Metal oxide cycles for high temperature heat and longer energy storage

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Summary:

I. Project presentation and metal energy cycle
II. Experimental investigation of iron combustion in a fluidized bed
III. Euler-Euler simulation of iron combustion in a fluidized bed
IV. Conclusions

Project MixMOXes :

Mixed Metal Oxides Energy Stations for zero-carbon thermal energy generation with integrated heat storage – EP/X000249/1

EPSRC
Engineering and Physical Sciences
Research Council

Objective:

Investigate and understanding of zero-carbon energy storage release through metal cycles (iron)

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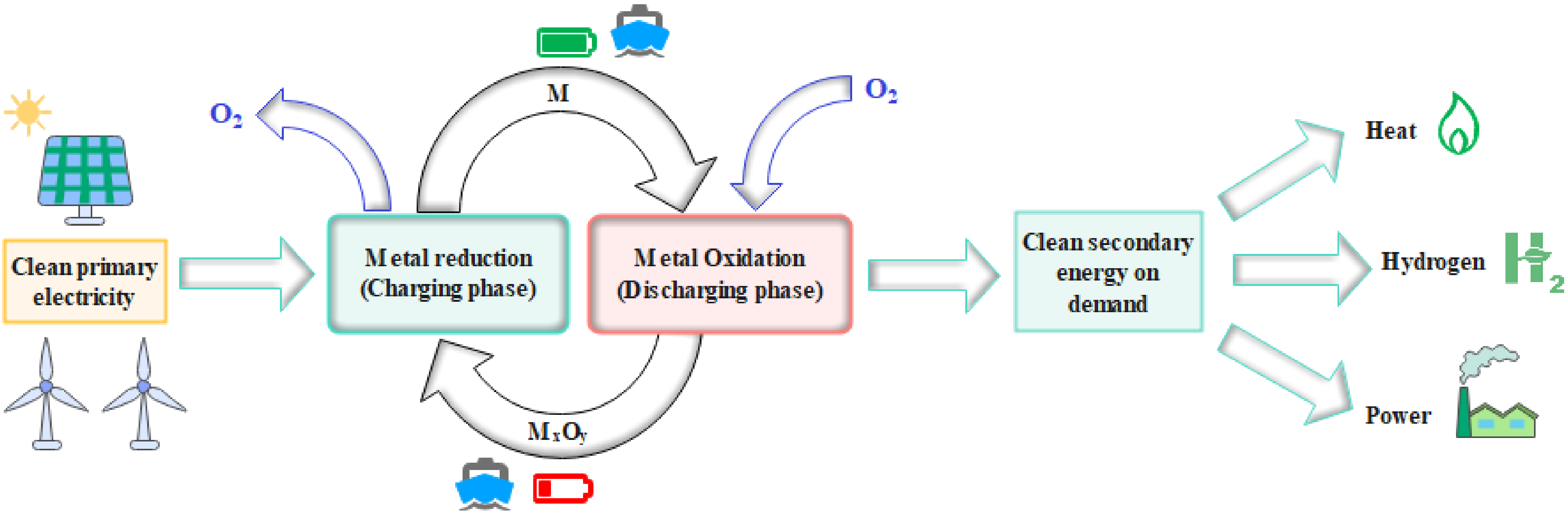
Metal oxides energy cycle

