

# Analysis of flame front velocities in planar iron particle cloud flames

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## Motivation

A redox cycle involving iron as a fuel is a promising strategy for storing and transporting energy from renewable sources. During the oxidation of micron sized iron particles, the metal and its oxides stays mostly solid or liquid, while heterogeneous combustion on the particles occurs. The flame propagation through an iron-air suspension behaves therefore differently compared to common solid fuel types. Within this work we conduct carrier-phase Direct Numerical Simulations (CP-DNS) of propagating flames through initially homogeneously distributed iron particles, and suggest a way to evaluate the flame velocity based on particle quantities.

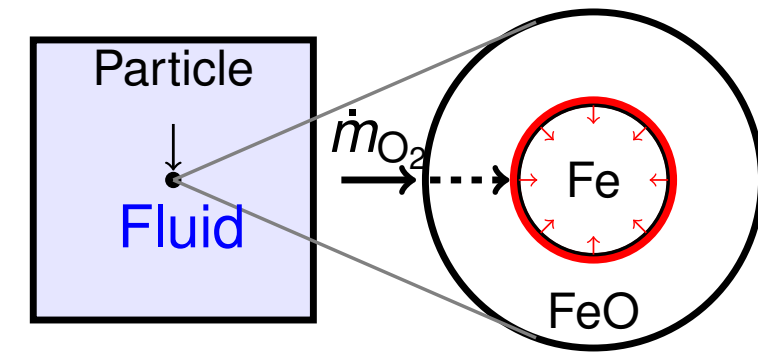
## CP-DNS approach

### Fluid phase [1,2]

- Low-Mach assumption,  $O_2/N_2$  mixture
- Governing equations for momentum, enthalpy, oxygen mass fraction are solved
- Particle feedback on fluid phase is implemented through non-uniform FFT

### Iron particles [3]

- Particle boundary layer modeled
- Iron combustion model includes Stefan flow, melting plateaus, radiation losses
- Particle momentum equation is solved, they can have a slip velocity



## Simulation setup

- 3D cube with 5 mm side length and periodic boundaries
- Iron-air mixture with  $\phi = 1$

### Initial fluid parameters:

- $u_{i,0} = 0 \text{ m s}^{-1}$ ,  $T_0 = 310 \text{ K}$ ,  $Y_{O_2,0} = 0.233$
- $32^3$  resolved Fourier modes

### Initial particle parameters:

- Initially homogeneously distributed
- $d_{p,0} = 10 \text{ }\mu\text{m}$ ,  $T_p(t=0) = T(t=0)$ ,  $\vec{u}_{p,0} = \vec{u}(\vec{x}_p, t_0)$

### Particle heating:

- A sheet with thickness 0.4 mm is initially heated for 0.05 ms with  $10^9 \text{ W m}^{-2}$
- $\zeta_1$ : Block profile with smoothed edges
- $\zeta_2$ : Gaussian distribution

