



Influence of turbulence on iron dust flame propagation

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ARTICLE INFO

Dataset link: <https://dx.doi.org/10.35097/e0fbwzmkftmhubne>

Keywords:

Iron particle combustion
Turbulent iron flame propagation
Carrier-phase DNS

ABSTRACT

We investigate the effect of turbulence and particle slip on propagating flames from micron-sized iron particles through carrier-phase direct numerical simulations (CP-DNS). We use a pseudo-spectral multiphase solver for the fluid equations, including heat, mass, and momentum transfer between the fluid and the particles, and model the iron combustion through a point-particle approach. In differently elongated domains with triply periodic boundary conditions, we initially let particles evolve and cluster in forced homogeneous isotropic turbulence (HIT) without chemical reaction. Then, we heat up a slice of particles to initiate combustion and examine flame propagation through forced turbulence. We vary the integral-scale Reynolds number Re_ρ , ranging from 57 to 250, independently from the Kolmogorov-based Stokes number $St = 1/4$ to 4, and compare the results to a case with planar flame propagation. The Stokes number has a strong impact on flame propagation speed, while no significant influence of the Reynolds number is observed across the investigated range. Particles at $St = 4$ reach a global oxidation progress of 80% around six times faster compared to the planar flame. The turbulent mixing at the smallest scales increases with St for a fixed initial particle size d_p , increasing the flame propagation speed. For a planar flame, particle slip enhances the propagation. We observe flame speeds in the range $7\text{--}13\text{ cm s}^{-1}$ for the planar flame, which is in a range similar to previous works. Moreover, we characterize turbulent flame fronts using temperature isocontours of the gas phase, and provide a first estimate for the turbulent flame front speed in HIT relative to the planar speed.

Novelty and significance statement: Iron particle cloud combustion is a promising concept for renewable energy storage and transportation. Many studies investigate single iron particle reaction properties or the combustion of small particle groups. This study aims to connect the knowledge from those models to more realistic, but generic turbulence, namely the flame propagation through homogeneous isotropic turbulence. We compute turbulent flame speeds for iron dust flames, connect them to the flame surface area, and investigate the effect of particle slip and small scale turbulence, which to the best of our knowledge has not yet been done before. These features need to be well understood for future designs of iron combustion chambers.

1. Introduction

The use of iron as a metal fuel within a redox cycle is a promising concept for long-distance transportation and seasonal storage of renewable energy [1,2]. Iron can be oxidized in powder form in, e.g., refitted coal power plants [3]. Due to the high boiling points, iron and its oxides remain mostly solid or liquid even during combustion, which makes the reaction fully heterogeneous and different from combustion of common solid fuels such as coal and biomass [1]. Many works have studied the combustion behavior of single particles [4–6] and proposed reduced order models for the combustion process [7–9]. Those models have been used, for example, in numerical simulations

to replicate experiments [10,11] and investigate how turbulence affects combustion [12,13]. In particular, particles are known to form clusters in turbulence [e.g.14–18], leading to faster ignition and longer burn times due to local oxygen depletion [19,20]. In the present work, we focus on the influence of turbulence and particle slip effects on iron flame propagation, which has not yet been thoroughly investigated. The study aims to address the following questions:

- Q1 How does flame propagation change with increasing integral scale Reynolds number of the gas phase?
- Q2 How does flame propagation depend on particle slip, characterized by the Stokes number?

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Q3 Does the flame speed scale with the flame surface area?

These questions have been widely discussed in literature for volatile-containing flames, but are still open questions for non-volatile iron particle combustion.

2. Modeling

We perform numerical simulations of combusting iron particle clouds using a carrier-phase DNS approach, which simultaneously solves the Eulerian gas phase and the Lagrangian particles in the two-way coupling regime within a pseudo-spectral framework [19,21]. We employ a previously validated, zero-dimensional model for iron particle combustion, as detailed in Section 2.2. We refer to [20] for a complete description of the two-phase model used. Since we use a similar setup, only the key features and differences are highlighted below.

2.1. Fluid model

The gas phase is a mixture of N_2 and O_2 , characterized by the fluid velocity field u_i , temperature T and oxygen mass fraction Y_{O_2} . Due to the high boiling points of Fe and its oxides, most of the reaction takes place in the solid or liquid phase on the particle. Therefore, gas chemistry is not taken into account in the Eulerian phase, chemical reactions are only included in the particle model. We apply the Low-mach approximation to divide the pressure $p(\vec{x}, t) = p_0(t) + \pi(\vec{x}, t)$ into a spatially constant thermodynamic pressure p_0 and the pressure fluctuation π . Compared to our previous work [20], we reformulated the energy equation to directly solve for temperature T instead of enthalpy ρh . The formulation matches the energy equation in temperature form for a binary mixture derived in [22]. Compared to the reference, we neglect the temperature increase through viscous dissipation ($\tau_{ij}\partial u_i/\partial x_j$) as well as any gas phase reaction and forcing, and added the source terms due to the particle phase. This formulation proved to be more stable for the configurations with flame propagation. The full derivation is provided in the Supplementary Material. The governing equations of the gas phase read

