Assessment of CFD phase models for simulating iron combustion in retrofitted coal combustion chambers

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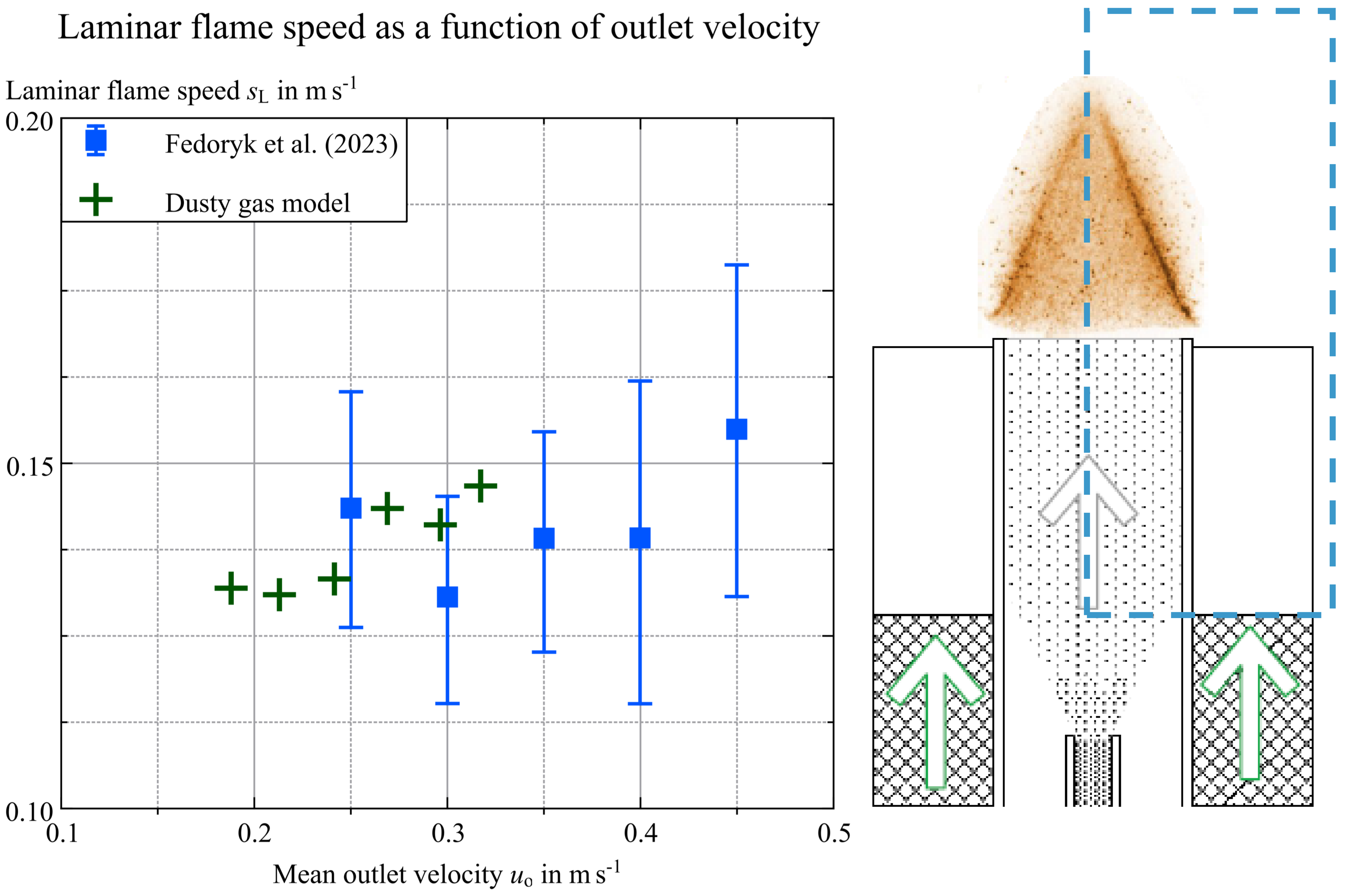

Figure 1: (left) Laminar flame speed of iron Bunsen burner flames as a function of the mean outlet velocity. CFD values are shown in green, whereas experimental results [1] are shown in blue. (right) The experimental modified Bunsen burner, with the simulated system overlaid in blue (adapted from [1]).

Motivation

The DLR project IronCircle® is investigating retrofitting coal-fired power plants to generate clean energy by burning iron. Our investigative methods include CFD simulations of iron combustion, which require multiphase models to accurately reflect the physics involved. This work examines potential models and their usage.

