# The use of iron powder as a cyclic energy carrier

## Dutch Section of the Combustion Institute webinar

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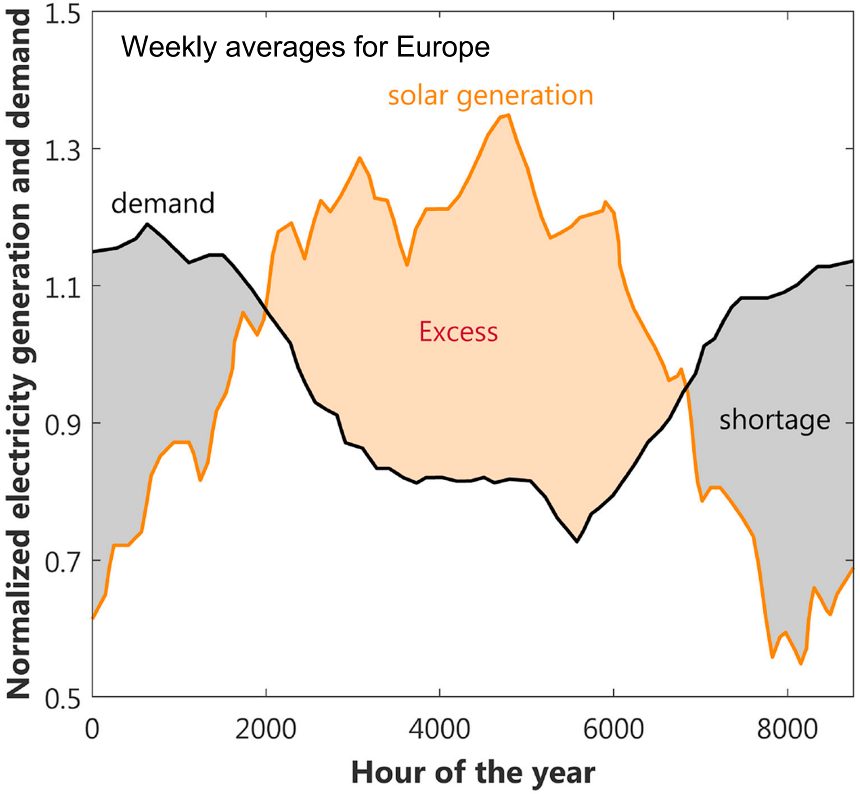
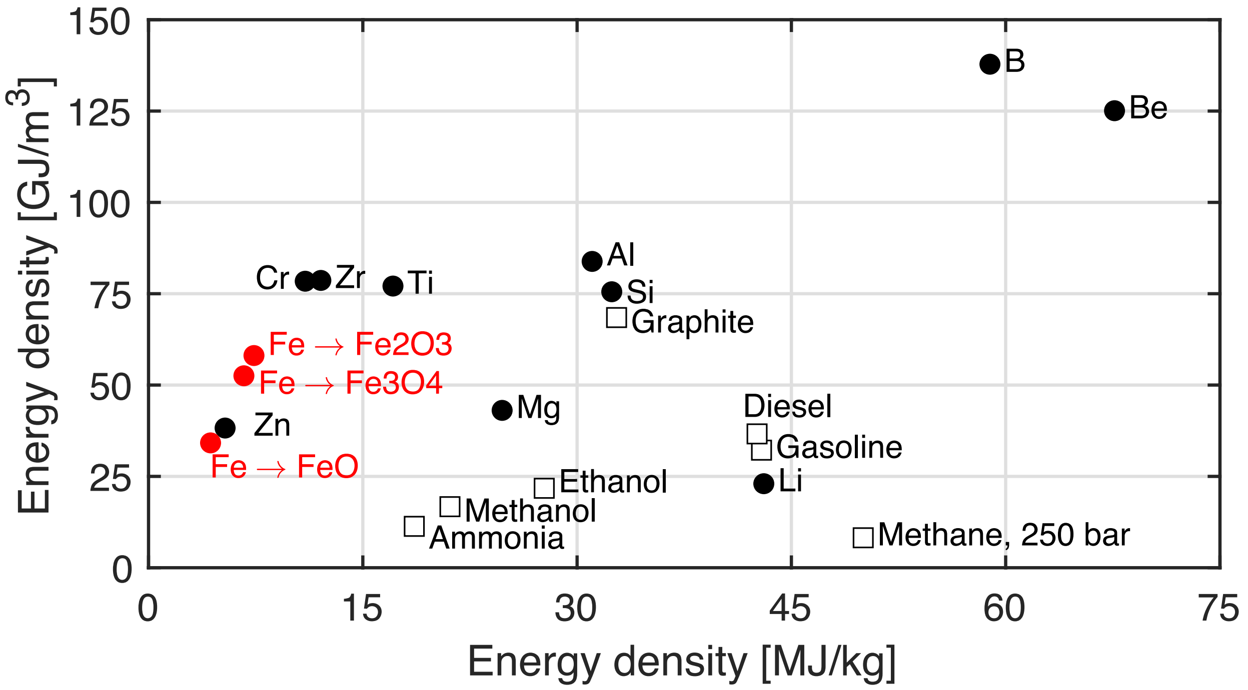
# Transitioning towards the use of sustainable energy

- Fossil fuels: producing $CO_2$, dependency on oil- and gas-producing countries...
- Sustainable energy sources (wind, solar) are intermittent (daily to yearly) and variable.
- Energy should be available when and where we need it: how can we store and transport this energy?
- How can we make use of existing infrastructure as much as possible?



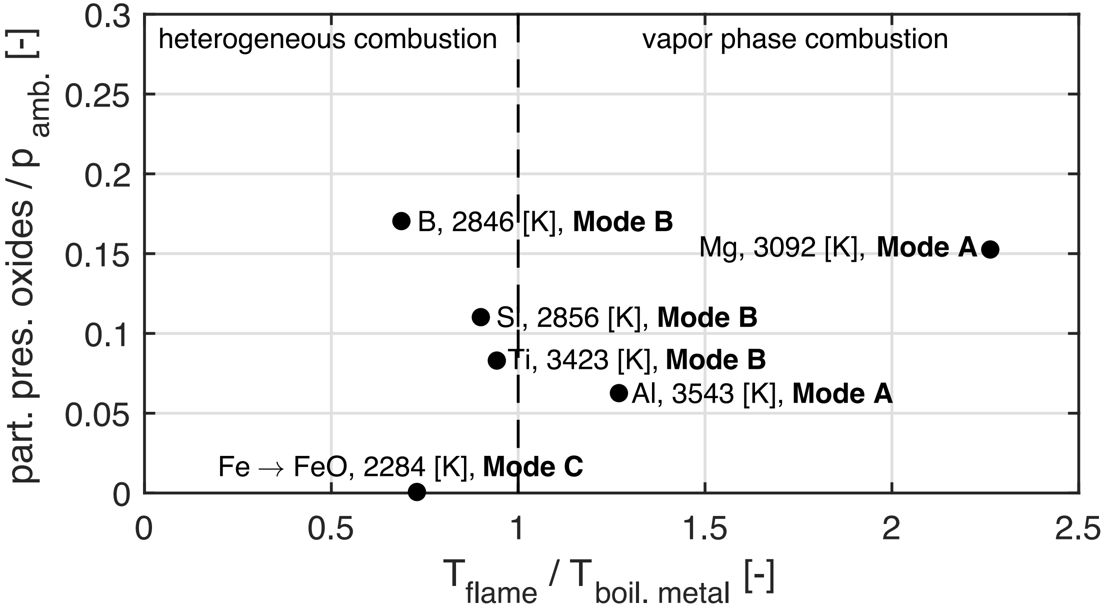
Gabrielli et al. (2020) Renew Sustain Energy Rev.

# Metal powders as energy carriers (1)

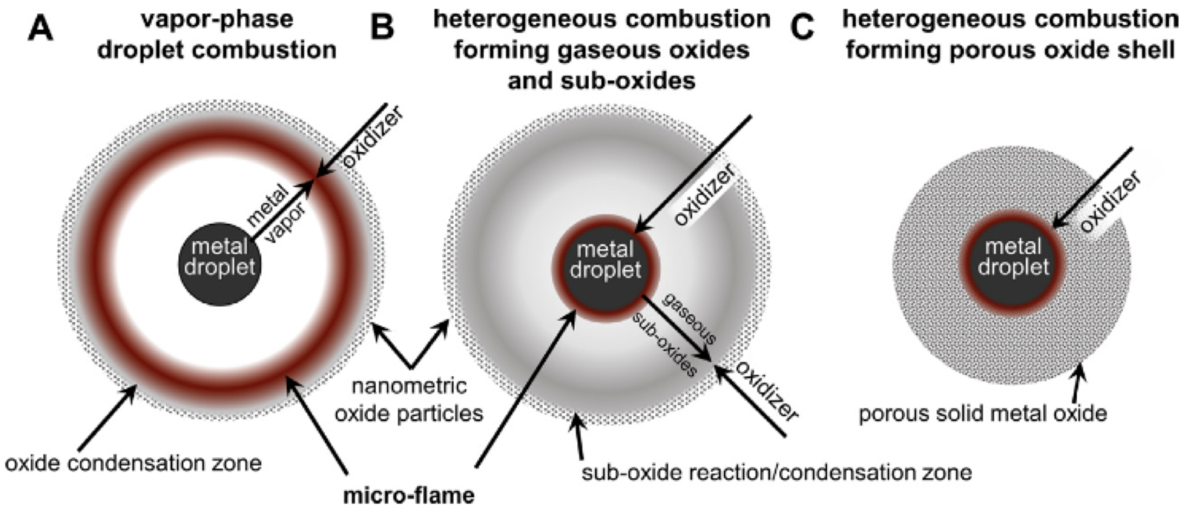


- Batteries: energy density O(1 MJ/kg, 1 GJ/m$^3$). Suitable for small-range e-mobility.
- Hydrogen: energy density O(100 MJ/kg, 1 GJ/m$^3$). Requires low-temperature/high-pressure storage.
- Ammonia, formic acid: toxicity...
- Metals: $CO_2$ free, similar volumetric energy density as fossil fuels, low gravimetric energy density.