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = S_{O_2} \quad (1a)$$

$$\frac{\partial(\rho Y_{O_2})}{\partial t} + \frac{\partial(\rho u_i Y_{O_2})}{\partial x_i} = \frac{\partial}{\partial x_i} \left(\rho D_{O_2} \frac{\partial Y_{O_2}}{\partial x_i} \right) + S_{O_2} \quad (1b)$$

$$\frac{\partial(\rho u_j)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_i} = -\frac{\partial \pi}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} + S_{j,u} + f_j \quad (1c)$$

$$\begin{aligned} \frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} &= \frac{1}{\rho c_p} \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial T}{\partial x_i} \right) + \frac{1}{\rho c_p} \frac{dp_0}{dt} + \\ &\frac{c_{p,O_2} - c_{p,N_2}}{c_p} D_{O_2} \frac{\partial Y_{O_2}}{\partial x_i} \frac{\partial T}{\partial x_i} + \frac{1}{\rho c_p} S_T \end{aligned} \quad (1d)$$

where ρ is the gas density, D_{O_2} the diffusivity of oxygen in air, λ the heat conductivity of the gas and $c_{p,i}$ and c_p the heat capacities of each species and the mixture, respectively. The stress tensor is given as

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \right) \quad (2)$$

with dynamic viscosity μ . The source terms due to the particle phase are

$$S_{O_2} = - \sum_{p=1}^{N_p} \delta|\vec{x}_p \frac{dm_p}{dt} \quad (3a)$$

$$S_{j,u} = - \sum_{p=1}^{N_p} \delta|\vec{x}_p \left(F_{i,drag,p} + \frac{dm_p}{dt} u_i|\vec{x}_p \right) \quad (3b)$$

$$S_T = - \sum_{p=1}^{N_p} \delta|\vec{x}_p \left(\dot{Q}_{conv,p} + \frac{dm_p}{dt} \Delta h_{O_2,p} \right). \quad (3c)$$

Following from the point-particle approximation, $\delta|\vec{x}_p$ is a Dirac delta centered at the particle position $\vec{x}_p$. $F_{i,drag,p}$ is the particle drag force, $\dot{Q}_{conv,p}$ the convective heat transfer between the particle and the gas phase, and $\Delta h_{O_2,p} = h_{O_2}(T_p) - h_{O_2}(T|\vec{x}_p)$ the enthalpy difference for the exchanged oxygen. The reader is referred to [20] for a detailed description of $F_{i,drag,p}$ and $\dot{Q}_{conv,p}$.

Before the particles are ignited and the flame front begins to propagate, the turbulent flow is statistically steady, homogeneous, and isotropic (HIT), sustained by a large-scale momentum forcing f_j , which allows to tune the flow statistics by adjusting the dissipation rate and the integral length scale [21,23].

2.2. Particle model

We use the first-order surface kinetics (FOSK) formulation [9] to model particle oxidation, which extends single particle models introduced earlier [7,24]. Only the reaction from Fe to FeO is considered, since this oxidation step has the highest energy release. Oxygen diffusion through the boundary layer limits the post-ignition reaction in both the present and more detailed particle combustion sub-models [8, 25], so the main conclusions of this work are expected to remain valid for those refined sub-models.

The state of each particle is described by the particle enthalpy H_p , particle mass m_p , iron mass $m_{p,Fe}$, particle position $x_{i,p}$ and velocity $u_{i,p}$. The oxidation reaction can be either limited by reaction kinetics at low particle temperatures or by diffusion of oxygen through the boundary layer to the particle surface for temperatures higher than around 1000 K. The particle enthalpy can change through convection, mass exchange with the gas phase, and radiation. We introduce a time-dependent heat flux $\dot{Q}_{heat}(\vec{x}_p, t)$ which heats the particles to initiate iron flame propagation in a cold mixture. Except for $\dot{Q}_{heat}$, the particle model is adopted from our previous work [20].

3. Computational setup

The domain is a triply periodic cuboid with dimensions L_1 , L_2 and L_3 . The momentum forcing sets the integral length scale ℓ through the forced wave numbers. For non-cubical domains, only wavelengths resolved in all three directions are forced, to ensure statistical isotropy. Therefore, ℓ can be adjusted by changing the minimum domain side length $\min(L_1, L_2, L_3)$, and the number and size of forced wave numbers. Through the employed method of forcing, the mean dissipation rate

$$\epsilon = \frac{1}{\langle \rho \rangle} \left\langle \frac{\partial u_i}{\partial x_j} \tau_{ij} \right\rangle \quad (4)$$

is set through the forcing strength, which determines the smallest turbulence scales, i.e., the Kolmogorov length η and time τ_η . Angular brackets denote the spatial mean over the domain.

In this work, we compare the flame propagation under different turbulent conditions and particle slip velocities. The separation between large and small scales of turbulence is characterized by the integral Reynolds number

$$Re_\ell = \frac{u_{rms}\ell}{\nu} \sim \left(\frac{\ell}{\eta} \right)^{4/3} \quad (5)$$

with the rms-velocity $u_{rms} = \sqrt{\langle u_i u_i \rangle}$ and $\nu = \mu/\rho$. The particle Stokes number

$$St = \frac{\tau_p}{\tau_\eta} \quad (6)$$

gives a measure of whether the particles follow the turbulent motion. $\tau_p = m_p/(3\pi\mu d_p)$ is the time scale of particle motion, with the particle mass m_p and diameter d_p .

