International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

Coupled CFD-DEM Simulation of Iron Powder Oxidation in a Fluidized Bed Reactor

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In the transition towards climate-neutral energy systems, metal fuels such as iron powder are emerging as promising renewable energy carriers due to their high energy density, recyclability, and CO_2-free combustion [1]. In particular, iron combustion offers the potential to provide carbon-neutral energy during periods of low solar and wind availability at comparatively low cost [2]. Computational Fluid Dynamics (CFD) plays a vital role in the design and optimization of such systems [3].

The objective of this study is the development of a numerical model for the oxidation of iron powder in a laboratory-scale bubbling fluidized bed reactor to investigate the oxidation of iron powder particles with a median diameter (d_{50}) of 200 µm. A coupled Computational Fluid Dynamics–Discrete Element Method (CFD-DEM) approach integrates ANSYS Fluent and ANSYS Rocky, augmented with a custom C++ module that enables two-way coupling between gas and particle phases. A reactive model is employed, incorporating a conversion rate derived from thermogravimetric analysis, which depends on particle diameter, temperature, porosity, and gas-phase concentration. Fluent computes the continuous gas phase on the CPU, while Rocky resolves individual particle dynamics and collisions on the GPU. The model accounts for local mass, volume, and enthalpy changes due to oxidation, allowing for spatially resolved analysis of temperature, pressure distribution, and solid-phase conversion.

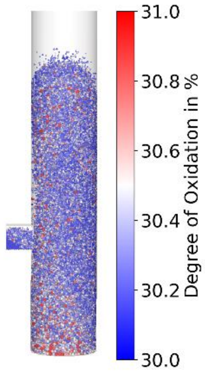

Figure 1: Degree of Oxidation of Iron Powder in a Fluidized Bed Reactor

The simulations provide insights into critical boundary effects and the impact of operating conditions on oxidation performance. By analyzing mixing behavior, residence time, and heat distribution, the model aims to be validated and refined against experimental data.

The findings support the conceptual design of larger-scale systems with a focus on process efficiency and reactor operability. Furthermore, the results can inform the retrofitting of existing coal-fired power plants to operate with iron as an alternative fuel. This work establishes a numerical foundation for scaling up iron powder combustion in fluidized beds, contributing to the development of design criteria for pilot and industrial reactors. Ultimately, the study supports the potential of iron as a circular, CO_2-free energy carrier and suggests that fluidized bed technology could be a promising platform for its implementation.

References

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