# Metal powders as energy carriers (2)



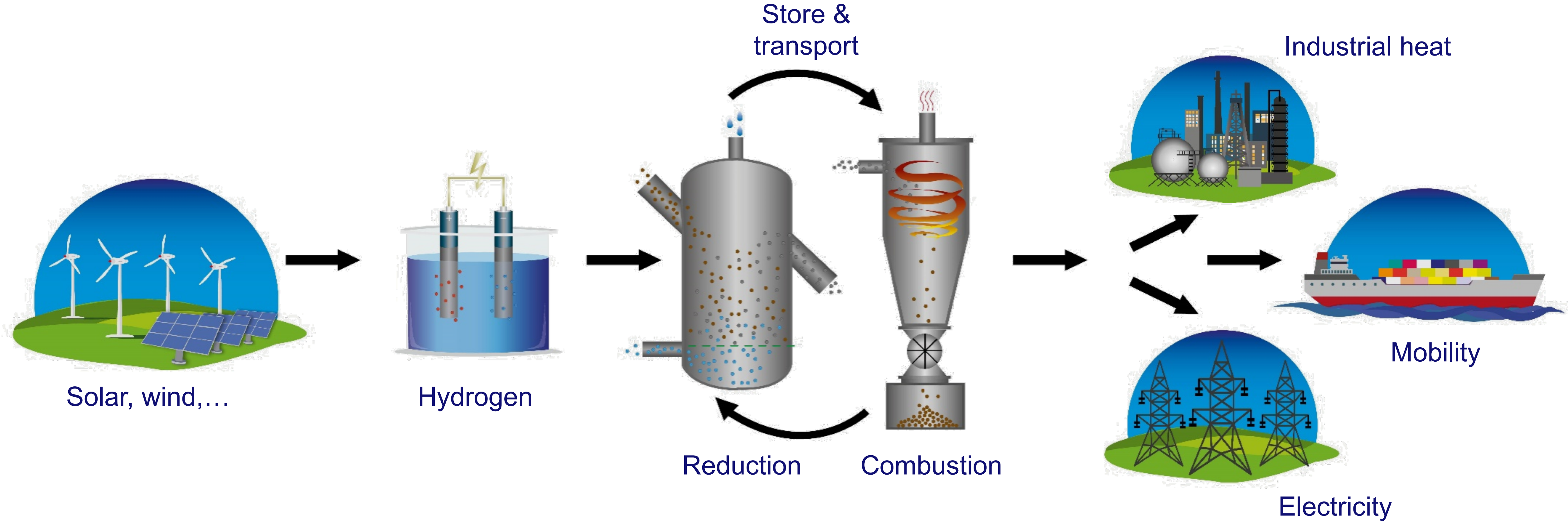
Selection of metals: Julien et al. (2017) Sustain Energy Fuels



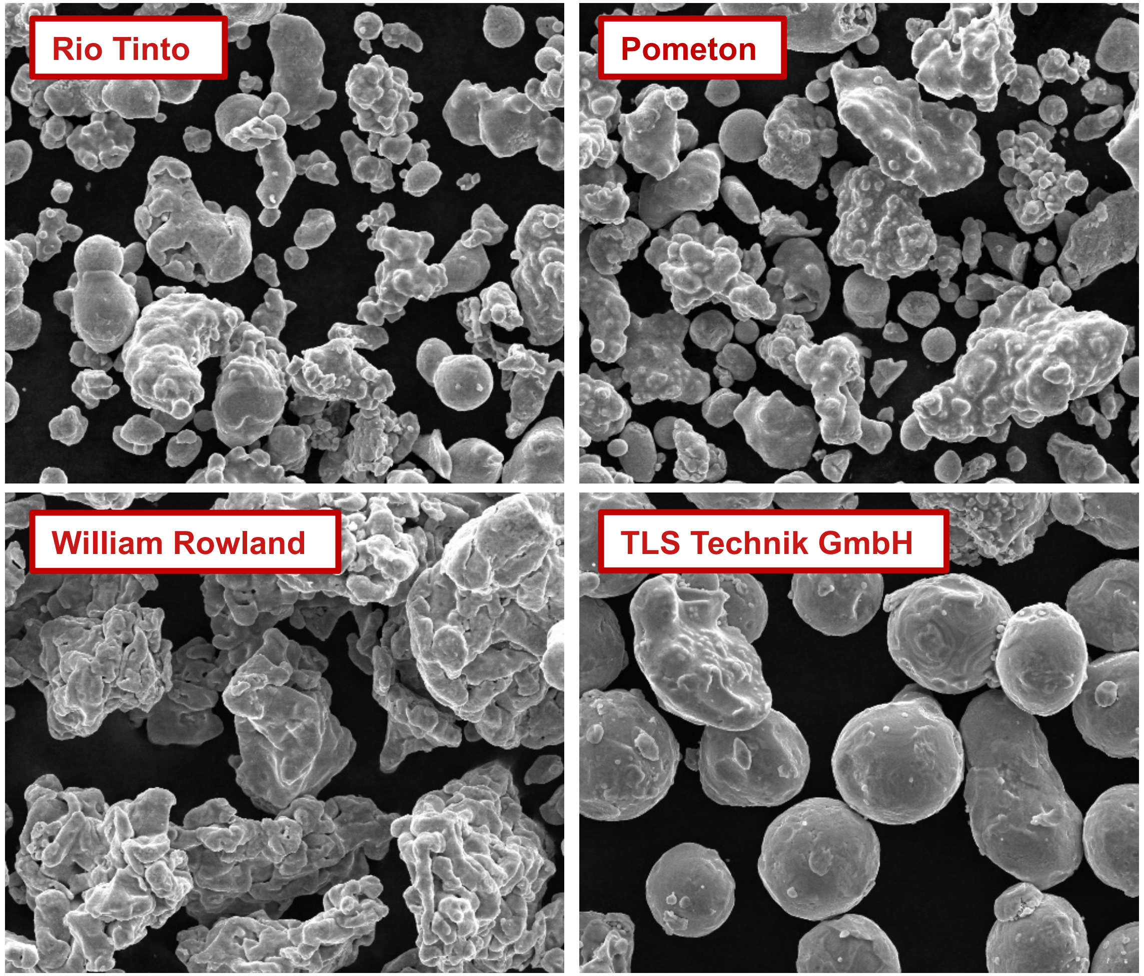
Bergthorson et al. (2015) Applied Energy.

- Except for iron, all other selected metals burn in vapor-phase and/or produce significant amounts of gaseous oxides (and nanoparticles)!
- Iron: safe, recyclable, cheap, compact.

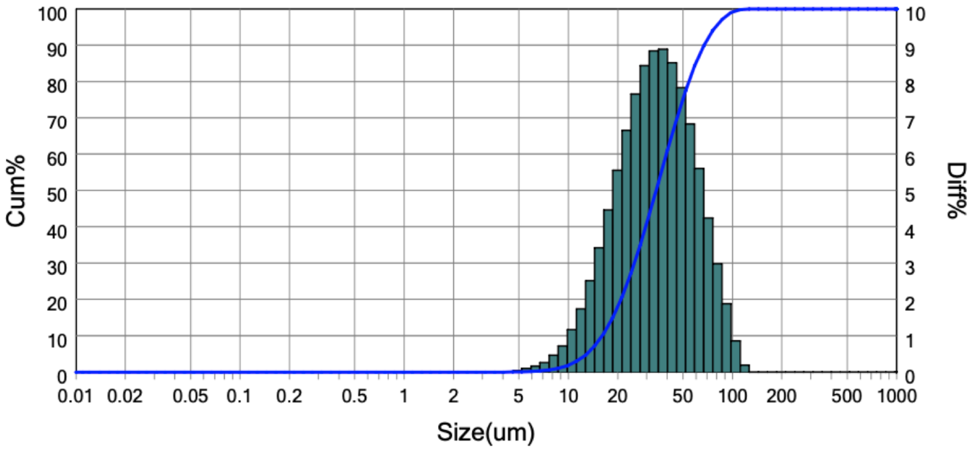
# Envisioned metal fuel cycle

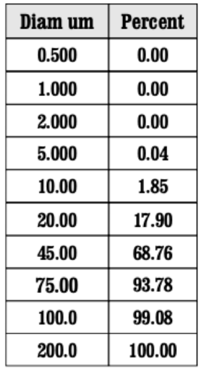


# How do (unburnt) iron particles look like?



Images: courtesy of C. Hessels (TUE).



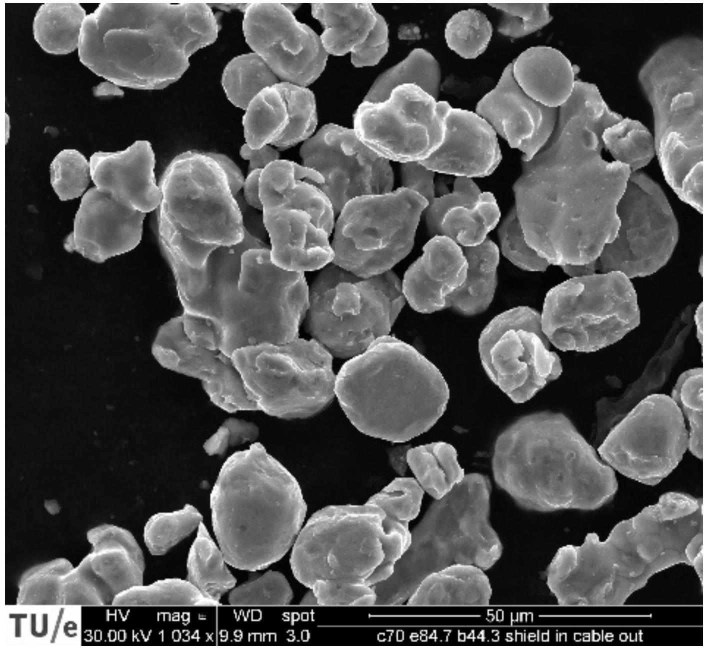


| Diam um | Percent |
|---|---|
| 0.500 | 0.00 |
| 1.000 | 0.00 |
| 2.000 | 0.00 |
| 5.000 | 0.04 |
| 10.00 | 1.85 |
| 20.00 | 17.90 |
| 45.00 | 68.76 |
| 75.00 | 93.78 |
| 100.0 | 99.08 |
| 200.0 | 100.00 |

**Important characteristics of powders:**

- Particle Size Distribution (PSD).
- Specific surface/porosity/morphology.
- Contamination by impurities (Si, Cr, Mn)

# What happens to particles during oxidation/reduction?



**Before combustion**

**After combustion**

Mainly spherical particles. Some particles seem to have ”exploded”

**After reduction**

Porous spherical particles. Reduction conditions (temperature, reducing agent) affect porosity.