We set Re_ℓ and St independently. For constant initial temperature $T_{=0}$ and initial iron particle diameter $d_{p,t=0}$, St depends only on $\tau_\eta = \sqrt{\nu/\epsilon}$, which we adjust by the forcing intensity. Due to the periodicity

Table 1

Case-specific parameters. The reported values of ϵ , η , u_{rms} , Re_ℓ and St are space-time averages computed over the statistically steady period of the inert pre-run simulations. The reference case *Lam* uses a zero-velocity field as the initial condition; therefore, no turbulent parameters are reported. N_p is adjusted to always obtain a global equivalence ratio of $\phi = 0.8$.

Parameter	Description	Case label					
		<i>Lam</i>	R_0S_0	<i>S-</i>	<i>S+</i>	<i>R-</i>	<i>R+</i>
$L_1 = L_2$ [cm]	Domain side length	7.5	7.5	15	3.75	7.5	15
$N_1 = N_2 \times N_3$ [-]	Resolved Fourier modes	96×192	96×192	96×96	96×384	96×192	192×192
$\eta N_1/L_1$ [-]	Resolution of dissipative scales	–	19.6	19.4	17.3	13.3	37.7
N_p [-]	Number of particles	7.43 M	7.43 M	29.7 M	1.86 M	7.43 M	29.7 M
$k_{max} L_1/(2\pi)$ [-]	Largest forced wavenumbers	–	$\sqrt{4}$	$\sqrt{3}$	$\sqrt{5}$	$\sqrt{8}$	$\sqrt{3}$
$k_{min} L_1/(2\pi)$ [-]	Smallest forced wavenumbers	–	0	0	$\sqrt{3}$	$\sqrt{6}$	0
ϵ [m ² s ⁻³]	Dissipation rate	–	0.156	0.0102	2.84	0.168	0.147
u_{rms} [m s ⁻¹]	rms-value of velocity	–	0.167	0.0792	0.364	0.137	0.217
Re_ℓ [-]	Integral Reynolds number	–	99.8	94.1	95.7	55.5	250
St [-]	Particle Stokes number	–	0.957	0.244	4.08	0.994	0.929

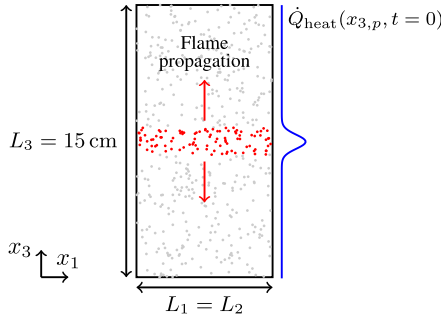


Fig. 1. Sketch of domain with Gaussian particle heating distribution. The thickness of the heating region is not to scale.

of our domain, pressure increases during combustion. The domain length $L_3 = 15$ cm in flame propagation direction is unchanged between simulations, resulting in a comparable pressure increase within our domain. We set a larger L_3 than in the similarly confined setup of [26], to slow down the pressure increase and therefore reduce effects of the periodic boundaries on particle slip. Re_ℓ is changed by employing different domain lengths in the other two directions $L_1 = L_2 \neq L_3$, resulting in cuboids with varying aspect ratios. In addition, we limit the forced wave numbers by $k_{min}^2 \leq k_i k_i \leq k_{max}^2$ and thereby adjust ℓ . The zeroth wave number $k_i k_i = 0$ is always excluded from the forcing, such that the mean of ρu_i is not forced; i.e., there is no mean flow in the computational domain.

Starting from a case at $Re_\ell = 100$ and $St = 1$ labeled as R_0S_0 , we vary the Stokes number to 1/4 (case *S-*) and 4 (case *S+*), while keeping Re_ℓ approximately constant. Also, we investigated two simulations where we vary Re_ℓ from 55 (case *R-*) to 250 (case *R+*) while keeping $St = 1$. One reference case without forcing named *Lam* uses a zero-velocity field with a random uniform particle distribution as the initial condition. In all other cases, the initial condition consists of a statistically steady HIT flow field laden with unreacted iron particles. These pre-run simulations were evolved for at least 15 eddy turnover times in forced HIT, with particle radiative heat losses turned off. For all initial fields, the gas and particle temperatures are set to 400 K. With the initial mass fraction of oxygen $Y_{O_2} = 0.233$, initial diameter $d_{p,i=0} = 25 \mu\text{m}$ and density $\rho_{Fe}(T_{p,0}) = 7834 \text{ kg m}^{-3}$ fixed between cases, the number of iron particles N_p is chosen such that the global equivalence ratio is always $\phi = 0.8$. A time step of $\Delta t = 10 \mu\text{s}$ is used for all main simulations.

All parameters for the specific cases, and the resulting flow conditions are summarized in Table 1, including the number of resolved Fourier modes N_i . For elongated domains, the resolution in each direction is constant so that $L_1/N_1 = L_2/N_2 = L_3/N_3$.

To ignite particles and initiate flame propagation, we heat the particles in a localized portion of the domain through a superimposed

heat flux

$$\dot{Q}_{\text{heat}} = \begin{cases} \pi r_p^2 \dot{q}_{\text{heat}} \zeta(x_{p,3}), & t \in (0, t_{\text{heat}}) \\ 0, & \text{otherwise.} \end{cases} \quad (7)$$

Here, r_p is the particle radius, $\dot{q}_{\text{heat}} = 2 \times 10^9 \text{ W m}^{-2}$ the imposed heat flux, and $t_{\text{heat}} = 0.1 \text{ ms}$ is the duration of heating. The intensity of heating is localized in space through

$$\zeta(x_{p,3}) = \exp\left(-\frac{(x_{p,3} - L_3/2)^2}{2l_{\text{heat}}^2}\right), \quad (8)$$

with $l_{\text{heat}} = 0.5 \text{ mm}$ defining the thickness of the heated region. The heated volume is therefore slightly less than 1% of the full domain. At $t = 0$, the start of the main simulations, the localized heat flux is switched on.