Dusty Gas

A single Eulerian phase models the continuum; particle trajectories are assumed to perfectly follow streamlines, allowing modelling a particulate system through a single set of Navier-Stokes equations for the Eulerian field. An extension to this model uses algebraic equations for particle velocities. The dusty gas model is accurate for small particles at low volume fractions. A relevant parameter is the Stokes number Stk: the ratio between the particle relaxation time and the characteristic flow time.

Euler-Lagrange

The Eulerian field representation of flowing continuums is combined with the Lagrangian representation of discrete point particles. Field values are calculated using Navier-Stokes equations, whereas each particle has its own equations of motion. Therefore, simulating large numbers of particles this way is often computationally expensive.

Euler-Euler

Particles and continuums are both modelled as fields, allowing identical particles to be solved for by a single set of Navier-Stokes equations. This constrains the overall number of equations required to model the system; however, the modelling of physics related to particle properties is limited.

Sectional Approach

An extension to Eulerian particle models, this approach groups particles into distinct fields based on a particular characteristic (e.g. diameter). Transport equations are solved for each field separately. At large particle numbers, the increase in equations needed to be solved is negligible compared to Lagrangian models.

Computational Set-Up

A mesh based on a modified Bunsen burner [1] and its surroundings was constructed and the combustion of iron particles under FeO-stochiometric conditions, modelled as a dusty gas, was simulated in OpenFOAM v11. Particle suspension combustion kinetics were modelled using a modified Arrhenius equation [2-4]:

$$\mathrm{Fe}_{(l)} \longrightarrow \mathrm{FeO}_{(l)}$$

$$r = k\,[\mathrm{Fe}_{(l)}]\,[\mathrm{O}_2]$$

$$k = 10^1 k_0\, A_p\, N_p$$

Modified Arrhenius equations [5] were further used to model phase changes in Fe and FeO:

$$\mathrm{Fe}_{(s)} \rightleftharpoons \mathrm{Fe}_{(l)}$$

$$\mathrm{FeO}_{(l)} \rightleftharpoons \mathrm{FeO}_{(s)}$$

Laminar flame speeds were determined using the outlet velocity/flame angle method [1]. As shown in Figure 2, mean outlet velocities were determined by taking half of the maximum z-component of velocity observed 1 mm below the Bunsen burner spout, while flame angles were determined by taking the angle of the heat release field $\dot{Q}$, limited to values above 10^4 W, against the vertical at the flame tip.

Results

Figure 1 shows numerical and experimental [1] laminar flame speeds plotted against outlet velocities. Our values tend to increase with increasing outlet velocity.

Our values broadly agree with the experimental values, although were not able to replicate stable flames for $u_0 \geq 0.35\ \mathrm{m\,s^{-1}}$ using the above parameters.

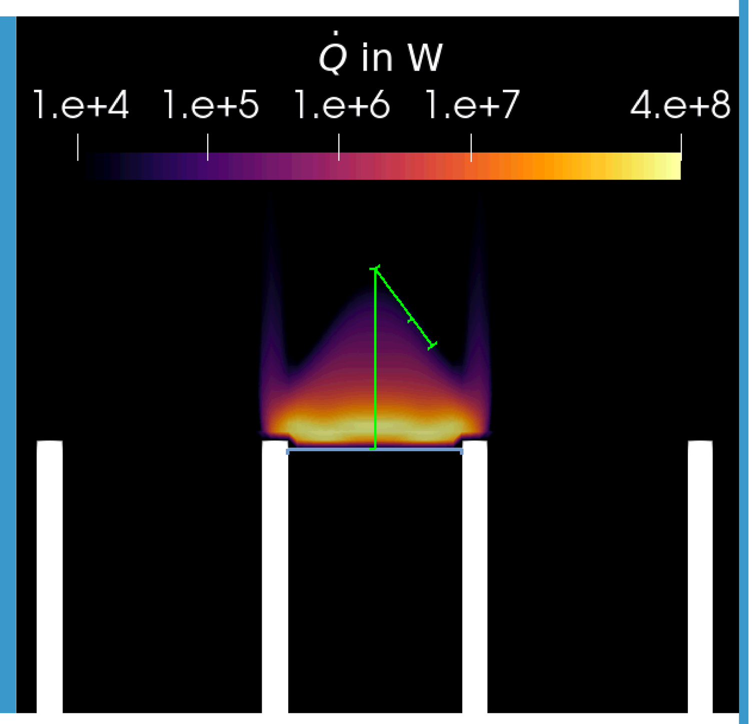

Figure 2: Visualisation of the heat release field $\dot{Q}$ of a simulated iron particle flame. The angle between the green lines represents the flame angle; the outlet velocities were sampled along the blue line.

Outlook

Both modelling the further oxidation of iron to Fe_2O_3 and the implementation of a sectional approach to assess effects of the particle size distribution on combustion are planned. Implementation of iron suspension combustion in an Euler-Euler model within the CFD software MFiX is underway.

References

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