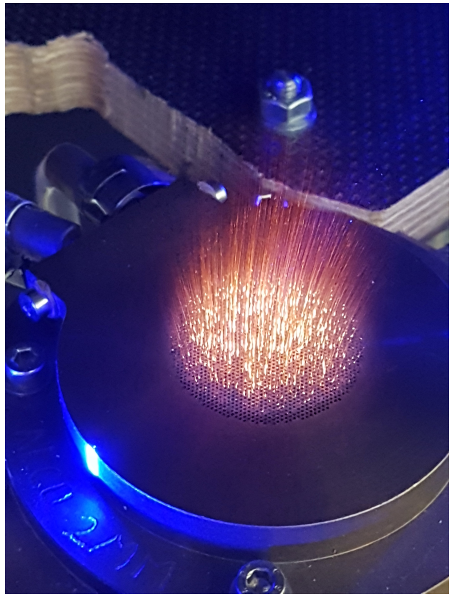
Images: courtesy of C. Hessels (TUE).

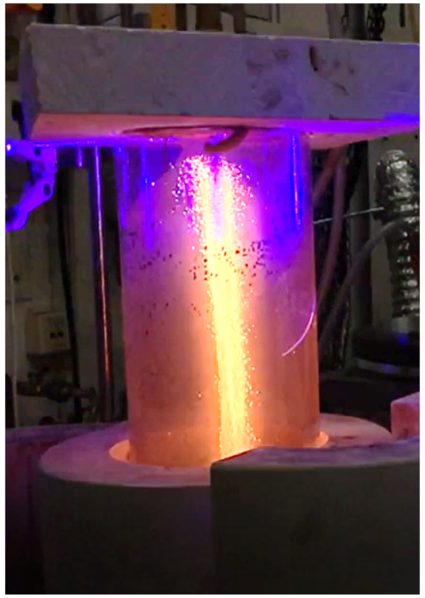
# Iron powder combustion: from particles to MW-scale

Modeling and experiments: **knowledge is (still) limited and only rudimentary models exist!**

- Single particle combustion.
- Flame propagation in clouds of particles.
- Large scale turbulent combustion of metal powder.

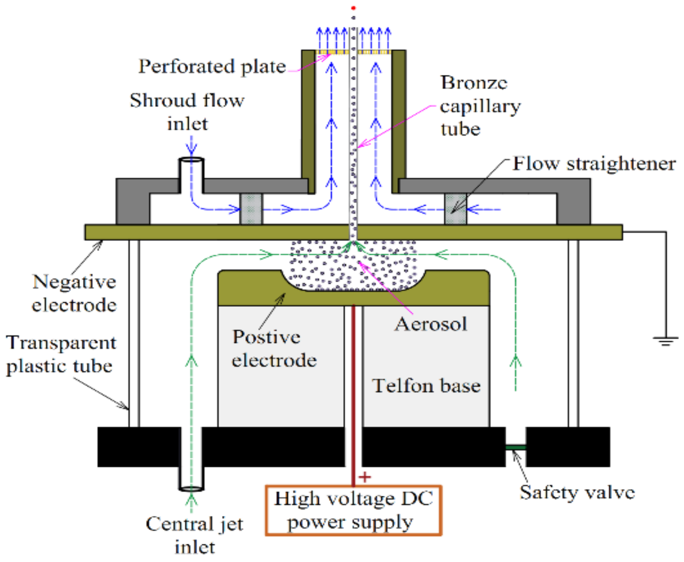

Single particle burner

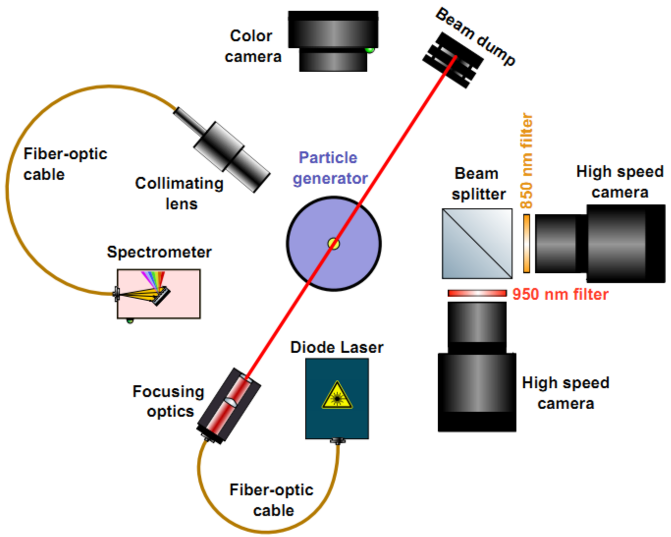

Laminar iron powder flame

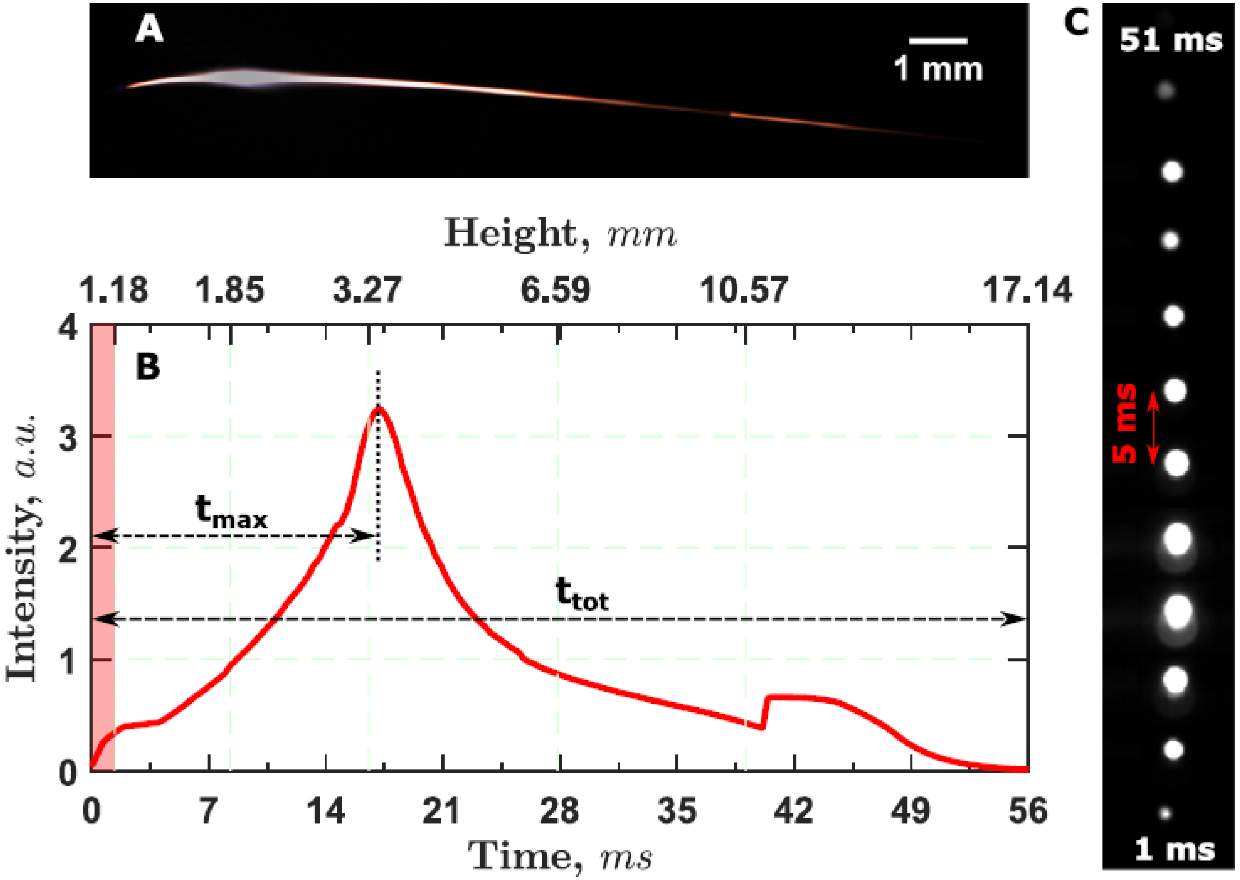

Tornado burner (3 kW)