This ignition process is illustrated in Fig. 1. The temperature of the particles in the heated region exceeds the ignition temperature, leading to oxidation and propagation of the flame away from the ignited region in both directions along the x_3 axis. Note that in our periodic domain, combustion products cannot expand freely as they would with an outlet boundary, and the two flame fronts eventually wrap around the domain borders and influence each other. These limitations are further discussed in the results.

The global combustion progress in the domain is defined through the global progress of Fe conversion.

$$C_{\text{ox}}^{\text{glob}}(t) = 1 - \frac{\sum_p m_{p,\text{Fe}}(t)}{\sum_p m_p(t=0)}, \quad (9)$$

while the single particle combustion progress is

$$C_{\text{ox}}(t) = 1 - \frac{m_{p,\text{Fe}}(t)}{m_p(t)}. \quad (10)$$

4. Results and discussion

Fig. 2 shows slices of the reference case *Lam* and the cases with varying St , extracted at an equal combustion progress of $C_{\text{ox}}^{\text{glob}} = 30\%$ for all cases, to allow for a fair comparison of all cases despite their inherently different flame propagation velocities. The time at which this combustion progress is reached is indicated below each slice. The particles are colored by their individual oxidation progress C_{ox} , the gas phase by Y_{O_2} . Slices of the cases with varying Re_ℓ are omitted here and presented in the Supplementary Material. For case *Lam*, the particle distribution is statistically homogeneous and a planar laminar flame front forms and propagates. Even though only 30% of the global iron mass has reacted, the combusted region occupies more than half of the domain since the hot products expand and compress the unreacted mixture, as in [27]. With increasing St the flame front becomes more wrinkled. At $St = 1/4$, the front shows large-scale wrinkling and the particles undergo moderate clustering, leading to locally higher temperatures and lower Y_{O_2} in the burned region. For $St = 1$, clustering

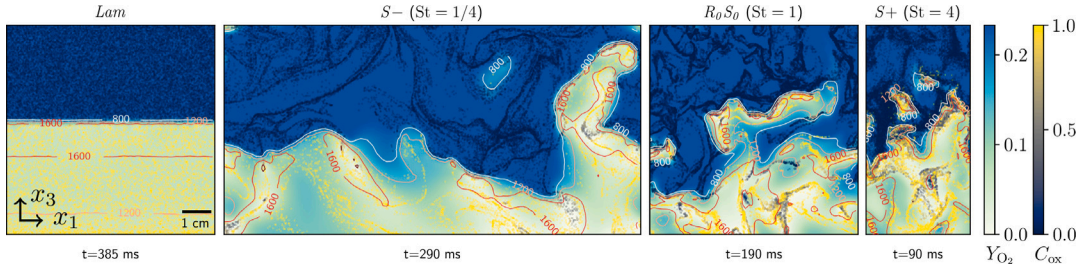


Fig. 2. Slices taken at times of equal global combustion progress $C_{\text{ox}}^{\text{glob}} = 30\%$. The actual times of the snapshots differ among simulations due to the different combustion speeds and are indicated below each slice. The flame propagates upwards. The contour color represents the oxygen mass fraction Y_{O_2} , the particle color represents the oxidation progress $C_{\text{ox}} = m_{\text{p,FeO}}/m_{\text{p}}$. The isolines show the gas temperature [K]. Due to the periodic setup, two flame fronts form after ignition; only the region $x_3 > L_3/2$ is shown here. The width of each slice is proportional to the domain length $L_1 = L_2$.

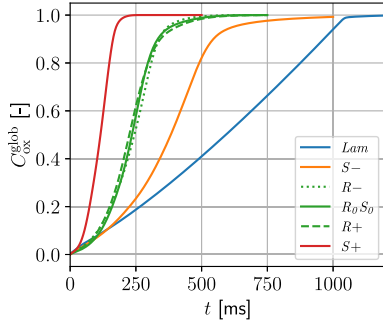


Fig. 3. Global combustion progress $C_{\text{ox}}^{\text{glob}}(t)$ for all cases.

of particles is strongest throughout the domain, as can be observed in the upper unreacted regions. This is known from literature [28,29] and quantified in our previous works [19,20]. The flame front is much more wrinkled, but the hot (reacted) regions and the cold (unreacted) zones are clearly separated. However, particle clusters in the hot region of the flow may remain partially unburned since local oxygen depletion hinders further oxidation. For $St = 4$, the flame front is heavily distorted showing features of corrugated flames. The separation between the burned and unburned zones is less evident since many fully oxidized particles are located in regions with otherwise cold gas and unreacted iron. In addition, there are more unburned particles inside the regions where $T > 800\text{ K}$, even close to the propagation front, where enough Y_{O_2} is still available. For such high Stokes numbers, the particle slip $\|\vec{u}|_{\vec{x}_p} - \vec{u}_p\|$ is statistically larger and therefore particles tend to move across the high gas temperature gradients. This is known to greatly enhance heat transfer for non-reacting particles [e.g.30–32]. Also, in our setup, the smallest turbulent scales decrease with increasing St as $d_p/\eta \sim \sqrt{St}$.