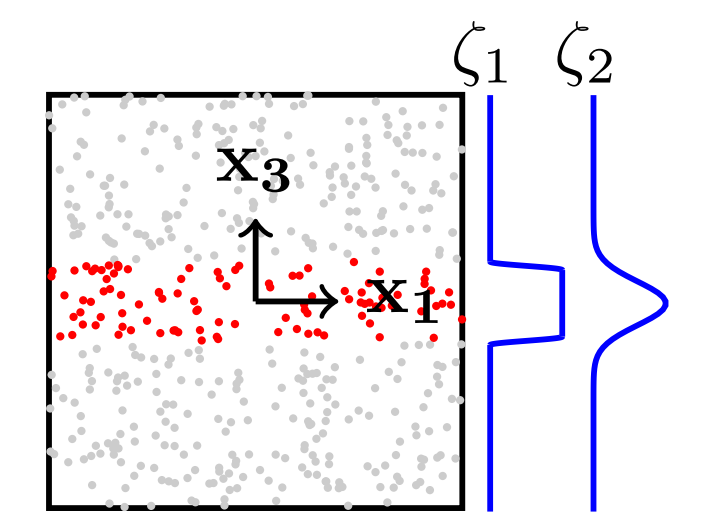


Fig.1: Particle heating distributions

## Planar flame propagation

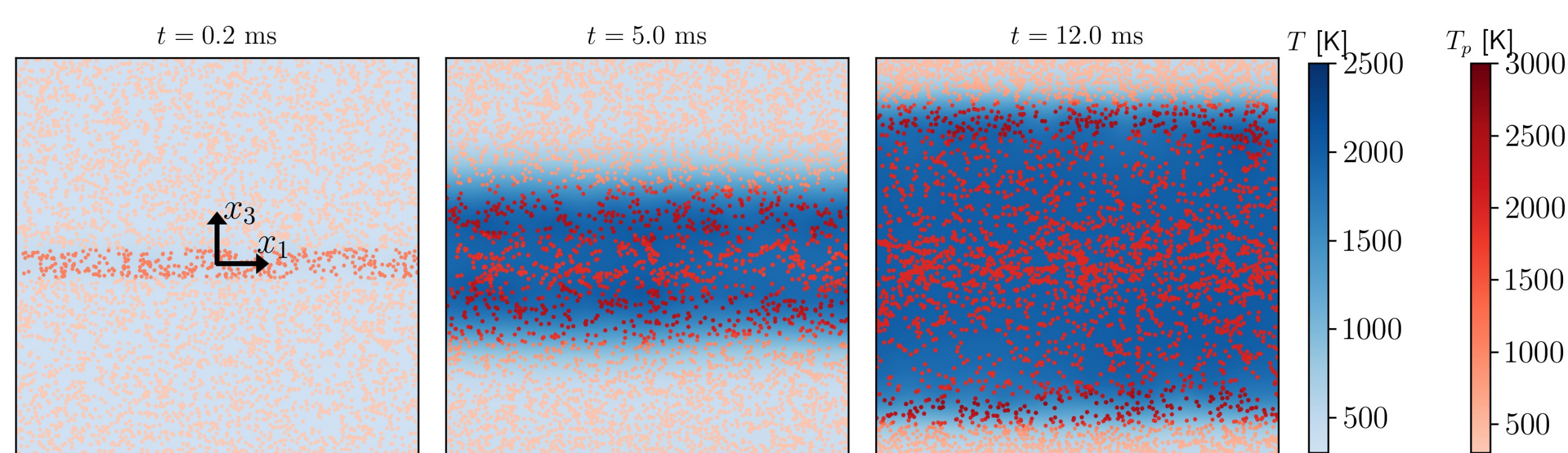


Fig.2: 2D temperature slices at different times for  $\zeta_1$  heating. A planar flame front, visible through the increase in temperature, propagates in both directions from the initially ignited zone.

- At  $t = 0.2 \text{ ms}$ , the particle heating is complete, leaving behind a slice of hot particles that initiates self-sustained flame propagation.
- The particle distribution evolves due to expansive and contractive fluid motion.
- There are no substantial inhomogeneities in the fluid temperature along the flame front.