100 kW proof-of-concept

# Single particle oxidation experiments: set-up

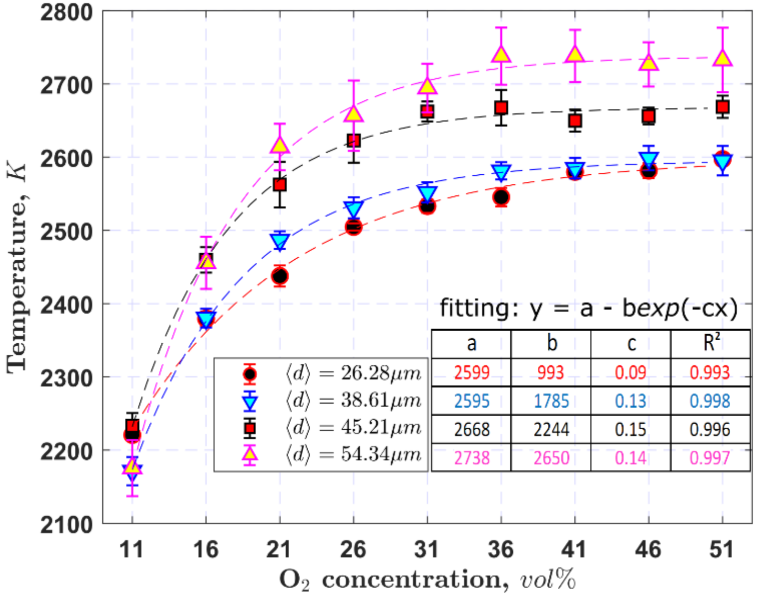




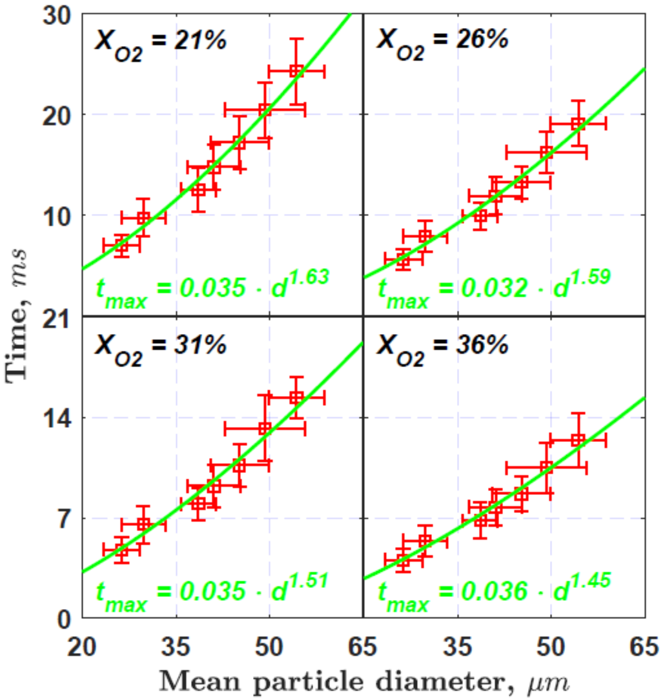


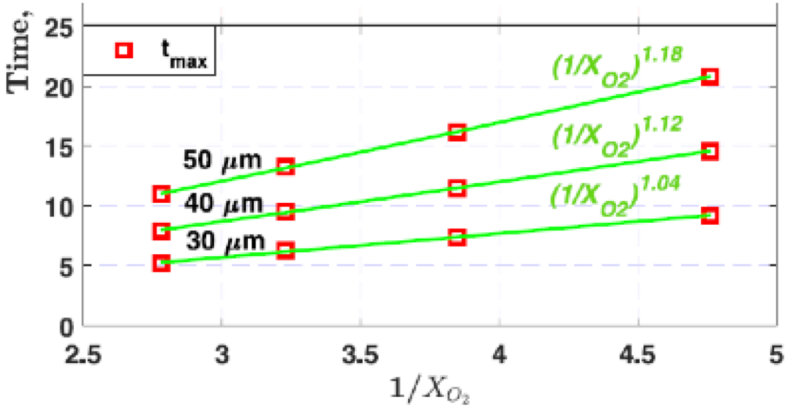
D. Ning et al. (2021) Combust Flame.
D. Ning et al. (2022) Combust Flame.

# Single particle oxidation experiments: important findings



| a | b | c | $R^2$ |
|---|---|---|---|
| 2599 | 993 | 0.09 | 0.993 |
| 2595 | 1785 | 0.13 | 0.998 |
| 2668 | 2244 | 0.15 | 0.996 |
| 2738 | 2650 | 0.14 | 0.997 |





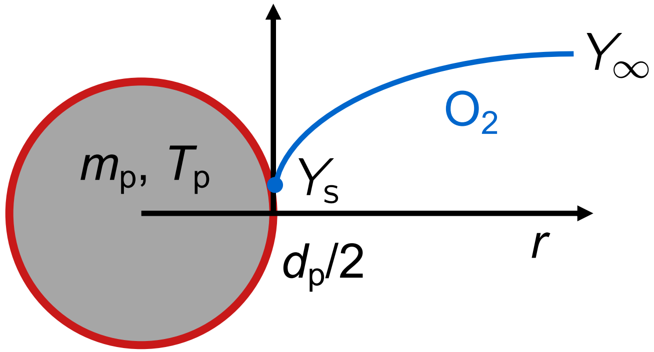
Combustion peak temperature depends on particle size and $O_2$ concentration.

Combustion time $t_{max}$ is proportional to diameter $d^{1.6}$. (Close to the analytical $d^2$-law for droplet combustion!)

Combustion time $t_{max}$ is inversely proportional to $X_{O2}$ in O2/N2 blends.

D. Ning et al. (2021) Combust Flame.
D. Ning et al. (2022) Combust Flame.

# Single particle oxidation modelling (1)



- Spherical particle $d_p$, $m_p$, $T_p$
- Surface reaction

$$\frac{\mathrm{d}m_\mathrm{p}}{\mathrm{d}t} = A_\mathrm{p} k Y_\mathrm{s} \qquad k = k_0 \exp\left(-E_a/RT\right) Y_\mathrm{u}$$

- Mass transfer

$$A_\mathrm{p} \beta (Y_\infty - Y_\mathrm{s}) = A_\mathrm{p} k Y_\mathrm{s} \qquad \beta = \frac{\mathrm{Sh} \rho D_{\mathrm{O}_2}}{d_p}$$

- Normalized Damköhler number

$$\frac{\mathrm{d}m_\mathrm{p}}{\mathrm{d}t} = A_\mathrm{p} \beta \, \mathrm{Da} \, Y_\infty \qquad \mathrm{Da} = \frac{k}{k + \beta}$$

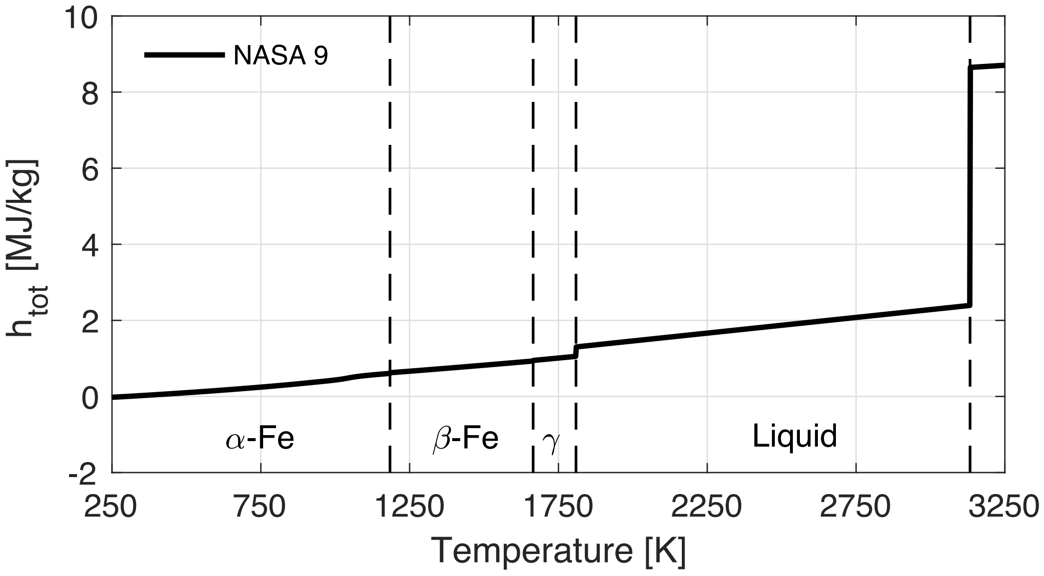
- Kinetically limited regime $k \ll \beta \quad \mathrm{Da} \to 0$
- Diffusion limited regime $\beta \ll k \quad \mathrm{Da} \to 1$

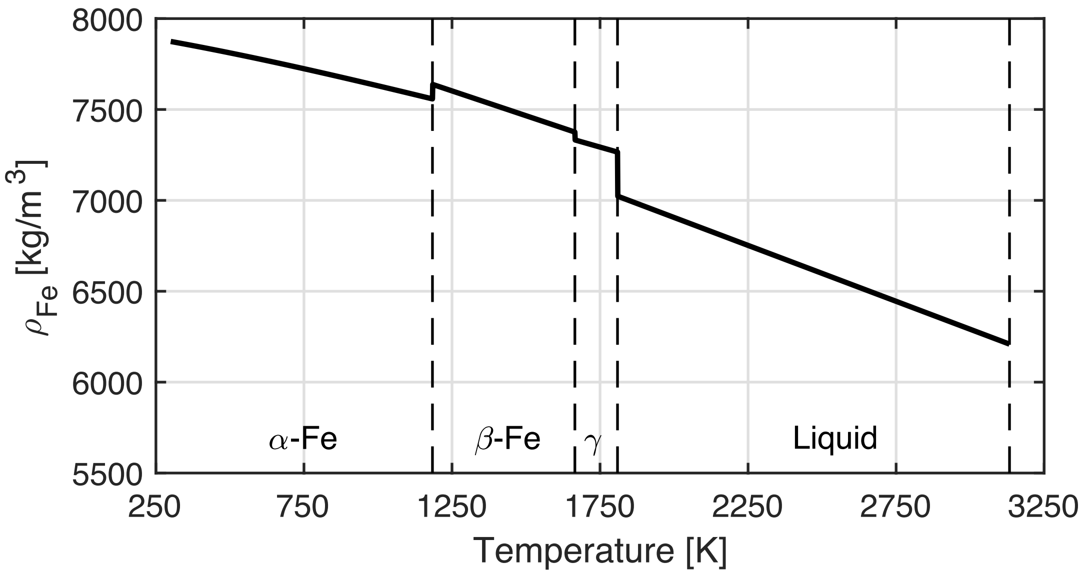
Hazenberg & van Oijen (2021) Proc. Combust. Inst.

