The influence of clustering on particle cloud combustion in homogeneous isotropic turbulence

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The imminent change towards power generation from renewable sources results in the need for large scale energy storage and transportation solutions due to the geographic dependence and fluctuation of energy production over time. The use of iron as a fuel within metal redox cycles is a promising concept, which includes the oxidation of iron, releasing the energy stored previously. One option for this process is the combustion of iron powder in e.g. retrofitted coal power plants. In technical applications of iron combustion, it is difficult to distribute the particles perfectly homogeneously and industrial burners are designed to work with highly turbulent flames. Therefore the interaction of turbulence, particle clustering and combustion characteristics is of high practical relevance, and this study will help to identify critical parameters for the turbulent cloud combustion.

In this work, we study the combustion of iron particles in homogeneous isotropic turbulence (HIT). With a carrier-phase DNS approach, we use existing iron particle combustion models [1,2] in a highly-scalable spectral solver that was initially developed for studying inertial particles in HIT [3]. In a first step, we perform HPC scaling tests to investigate the parallel performance of the solver at high Reynolds numbers, requiring large grid sizes of $> 1024^3$ resolved Fourier modes, while handling $> 10^9$ particles. The scaling of first simulations with 512^3 resolved Fourier modes and 29M particles is presented in Fig. 1. It shows good scaling between 128 and 4096 cores, with 81% scaling efficiency for a 32-fold increase of the number of parallel cores.

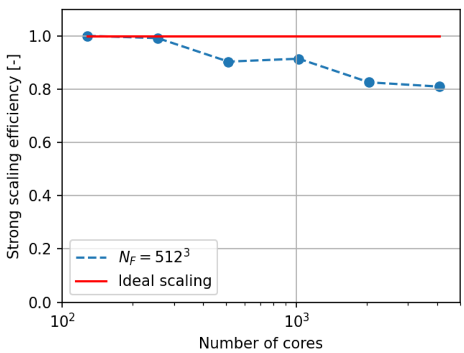

Figure 1: Strong scaling efficiency of HIT code with 512^3 resolved Fourier modes in the fluid domain and 29M particles. The number of cores varies between 128 and 4096.

Our previous work established a link between the ignition delay time and the particle Stokes number for globally lean mixtures, with a higher extent of particle clustering leading to earlier ignition [4]. Now we extend the setup to investigate the full combustion process across a wide range of equivalence ratios. Figure 2 shows 2D example slices of gas temperature, oxygen mass fraction and velocity magnitude through the 3D HIT domain with a particle Stokes number of one, where considerable particle clustering occurs. This clustering leads to localised oxygen depletion that will affect the local flame structure and flame propagation properties. Voronoi analysis for quantifying clustering will be used to characterise the impact of clustering on the turbulent flame properties for initially monodisperse iron particle clouds. Subsequently we will explore polydispersity effects by considering the experimental particle size distribution of Fedoryk et al. [5] and Luu et al. [6]. For polydisperse clouds clustering is expected to be less prominent, but spatial separation of different particle sizes is still likely to influence the cloud combustion characteristics.

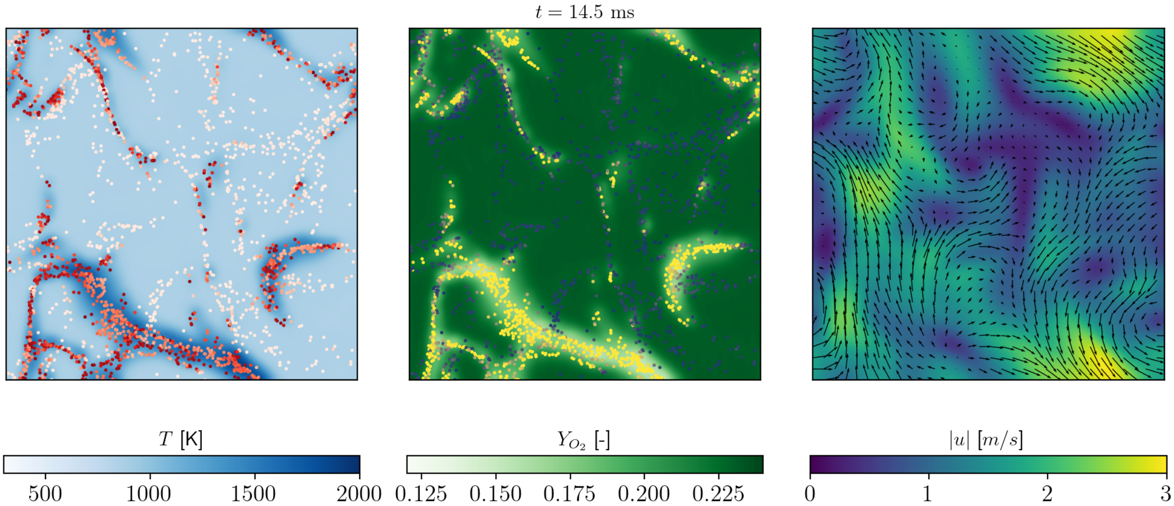

Figure 2: Instantaneous snapshots of iron particle combustion in HIT, where considerable particle clustering can be observed. The particle Stokes number is 1, where clustering is most prominent. The temperature T, the oxygen mass ratio Y_{O_2} and the fluid velocity magnitude $|u|$ are shown.

References

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