Qualitative observations from Fig. 2 are quantified in Fig. 3, which shows global combustion progress $C_{\text{ox}}^{\text{glob}}$ as a function of time for all cases. For *Lam*, without initial fluid motion, oxidation is the slowest and combustion progresses faster for increasing St . A conversion rate of $C_{\text{ox}}^{\text{glob}} = 80\%$ is reached approximately six times faster for the case *S+* compared to *Lam*, and the results do not suggest a saturation of the increase in oxidation speed for higher St in the investigated parameter range. The combustion progress seems unaffected by a change in Re_ℓ at constant $St = 1$, as the three cases *R-*, *R₀S₀* and *R+* show almost identical $C_{\text{ox}}^{\text{glob}}$ over time. This suggests that particle oxidation is mainly affected by small turbulent scales, and mildly influenced by the size of the largest scales ℓ , which will be further evaluated later.

Fig. 4 shows a scatter plot of the particle temperature versus C_{ox} , at the time of global oxidation of $C_{\text{ox}}^{\text{glob}} = 80\%$. The color indicates the $\log_{10}$ of $\hat{V}$, the Voronoi volume normalized by its mean, which is a measure of local clustering [19,33,34]. Particles in clusters have a smaller Voronoi volume and are colored in blue, while red indicates particles in regions

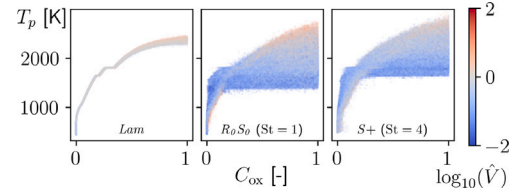


Fig. 4. Particle temperature vs. oxidation progress at $C_{\text{ox}}^{\text{glob}} = 80\%$, colored by normalized Voronoi volumes $\hat{V}$. Blue/red colors represent particles inside/outside clusters.

with a low particle number density. Reacting particles with sufficient oxygen available in their surroundings follow a well-defined curve in the T - C_{ox} plane, as observed for case *Lam*. However, in the turbulent cases, a large fraction of particles deviate from this curve, especially at intermediate C_{ox} . Most of these particles are clustered, where O_2 diffusion from oxygen-rich regions is the limiting factor for further progress of the reaction [20]. Here, only the cases *R₀S₀* and *S+* are shown, as the other turbulent cases yield very similar results.

4.1. Particle slip effects

For heterogeneous iron dust flames, where oxidation takes place solely on the particle itself, the flame propagation speed is limited not only by the reaction time of a single particle but also by the heat transfer from hot oxidized particles towards cold unburned particles [35]. This heat is conducted and convected through the gas phase. The relative motion of inertial particles can increase or limit this heat transfer, which is characterized by the two quantities

$$q_0 = \vec{u}_{\text{slip}} \cdot \vec{n}_T \quad (11a)$$

$$q_1 = \vec{u}_{\text{slip}} \cdot \vec{n}_T (T_p - T|_{\vec{x}_p}) \quad (11b)$$

with the particle slip velocity $\vec{u}_{\text{slip}} = \vec{u}_p - \vec{u}|_{\vec{x}_p}$ and the normal vector of the temperature gradient evaluated at the particle position

$$\vec{n}_T = \frac{\vec{\nabla} T|_{\vec{x}_p}}{\|\vec{\nabla} T|_{\vec{x}_p}\|} \quad (12)$$

The quantities in Eq. (11) can be evaluated for each particle over time, and are similar to the *particle heat fluxes* q_n introduced in [21]. The quantity q_0 is the scalar product of the slip velocity and the normalized temperature gradient and quantifies the motion of inertial particles through the iso-surfaces of the gas temperature. If a particle slips towards higher gas phase temperatures, q_0 is positive. If a particle moves relative to the gas phase towards colder regions, q_0 becomes negative. The quantity q_1 is the temperature difference between the gas and the particle multiplied by q_0 and can be interpreted as a heat flux induced by the motion of the particles relative to the fluid. For $q_0 < 0$ and $T_p - T|_{\vec{x}_p} > 0$, (i.e., a hot particle moves towards colder gas),

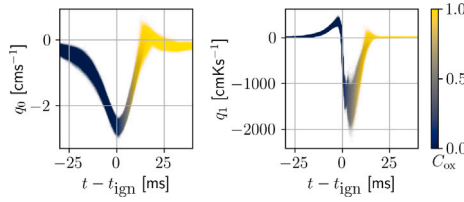


Fig. 5. Particle motion relative to temperature gradient q_0 and particle heat flux q_1 , for planar flame propagation *Lam*. Time is shifted by the individual particle ignition time t_{ign} .

q_1 is negative. The same is true for $q_0 > 0$ and $T_p - T|_{\bar{x}_p} < 0$ (i.e., a cold particle moves into a hot region). Therefore, $q_1 < 0$ corresponds to a mixing process in which particles transport heat across temperature gradients in the gas phase, thus diminishing the gradients.