# Single particle oxidation modelling (2)

Other model “ingredients”:

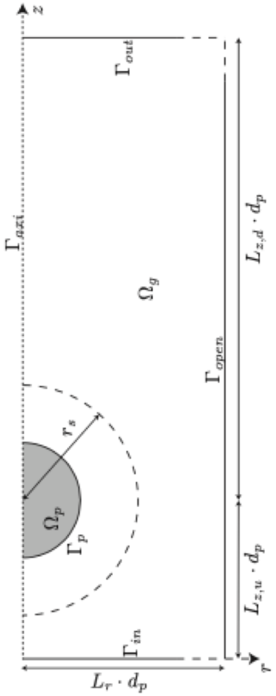
- Particle temperature equation includes convective and radiative heat transfer.
- Slip velocity, Stefan flow correction.
- Detailed gas phase properties (thermodynamic- and transport properties).
- Detailed solid phase properties (density, specific heat/total enthalpy).

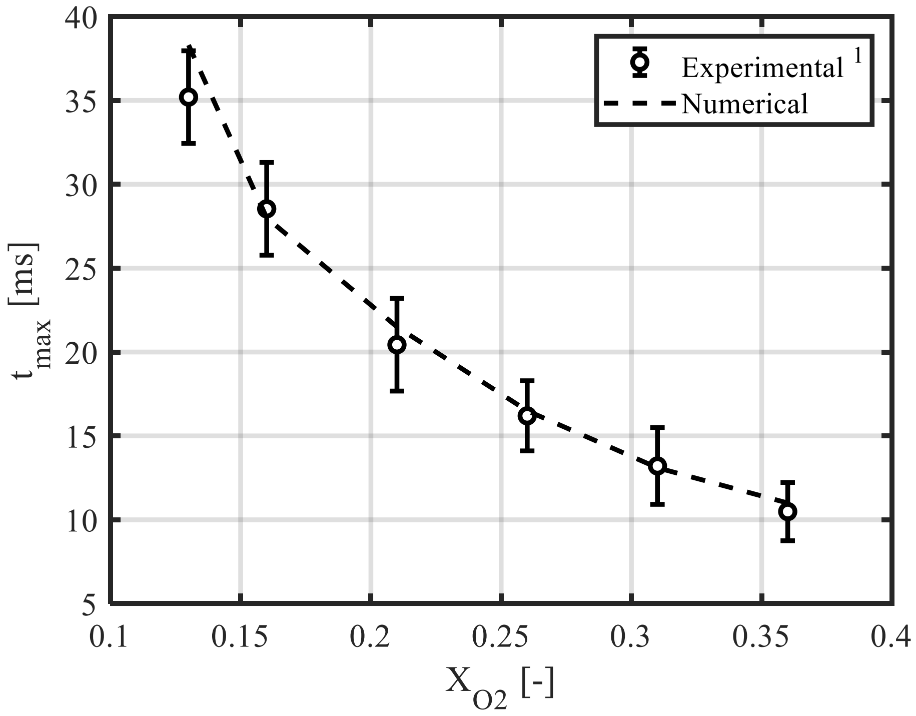


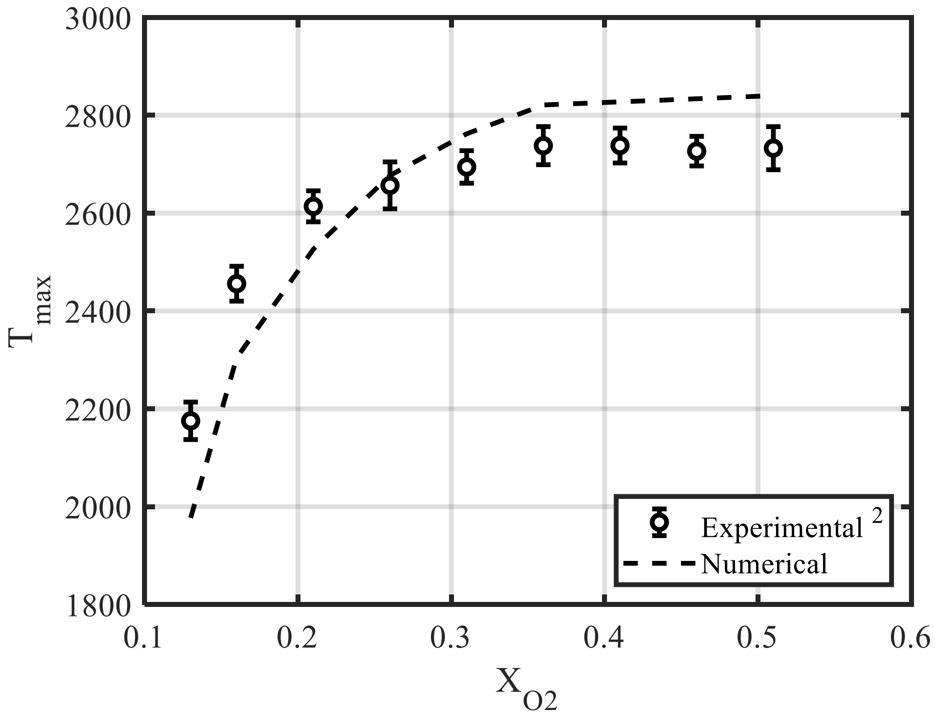


# Resolved single particle simulations (1)

- Comparison with laser-ignited particle combustion experiments
- Combustion time $t_{\max}$ and maximum temperature $T_{\max}$ for $d_p$ = 54 µm.

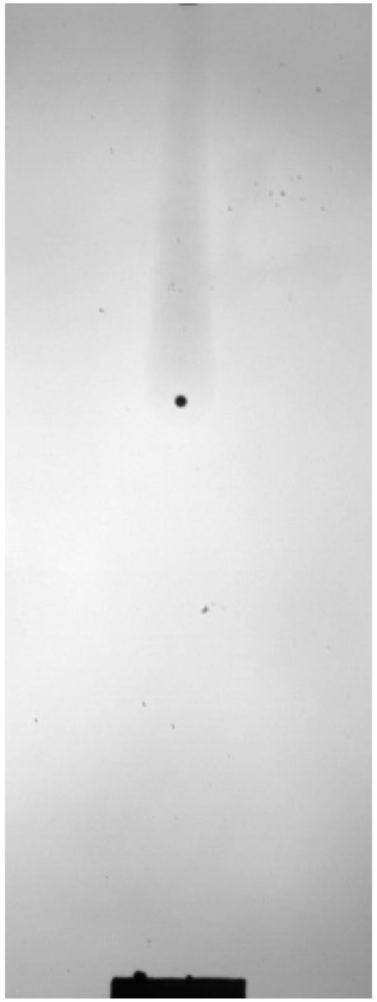




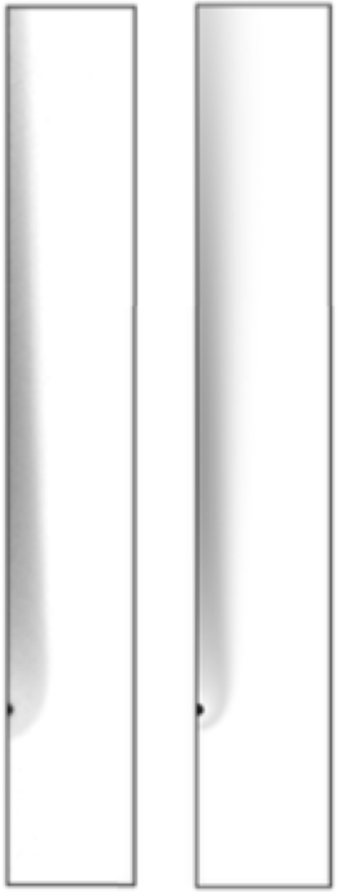


Thijs et al. (2022) Proc. Combust. Inst.

# Resolved single particle simulations (2)



Movie: courtesy of D. Ning (TUE).



Exp. Sim.

