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Towards the numerical simulation of iron particle combustion

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Our work focuses on the modelling of iron particle combustion, a process providing potentially carbon-free thermal power. The numerical developments are structured around two principal steps: 1) the development and validation of a 0D model for the combustion of a single iron particle and 2) the integration of this model into a CFD solver to perform direct numerical simulation (DNS) of iron particle-laden flows.

The single particle model [1] accounts for sequential oxidation reactions (Fe $\rightarrow$ FeO $\rightarrow$ Fe_3O_4 $\rightarrow$ Fe_2O_3), heat transfer, solid–liquid phase changes and dissociative evaporation. It employs a pragmatic optimisation strategy regarding the principal driver of heat release, the absorption of oxygen from the surrounding atmosphere. Mass and enthalpy balances for the particle yield the particle temperature evolution, which has been validated against experimental data and compared with state of the art models across a wide range of operating conditions. The optimisation of the model is realised via the reduction of oxygen absorption flux through the quantity γ, which was modelled as piecewise constant, changing once at a predetermined burn time based on experimental measurements. The initial value and transition time of γ are parameterised as functions of particle diameter and the ambient oxygen molar fraction.

The model is being deployed in the DNS-DPS solver ASPHODELE [2] using an Eulerian approach for the carrier phase and a Lagrangian approach for the dispersed phase. Two-way coupling is considered through exchange of mass, momentum, and energy between both phases. This integration aims to investigate the propagation mechanisms of reactive fronts in iron-particle-laden flows. Simulations will be conducted with various spray characteristics, both in laminar and turbulent regimes. A first validation case in a homogeneous 2D spray has shown good agreement between the simulated reactive front propagation speed and experimental observations.

References

[1] Kuhmann M et al. Optimised 0D model for the simulation of single iron particle combustion. *Fuel*. 2025; 381:133436.

[2] Bouali Z et al. Development of an extended reactor configuration to analyze preferential segregation impact on spray autoignition. *Fuel*. 2021; 302:120869.