Fig. 5 shows q_0 and q_1 scattered over time from the individual ignition time, for the planar flame propagation case *Lam*. t_{ign} is defined for each particle as the time with the maximum temperature increase dT_p/dt . Only particles that ignite while the overall combustion progress is in the range of $0.2 < C_{\text{ox}}^{\text{glob}}(t) < 0.8$ are plotted. This excludes the influence of the initial artificial heating $\dot{Q}_{\text{heat}}$ and late burnout, during which the periodicity of the domain might affect flame propagation. For case *Lam*, the particles and the fluid flow are statistically homogeneous orthogonal to the propagation direction x_3 , as shown earlier in the leftmost slice of Fig. 2. Therefore, both the slip velocity vector and the normalized temperature gradient are expected to be parallel to x_3 and $\|q_0\| \approx \|\vec{u}_{\text{slip}}\|$ holds. For times $|t - t_{\text{ign}}| > 20$ ms, the particles are far away from the flame front. Since for case *Lam* without any turbulent forcing, no strong velocity gradients are present away from the planar front, the particles can follow the slow motion of the gas phase, and the slip velocity (and therefore q_0) becomes zero. At the flame front, the heat release of the particles induces fast thermal dilatation, which the particles cannot follow perfectly. In this case, q_0 becomes negative, as the particles tend to stay in the colder part of the flame slightly longer due to their inertia. For $t < t_{\text{ign}}$, the particles are unburned, cold, and heat up through heat conduction in the gas phase. Around $t = t_{\text{ign}}$, the particles heat up very fast through their reaction, and the sign of $T_p - T|_{\bar{x}_p}$ flips. Also, q_1 , initially positive, then becomes negative. From this we can deduce that during preheating, the particle slip slows down the heat transfer ($q_1 > 0$) and therefore also the ignition propagation, while during reaction the slip enhances the heat transfer to the colder region ($q_1 < 0$). Compared to a theoretical flame without particle slip, the particles in the preheat zone are located in colder fluid, as they cannot effectively follow the fluid expansion towards higher T . However, in the reacting zone, the particles burn in a colder environment compared to a hypothetical no-slip dust flame. Here, slip enhances heat transfer and ignition propagation. q_1 stays below zero for much longer and with a higher absolute value, suggesting that the particle slip for the presented planar iron cloud flame increases flame speed.

While for case *Lam* both q_0 and q_1 scatter only slightly, the turbulent motion of all other cases introduces additional particle slip. These fluctuations of $\vec{u}_{\text{slip}}$ increase with *St*. Hence, we now evaluate the mean values $\bar{q}_n$, which are averages over all particle data at the same time relative to ignition $t - t_{\text{ign}}$.

Fig. 6 shows $\bar{q}_0$ and $\bar{q}_1$ over time for all investigated cases. The average of case *Lam* is by construction very similar to Fig. 5. In the left subplot of Fig. 6 at times before ignition, $\bar{q}_0$ increases for higher *St*, while Re_φ does not have a significant influence. Generally, if unreacted particles move through a hot gas region, they heat up and eventually ignite. For high *St*, high values of $\bar{q}_0$ before t_{ign} in Fig. 6 suggest that this relative particle motion is a relevant mechanism for ignition propagation, compared to heat conduction in the gas phase for *S-* and *Lam*, where $\bar{q}_0$ is negative. For case *S+* with *St* = 4, just after

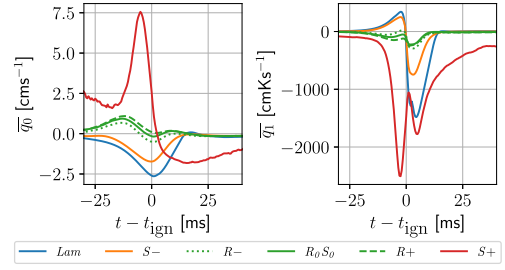


Fig. 6. Mean of particle motion relative to temperature gradient $\bar{q}_0$ and particle heat flux $\bar{q}_1$ for all cases. For $\text{St} \gtrsim 1$, the slip velocity before ignition tends to be in the direction of higher temperatures, leading to faster ignition.

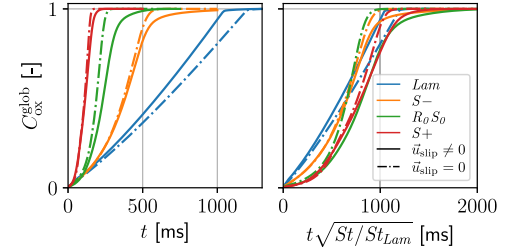


Fig. 7. Global combustion progress $C_{\text{ox}}^{\text{glob}}(t)$ for different cases, with particle slip turned on and off. On the right the time is scaled to collapse all simulations on case *Lam*.

ignition, particles return on average to colder regions due to their inertia ($\bar{q}_0 < 0$), further enhancing the mixing of heat ($\bar{q}_1 < 0$).

Furthermore, increasing *St* decreases η , leading to stronger turbulent mixing at the smallest scales. To distinguish between slip effects and turbulent mixing, we run additional cases where we force the inertial particles to behave as flow tracers, with $\vec{u}_p = \vec{u}|_{\bar{x}_p}$. We use initial turbulence fields identical to the main cases to keep d_p/η comparable, but with initially random homogeneous particle positions.