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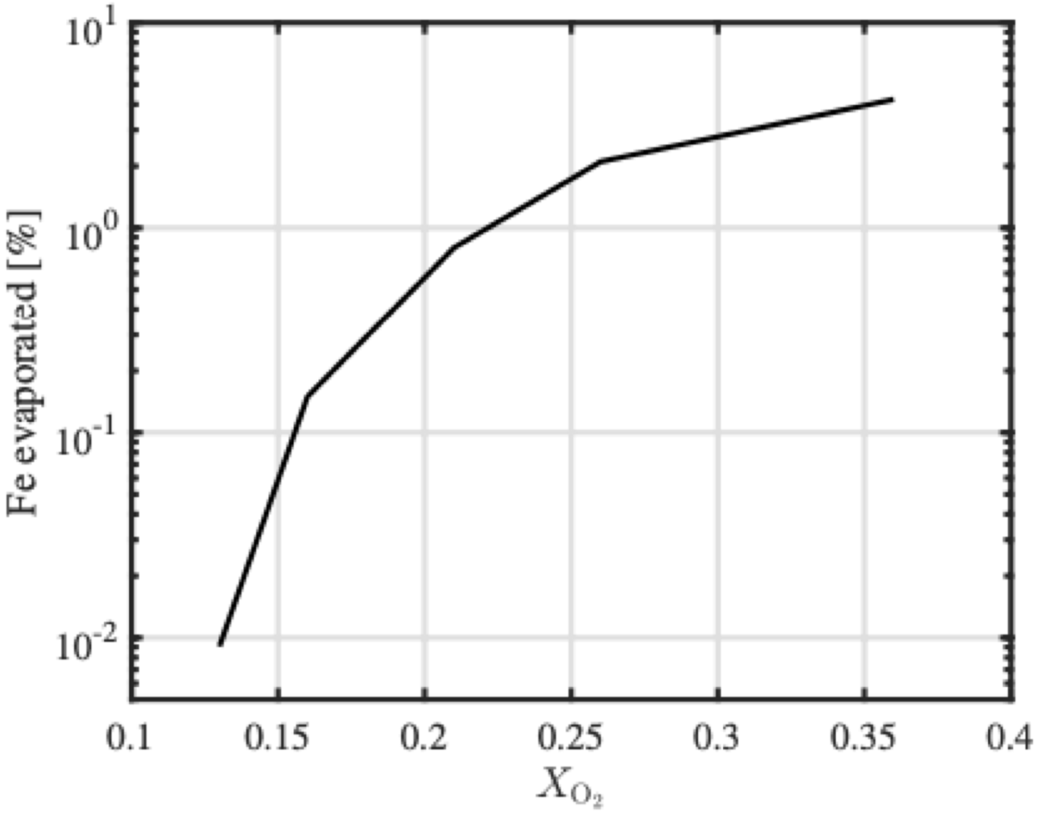
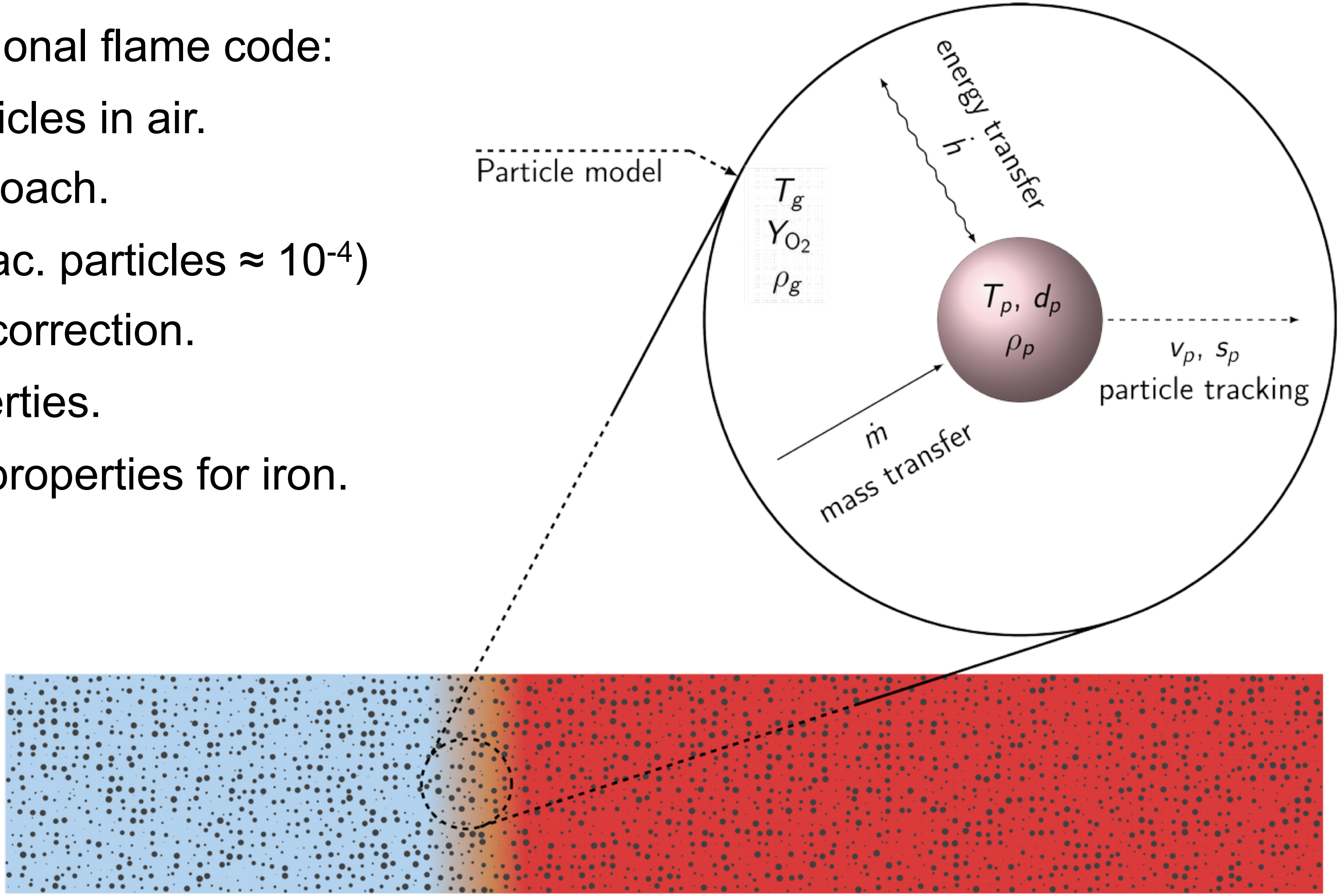


Prediction of amount of evaporated Fe.

# Flame propagation in iron dust clouds

Implementation in 1-dimensional flame code:

- (Poly-)dispersed iron particles in air.
- Eulerian-Lagrangian approach.
- Two-way coupling (vol. frac. particles ≈ $10^{-4}$)
- Slip velocity, Stefan flow correction.
- Detailed gas phase properties.
- Temperature-dependent properties for iron.



Hazenberg & van Oijen (2021) Proc. Combust. Inst.

# One-dimensional iron aerosol flames (metalets)

- Steady 1D planar flame propagation, continuous regime (not discrete).
- Like flame propagation in droplet mists:

Gas phase species

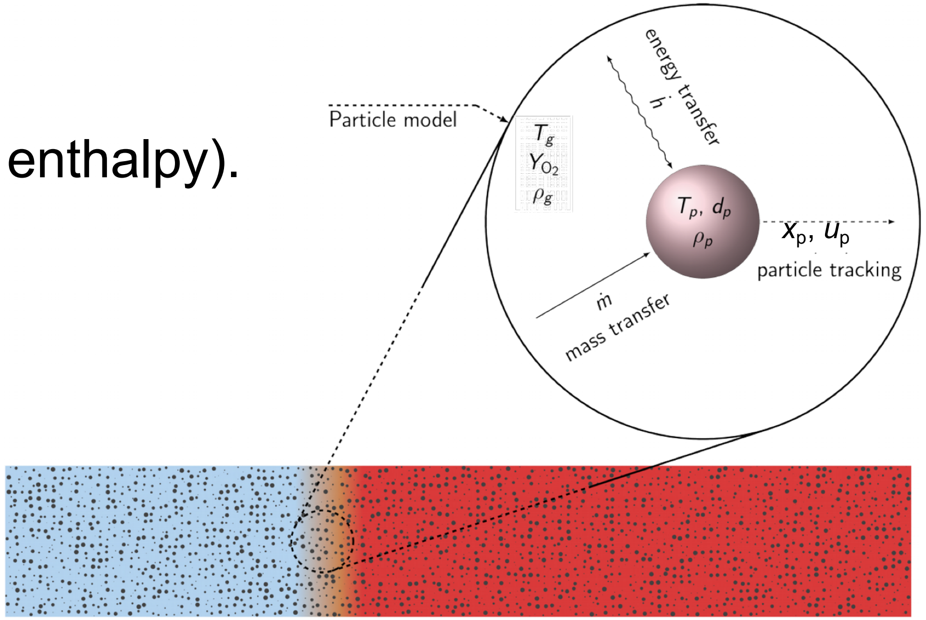
$$\frac{\mathrm{d}}{\mathrm{d}x}(\rho u Y_i) - \frac{\mathrm{d}}{\mathrm{d}x}\left(\rho D \frac{\mathrm{d}Y_i}{\mathrm{d}x}\right) = \omega_i + S_\mathrm{m}$$

- $S_\mathrm{m}$ is mass transfer rate from particles to gas (same for enthalpy).
- Track particle through computational domain:

Particles

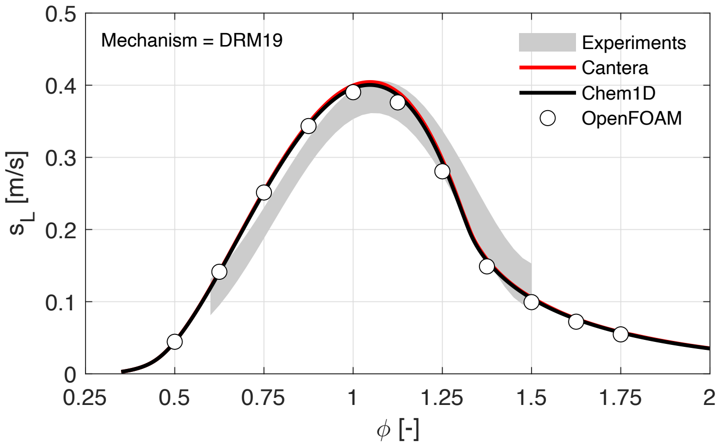
$$\frac{\mathrm{d}x_\mathrm{p}}{\mathrm{d}t} = u_\mathrm{p} \qquad \frac{\mathrm{d}u_\mathrm{p}}{\mathrm{d}t} = \frac{3}{4}\frac{C_d}{d_\mathrm{p}}\frac{\rho}{\rho_\mathrm{p}}|u - u_\mathrm{p}|(u - u_\mathrm{p})$$

- Calculate heat and mass transfer terms $S_\mathrm{h}$ & $S_\mathrm{m}$ for each computational cell.



Sacomano Filho et al. (2018) Combust. Theory Model.