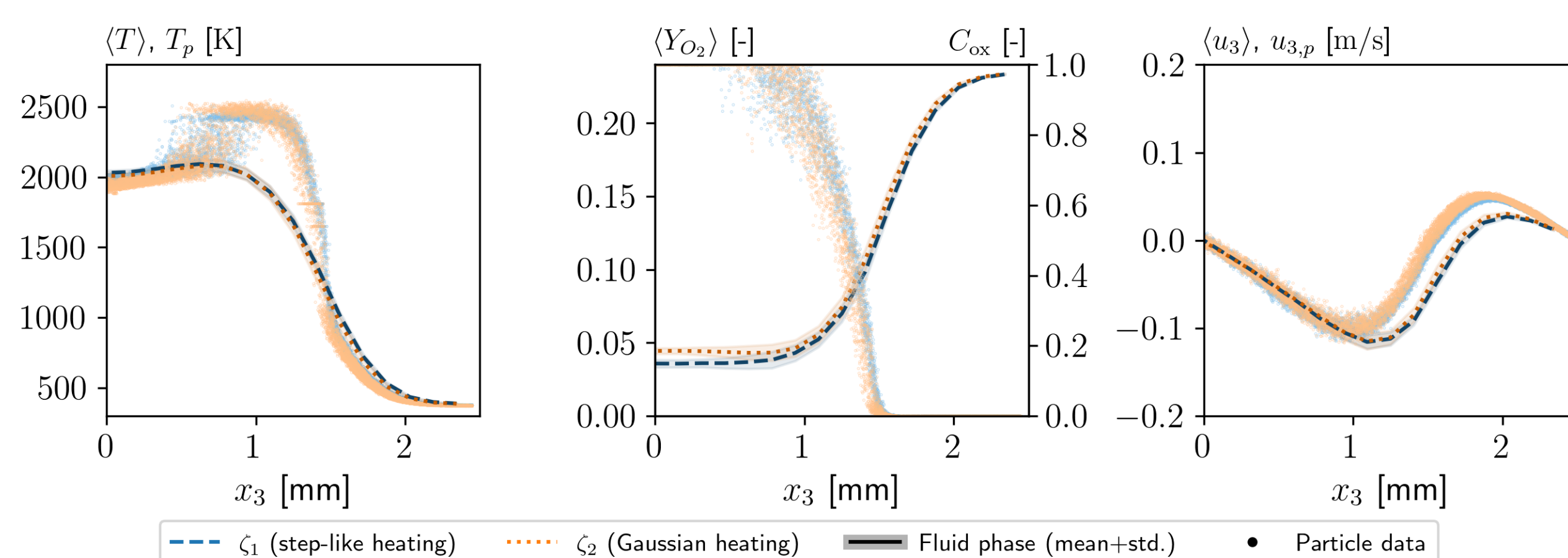


Fig.3: Mean fluid and particle properties at  $t = 7.8 \text{ ms}$  ( $\zeta_1$ ) /  $t = 8.2 \text{ ms}$  ( $\zeta_2$ ) over  $x_3$ -component. Even though the initial heating differs, the resulting flame fronts look similar. Only the upper part  $x_3 > 0$  of the domain is shown.

- Fluid quantities are averaged to obtain 1D profiles of temperature, oxygen concentration, and velocity across the flame front, as shown in Fig. 3.
- Variations in initial heating do not lead to significant deviations at later times.

➔ How can an iron particle flame velocity be calculated when both the particle and gas phase are moving?

## Calculating a heterogeneous flame front velocity

### Calculation procedure

- Only consider particles currently reacting  $\rightarrow C_{ox} = m_{p,FeO}/m_p \in (0.2, 0.8)$
- Divide the domain in  $N_{Box}$  boxes along each direction, each particle is located in a box depending on the position  $\vec{x}_p$

$$f_i = \frac{\text{Mean part. position} \langle \vec{x}_{i,p} \rangle_{Box}^{(n)} - \text{Mean part. position, last step} \langle \vec{x}_{i,p} \rangle_{Box}^{(n-1)}}{\Delta t} - \text{Mean fluid velocity at part. position} \langle u_i(\vec{x}_p) \rangle_{Box}^{(n)} \quad (1)$$

- To avoid artefacts at box boundaries, this computation is performed  $N_{shift}^3$  times, shifting the box center by  $L_{Box}/N_{shift} = L/(N_{Box}N_{shift})$  along each direction