Left in Fig. 7, the oxidation progress over time is compared for the cases with and without slip. For *Lam*, where turbulence does not play a major role, setting the particle slip to zero indeed slows down the combustion, matching the analysis of Fig. 5. For the turbulent cases however, combustion is faster when particles behave as tracers. Clustering only occurs for inertial particles, so combustion with slip is slower than without slip, most prominent for case R_0S_0 with *St* = 1, where clustering is strongest. This suggests that the main reason for faster combustion with increasing *St* is the stronger turbulent small-scale mixing. To assess that, on the right panel of Fig. 7 we rescale time by $\sqrt{\text{St}/\text{St}_{\text{Lam}}}$ with $\text{St}_{\text{Lam}} = 1/12$ as empirical factor to collapse $C_{\text{ox}}^{\text{glob}}$ from turbulent combustion on *Lam*, for which the Stokes number is not well defined. This factor is related to the higher effective diffusivity through turbulence over plain molecular diffusivity. The collapse of $C_{\text{ox}}^{\text{glob}}$ as a function of $t\sqrt{\text{St}/\text{St}_{\text{Lam}}}$ for all cases suggests that the flame speed scales with the Kolmogorov speed $u_\eta \sim \sqrt{\text{St}}$. However, a single scale may not fully characterize the flame speed behavior [36], further analysis will be subject of future work.

This can be connected to the qualitative observations made earlier. A detailed view of the reaction zone for case *S+* with and without particle slip is shown in Fig. 8. Many fully oxidized particles are located in cold fluid regions, and unreacted particles can be found in the hot gas regions. Interestingly, this is also the case for the simulation without particle slip.

4.2. Flame propagation speed

Due to the periodic boundaries, fluid expansion at the reaction zone compresses the mixture. In a 1D flame propagation study in a similarly

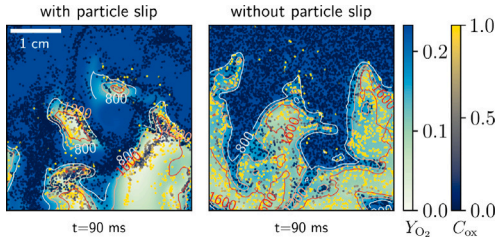


Fig. 8. Section of the flame front for case $S+$ at $C_{\text{ox}}^{\text{glob}} = 30\%$, with and without particle slip. Because of small scale turbulence at high Stokes numbers $St = 4$, many oxidized particles are located in cold gas regions, and unreacted particles are placed in hot regions, even without particle slip.

confined domain, the flame speed was defined through positions of igniting particles [27]. Here, we define the turbulent iron dust flame speed globally in the domain through the overall mass conversion rate as

$$s_C = \frac{dC_{\text{ox}}^{\text{glob}}}{dt} \frac{L_3}{2}, \quad (13)$$

which is not directly affected by thermal dilatation. The factor $L_3/2$ introduces a length scale to the dimensionless parameter $C_{\text{ox}}^{\text{glob}}$ which corresponds to the distance in x_3 -direction both flame fronts travel, while $C_{\text{ox}}^{\text{glob}}$ increases from 0 to 1.

The global flame speed s_C is plotted as a function of time for all cases in Fig. 9. For planar flame propagation (case Lam), the resulting speed is in the range of $7\text{--}13\text{ cm s}^{-1}$. By definition, s_C drops to zero when $C_{\text{ox}}^{\text{glob}} = 1$ is reached. The flame speed increases slightly during the simulation, which can be linked to the pressure increase during combustion. For case Lam , the maximum pressure at the end of combustion is 2.3 bar (3.5 bar for $S+$), and throughout the flame propagation the thermal dilatation compresses the unburned mixture. Therefore, the distance between particles in the unreacted mixture decreases, and also the temperature of the cold gas-particle mixture rises. The decrease in spacing of unburned particles can also be observed in Fig. 2, when comparing the particle density in the hot and cold regions. Both effects lead to an increase of the flame speed.

Although perfect agreement is not expected due to the difference in setups, the speed is in a similar range as literature data. Compared with 1D-simulations of laminar flame propagation using the same model [9], yielding a speed of $\sim 6\text{--}8\text{ cm s}^{-1}$ for $d_p = 10\text{ }\mu\text{m}$ and $\sim 2\text{--}3\text{ cm s}^{-1}$ for $d_p = 40\text{ }\mu\text{m}$, the presented simulation shows a faster flame propagation. However, experiments with particle sizes of 5 to $30\text{ }\mu\text{m}$ show a flame speed of 15 cm s^{-1} [37]. The simplistic iron oxidation sub-model used in the present study may not capture all the physics involved in particle ignition and flame propagation, e.g. the possible effect of oxide layers on particle ignition [8]. However, while the absolute predictions of flame speed in the present study may vary due to such effects, the overall trends are not expected to differ. With the introduced definition of s_C , the flame speed directly corresponds to the overall Fe oxidation speed, so as already discussed in Fig. 3, for higher Stokes numbers the flame speed increases, but is unaffected by changes of Re_ℓ . For case $S+$ with $St = 4$, s_C reaches values up to 69 cm s^{-1} . As discussed previously, this increase is attributed to higher turbulent small scale mixing of heat in the reaction zone. Due to the periodic domain, the two flame branches interact once the global conversion reaches $C_{\text{ox}}^{\text{glob}} \approx 50\%$, causing the flame speed to drop towards the end of combustion.