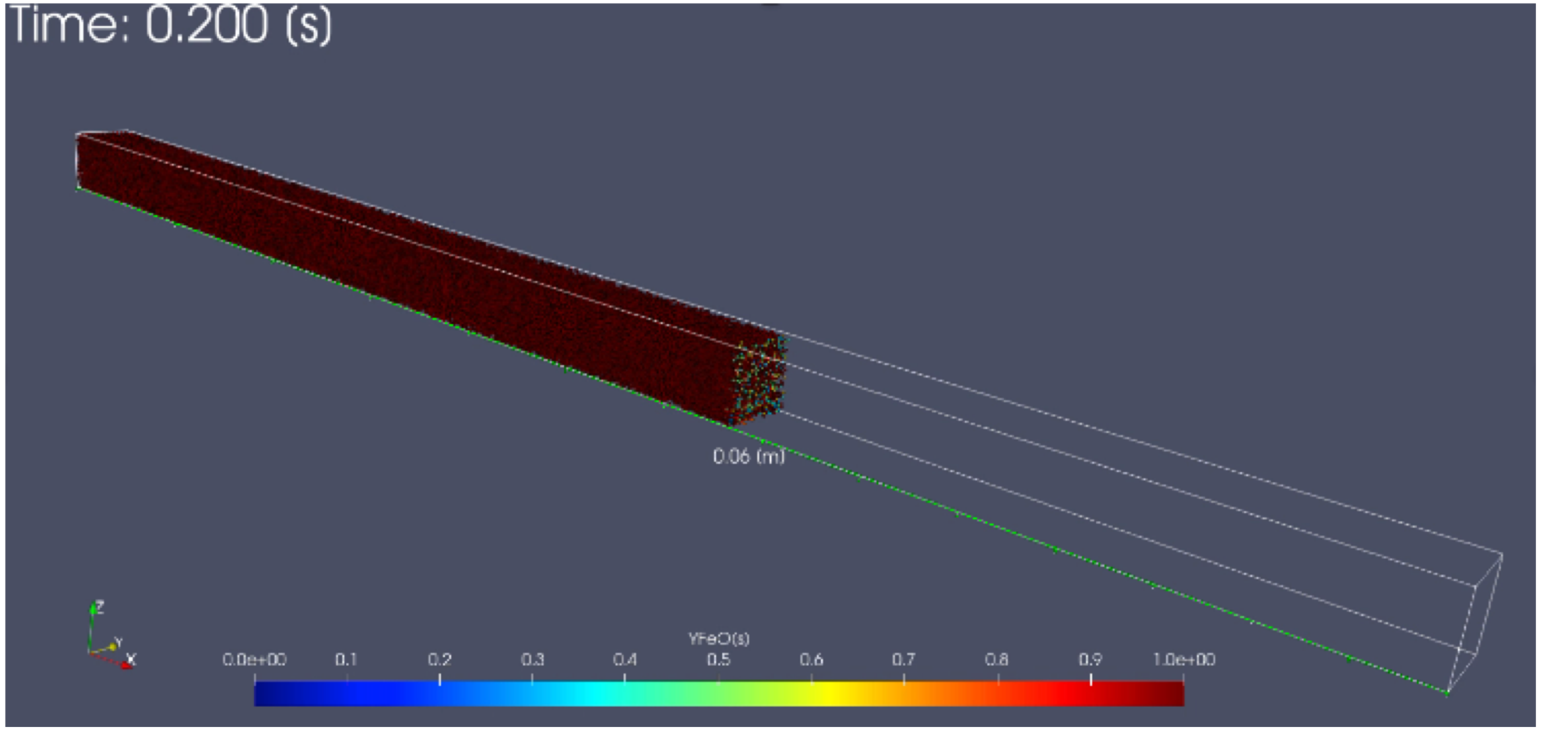
# 3-D CFD modeling: OpenFOAM implementation



Code has been extensively validated for $CH_4$-air flames.

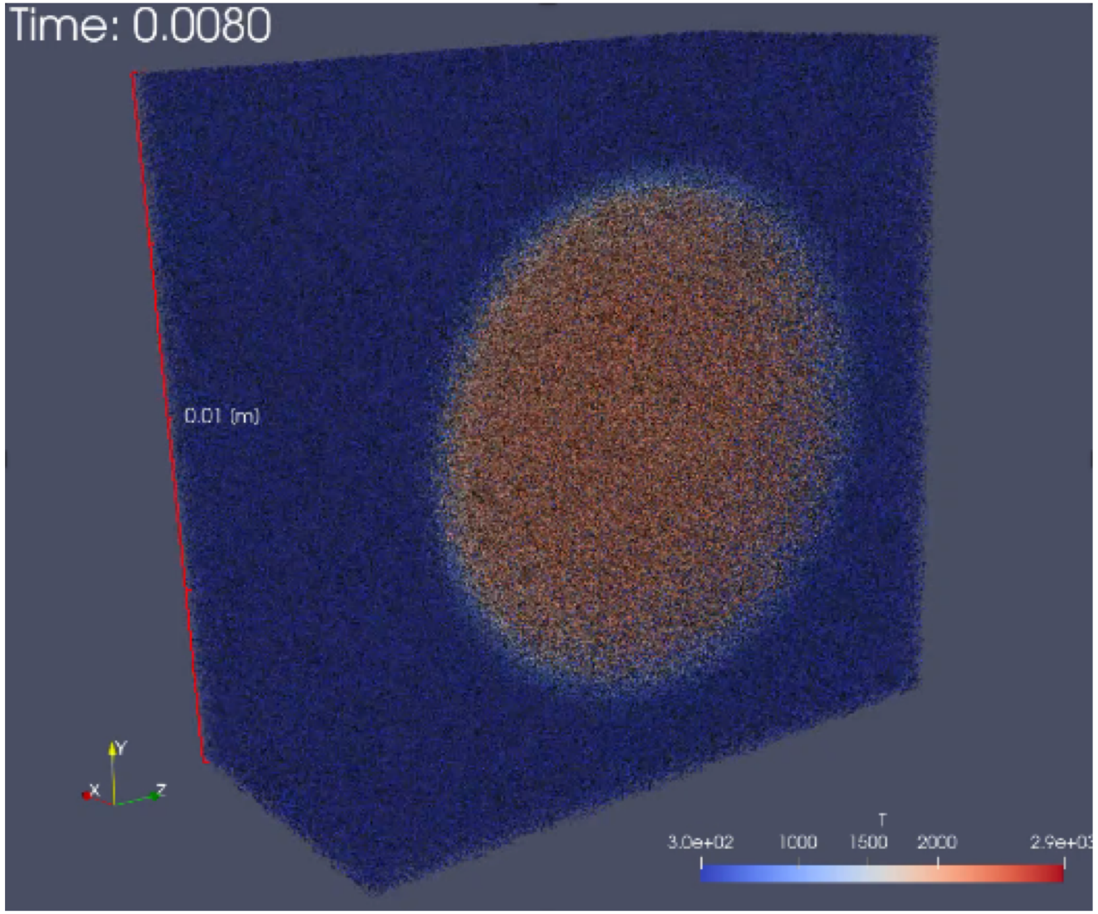
Heterogeneous combustion:

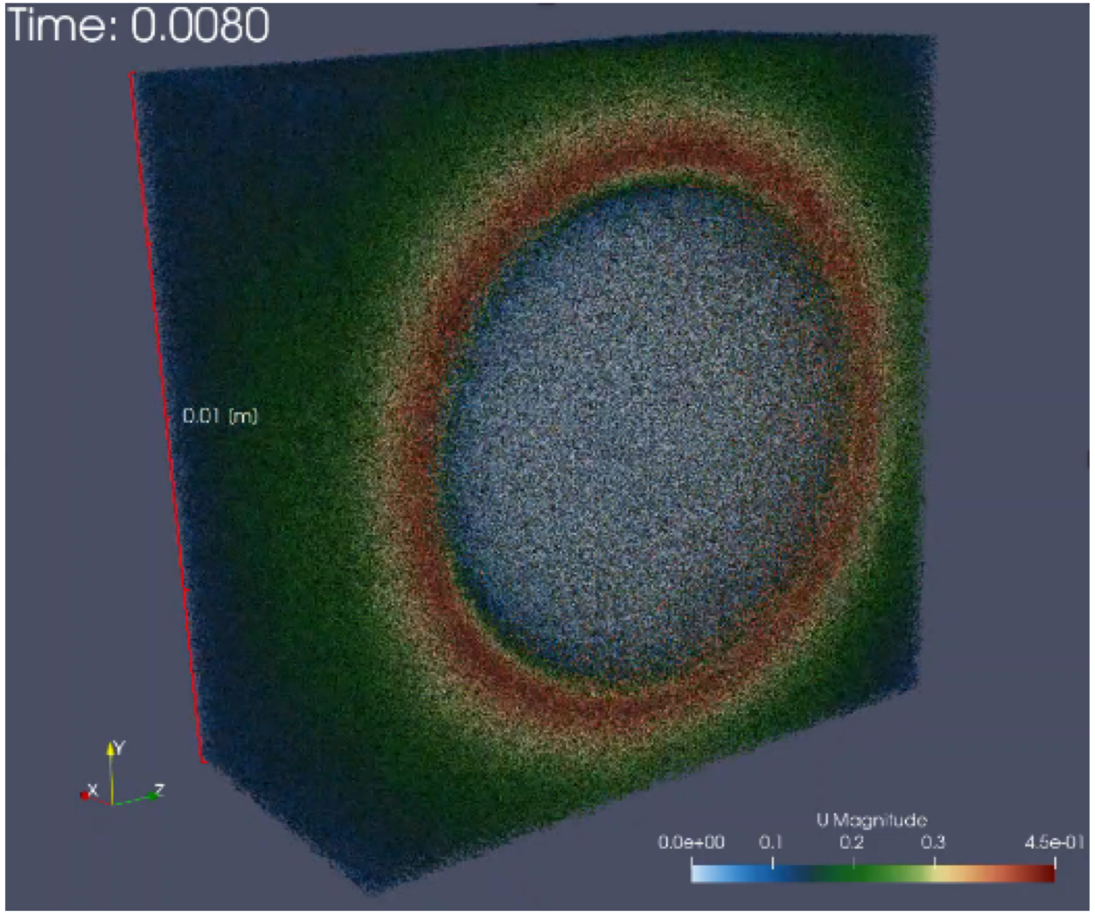
- Euler-Lagrange approach.
- Includes two-step oxidation model for Fe to $Fe_3O_4$.
- Radiation models included.



Particles: mean $d_p$ = 3.7 μm, 600 gr/$m^3$, inter-particle dist. = 70.4 μm.
Oxidizer: ambient air.

