometric conditions. Red, green and blue lines mark temperatures close to ignition, thermal runaway and particle surface temperatures.

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Clusters
Lichtenberg II Cluster Darmstadt

Software
ANSYS

Institute
Simulation of Reactive Thermo-Fluid Systems

University
Technische Universität Darmstadt

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Introduction

Iron powder can help in a clean and sustainable generation of heat and power and holds the potential to replace hydrocarbon-based fuels. It can be combusted and then recycled using renewable energy sources such as wind and solar. However, knowledge of the combustion of iron particles needs to be improved and faces several challenging questions for the design of efficient and safe devices. In this project, we analyzed two such issues, which is the mode of flame propagation and the effect of flame curvature using boundary-layer resolved (BLR) simulations of the particle, including the heterogeneous reaction of iron with oxygen. Depending on the conditions, an iron dust flame can propagate in either the continuous mode with neighboring particles burning simultaneously or in a discrete mode with each particle burning separately, i.e., as a percolating wave. This necessitates the usage of experimentally validated numerical models in order to explore and understand the physics of its combustion. As iron powder combustion could consist of several hundred particles, in this project the usage of HPC resources was absolutely crucial for the simulation of highly resolved grids.

Methods

In this project, boundary-layer resolved (BLR) simulations of up to 900 particles were conducted. Unsteady flow, species, and energy equations were solved using second-order discretization schemes. A heterogeneous combustion model for the iron particle was implemented and applied at the particle boundary. This, in effect, resulted in Direct Numerical Simulations of iron dust combustion. High-Performance Computing resources made available at the Lichtenberg cluster allowed for the possibility to solve a high number of particles using parallelization.

Results

During this project, BLR simulations of planar and curved iron dust flames were conducted. Curved flames can arise in stabilized flames as well as during the initial stages of ignition. The 3D symmetric computational setup comprised an equidistant rectangular grid of particles with ignition initiated by the central particle. This study was designed in a way that a systematic comparison can be made between the two types of flames. Over 900 boundary-layer resolved particles were simulated with a mesh count of around 8 million.

Discussion

Key insights obtained from this project regarding propagating iron flames indicate that curved flames exhibit a lower flame speed compared to planar flames. While only continuous flames were observed, with no curved discrete flames detected, planar flames demonstrated both continuous and discrete modes, separated by a quantifiable limit. Additionally, curvature effects were evident, as no propagating curved flame was found below

an equivalence ratio of 0.7. This absence is attributed to the lack of ignition at leaner equivalence ratios, where larger particle distances necessitate heating a greater volume within the cylindrical space. Furthermore, the results suggest that, similar to gaseous flames, iron flames experience curvature effects in their macrostructure due to the redistribution of gaseous species, such as oxygen, within the microstructure.

Publications

Vance, F. H.; Scholtissek, A.; Nicolai, H.; Hasse, C.: "A numerical analysis of multi-dimensional iron flame propagation using boundary-layer resolved simulations", Fuel 369 (2024), pp. 131793. https://doi.org/10.1016/j.fuel.2024.131793

Vance, F. H.; Scholtissek, A.; Nicolai, H.; Hasse, C.: "Propagation of iron dust flames in a narrow channel", 2nd MeCRE Workshop 2024, Darmstadt.

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