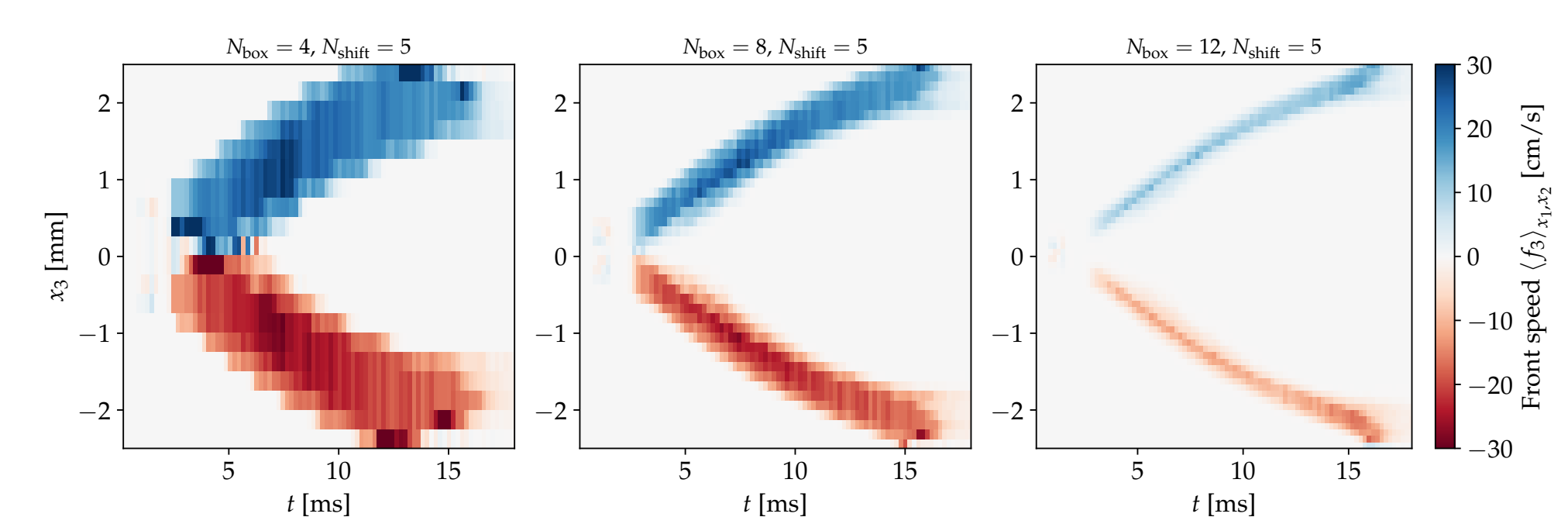
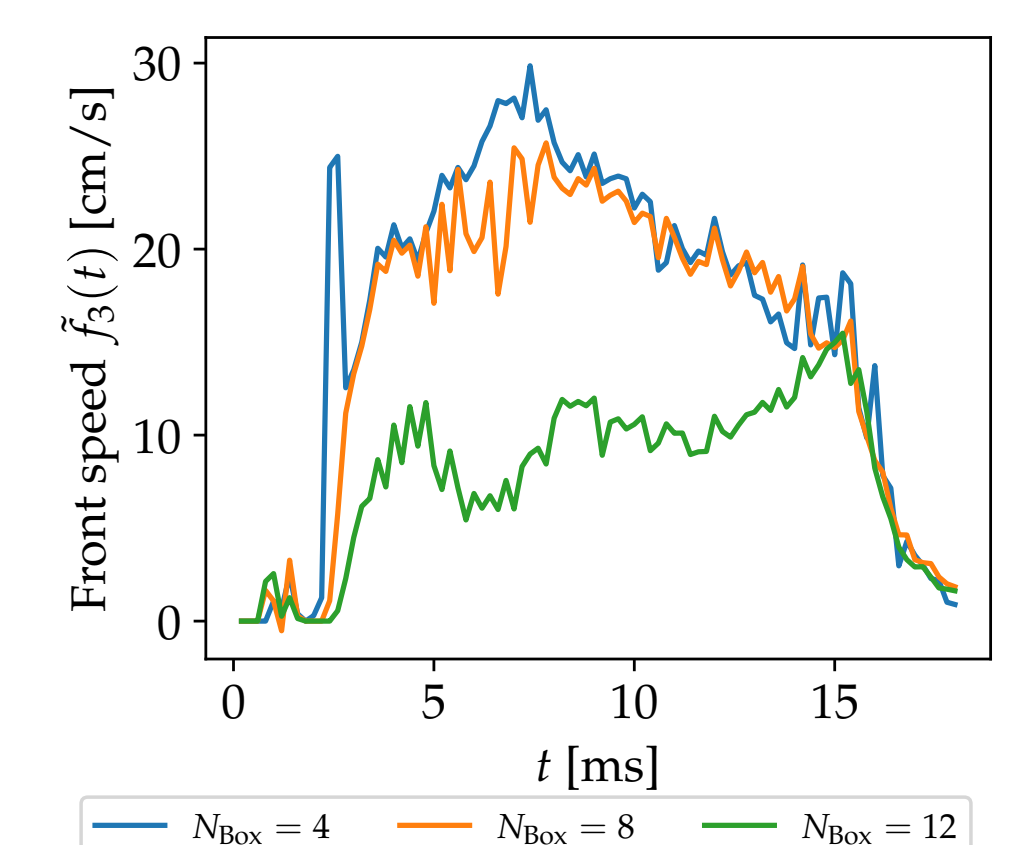


Fig.4: Front velocity distribution over time for different box sizes  $L_{Box} = L/N_{Box}$

- Propagation velocities based on particle phase
- Calculated flame velocities range between  $15\text{-}25 \text{ m s}^{-1}$
- Higher values than other numerical and experimental work [4]
- Calculation will be used for
  - Larger domains
  - Flame propagation through homogeneous isotropic turbulence (HIT)



## Conclusion

- We present a setup with a planar iron particle combustion front
- The shape of the initial heating does not influence combustion at later times, as long as the flame propagation is initiated
- We propose a procedure to calculate the flame propagation based on particle quantities
- First results show flame velocities comparable but larger than other works

## References

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