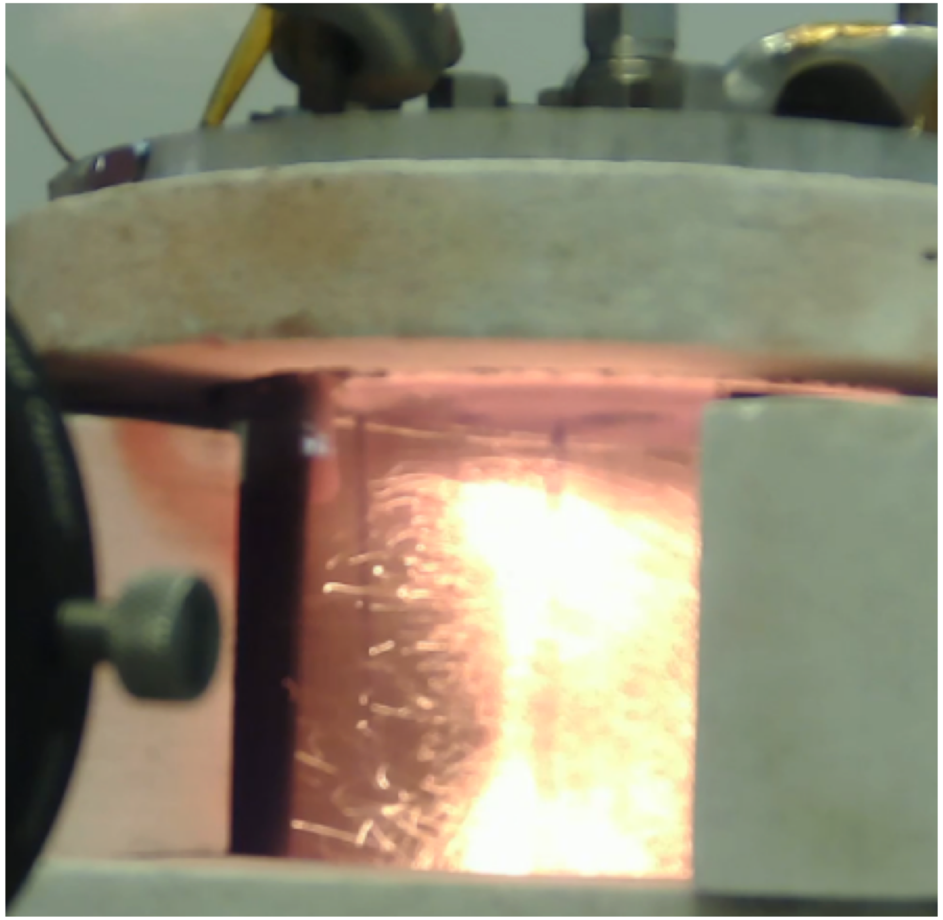
# OpenFOAM simulations of lab-scale experiments

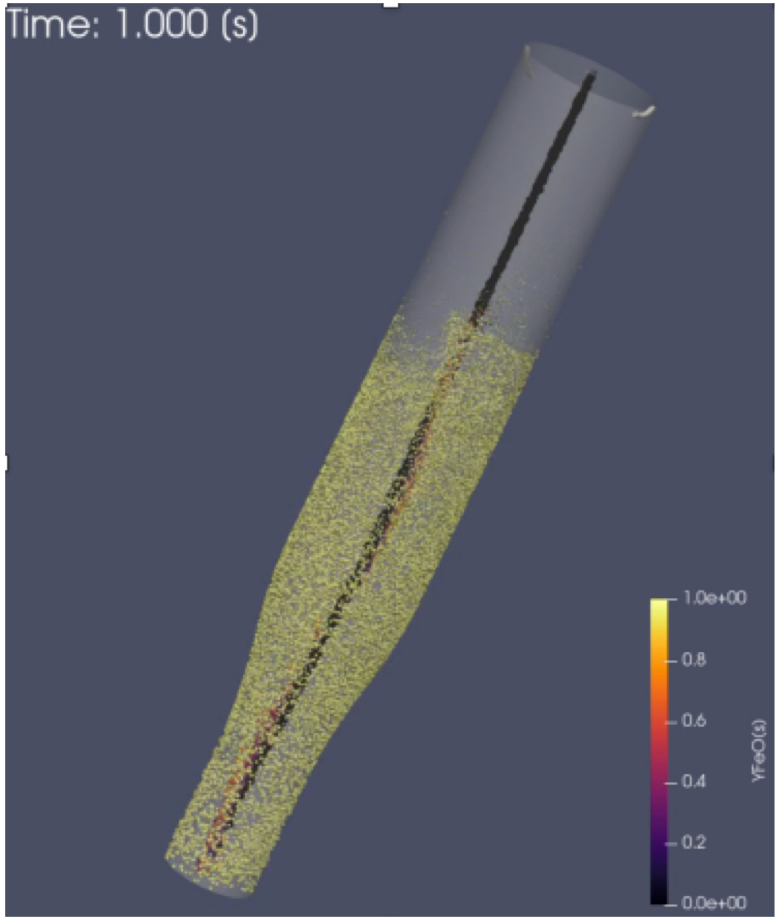


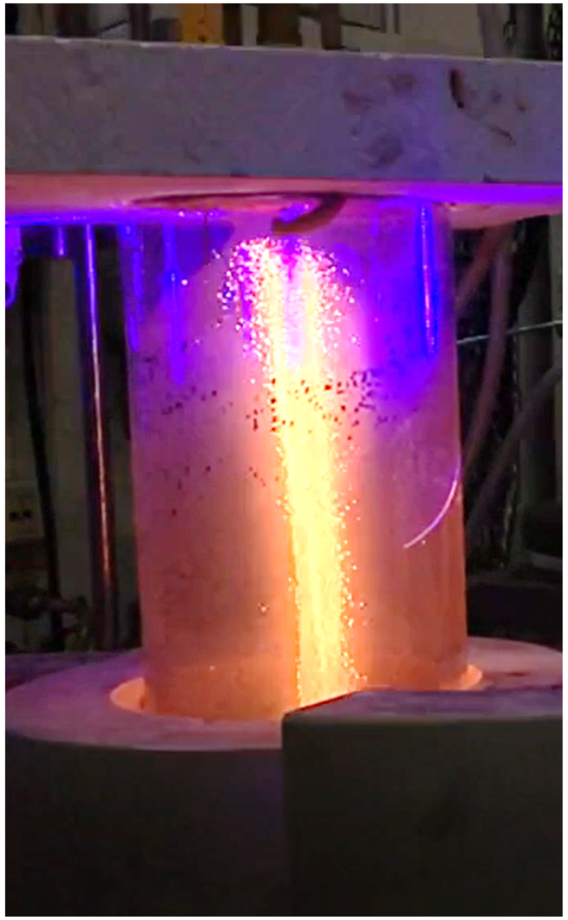


Experiments by Sun et al. (1998). Particles: mean $d_p$ = 3.7 µm, 900 gr/m$^3$, inter-particle dist. = 61.5 µm. Oxidizer: ambient air. **Cubic cm contains approx. 4.3 million particles!**

# Scaling it up...





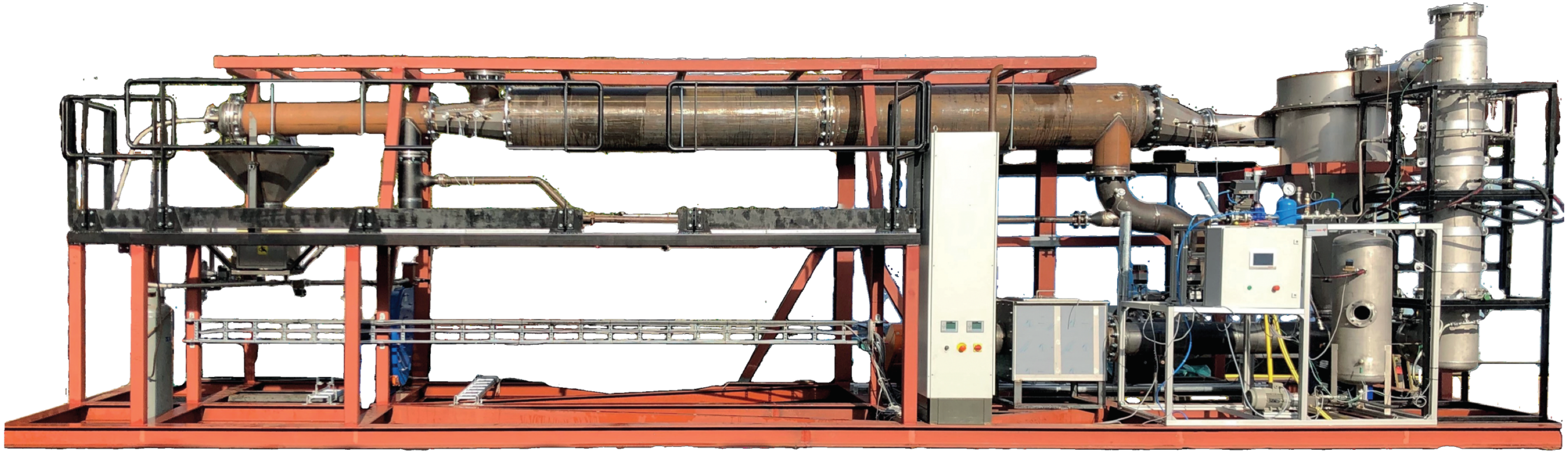


Original burner design: T. Spee (TUE).
Images experiments: courtesy of M. Baigmohammadi (TUE).

Tornado burner (approx. 3 kW thermal power).

# And up...

- **Metalot**: Network organization, demonstration and scaling up, bringing metal power technology to market.
- **MP100**: 100 kW iron fueled boiler system demonstrated by Metal Power Consortium at Royal Swinkels Brewery.
- MP100 is currently being redesigned, built and tested to operate at higher loads (up to 500 kW).



# Summary

- Metal fuel cycle: storing and transporting carbon free energy.

- Iron is the most promising metal fuel!

- To develop iron fuel technology, accurate measurements are needed:
  - Single particle combustion: detailed oxidation process behavior.
  - One-dimensional aerosol flames: flame/percolation wave speeds.
  - Lab-scale burners for iron powder.
  - Incorporate PSA/SEM/XRD/porosity measurements for (un-)burnt particles.

- Numerical tools of various complexity are being developed and validated to enable highly accurate predictions (and to be able to steer combustor development).

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