4.3. Flame front surface area

For premixed gas flames, the turbulent flame speed is strongly correlated with the surface area of the wrinkled flame front, which increases for higher Re_λ [38]. In the following, we investigate the analogy between wrinkled premixed gas flames and iron dust flames. Since the

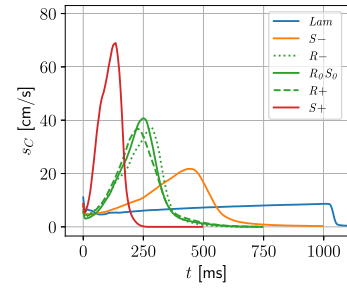


Fig. 9. Comparison of flame propagation speed, based on overall mass conversion, i.e., Eq. (13).

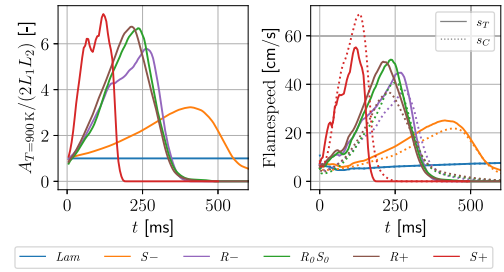


Fig. 10. Left: Normalized surface area of the $T = 900\text{ K}$ contour. Right: Turbulent flame speed s_T calculated from surface area $A_{T=900\text{ K}}$ compared to s_C as in Fig. 9.

discretely reacting particles do not form a well-defined surface, we use isocontours of the gas temperature to define a continuous flame surface. The gas temperature has already been used to quantify the propagation of iron flames in the context of particle group combustion [39]. From the isocontour surface area $A_{T=900\text{ K}}$, we compute an estimate of the flame speed as

$$s_T(t) = \frac{A_{T=900\text{ K}}(t)}{2L_1L_2} s_C^{\text{Lam}}(t), \quad (14)$$

where $s_C^{\text{Lam}}(t)$ is the flame speed of case Lam evaluated at the same combustion progress $C_{\text{ox}}^{\text{glob}}$, accounting for its increase due to pressure rise.

Fig. 10 shows the area of the flame fronts $A_{T=900\text{ K}}$ on the left for all cases and the comparison between s_C and the estimated flame speed s_T on the right. The area remains constant for Lam , but increases by up to a factor of 7 for R_0S_0 , $R+$ and $S+$, in which the flame surface is highly wrinkled, as observed earlier in Fig. 2. On the right of Fig. 10 the flame speeds are shown, both the calculated s_C and s_T , the estimation through the isocontour surface area. The speeds agree reasonably well, best for $S-$. For cases with $St = 1$, the flame speed is overpredicted, which can be caused by the formation of clusters, where ignited particles cannot fully burn out due to the lack of Y_{O_2} . s_T matches better at earlier times for each case, since for $C_{\text{ox}}^{\text{glob}} > 50\%$ the two flame branches influence each other through the periodicity of our domain.

5. Conclusion

We studied the effect of turbulence and Stokes number on the flame propagation in iron particle combustion using a carrier-phase DNS approach. Adjusting the domain size and turbulent forcing, we changed the Reynolds number independently of the Stokes number and investigated the parameter range $57 \leq Re_\ell \leq 250$ and $1/4 \leq St \leq 4$, as well as a planar reference case. The observed planar flame

speed $7 - 13 \text{ cm s}^{-1}$ agrees with other experimental and numerical works. Defining the flame surface as the isocontour $T = 900 \text{ K}$ in the gas phase, we give an estimate of the turbulent flame speed relative to the planar propagation speed. In summary, this work answered our three posed research questions:

- Q1 The flame speed is largely unaffected by Re_ℓ at constant St in the range $57 \leq \text{Re}_\ell \leq 250$.
- Q2 The flame speed increases with St since the smaller turbulent scales increase the local heat transfer, resulting in over six times faster overall combustion for $\text{St} = 4$ compared to a planar flame. Particle slip increases the flame speed for the investigated planar flame configuration.
- Q3 The flame speed scales with the flame surface area defined by a selected gas temperature isocontour, and this estimate of the turbulent flame speed matches reasonably well the value obtained directly from the global oxidation progress. However, the effects of particle slip and clustering need to be considered for more accurate flame speed predictions in heterogeneous iron dust flames.

For realistic burners this implies that small scale turbulent mixing seems to be the key factor for fast iron particle cloud combustion. While the absolute values of flame speed reported may be related to the comparatively simple iron oxidation sub-model, the presented trends are likely qualitatively robust. A detailed analysis of the relationship between clustering and flame surface area, aimed at improving estimates of turbulent flame speeds, as well as the differences for other sub-models, is reserved for future work.

CRedit authorship contribution statement

Gabriel Thäter: Software, Validation, Formal analysis, Methodology, Visualization, Writing. **Maurizio Carbone:** Software, Validation, Formal analysis, Writing – review & editing. **Alessandra Zanini:** Formal analysis, Methodology. **Oliver T. Stein:** Conceptualization, Supervision, Writing – review & editing. **Bettina Frohnapfel:** Conceptualization, Supervision, Funding acquisition, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The authors gratefully acknowledge the financial support of the Helmholtz Association of German Research Centers (HGF), within the MTET program and HPC time via bwHPC.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at <https://doi.org/10.1016/j.proci.2026.106663>.

Data availability

The postprocessed data used in this work is accessible at <https://dx.doi.org/10.35097/e0fbwzmktfmhubne>, including all scripts necessary to create the figures in this publication.

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