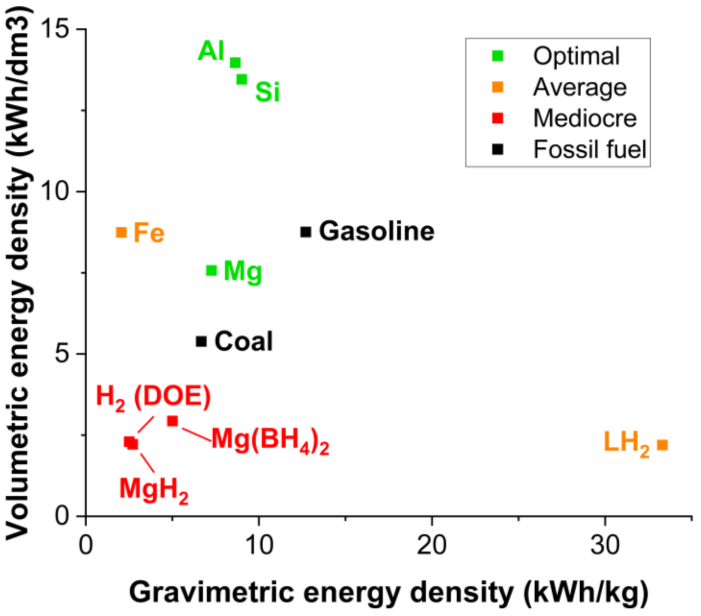


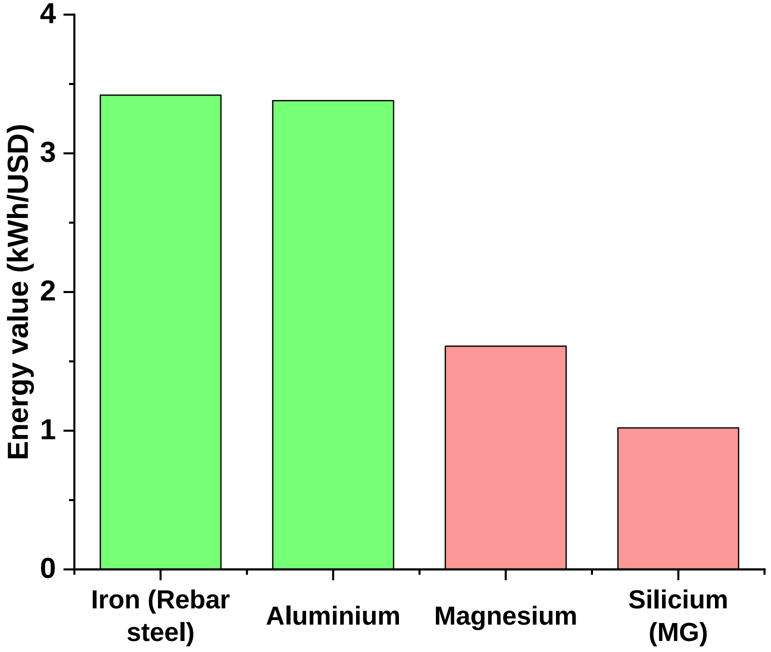
$$Fe + \frac{3}{4}O_2 \leftrightarrow \frac{1}{2}Fe_2O_3$$

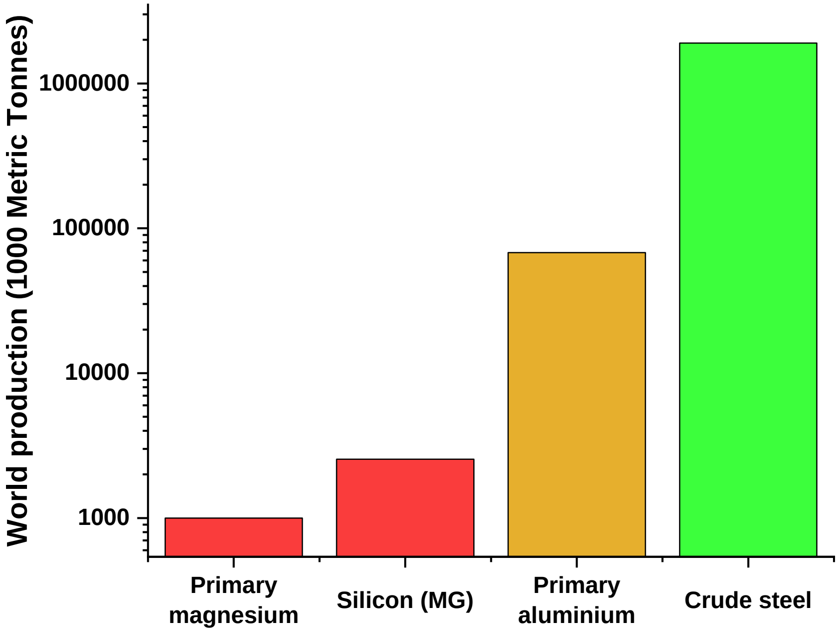
Wronski T. & Sciacovelli A., Analysis of the potential of four reactive metals as zero carbon energy carriers for energy storage and conversion, 2024.

Metal oxides energy cycle

➔ Compromise between energy densities, price, and availability





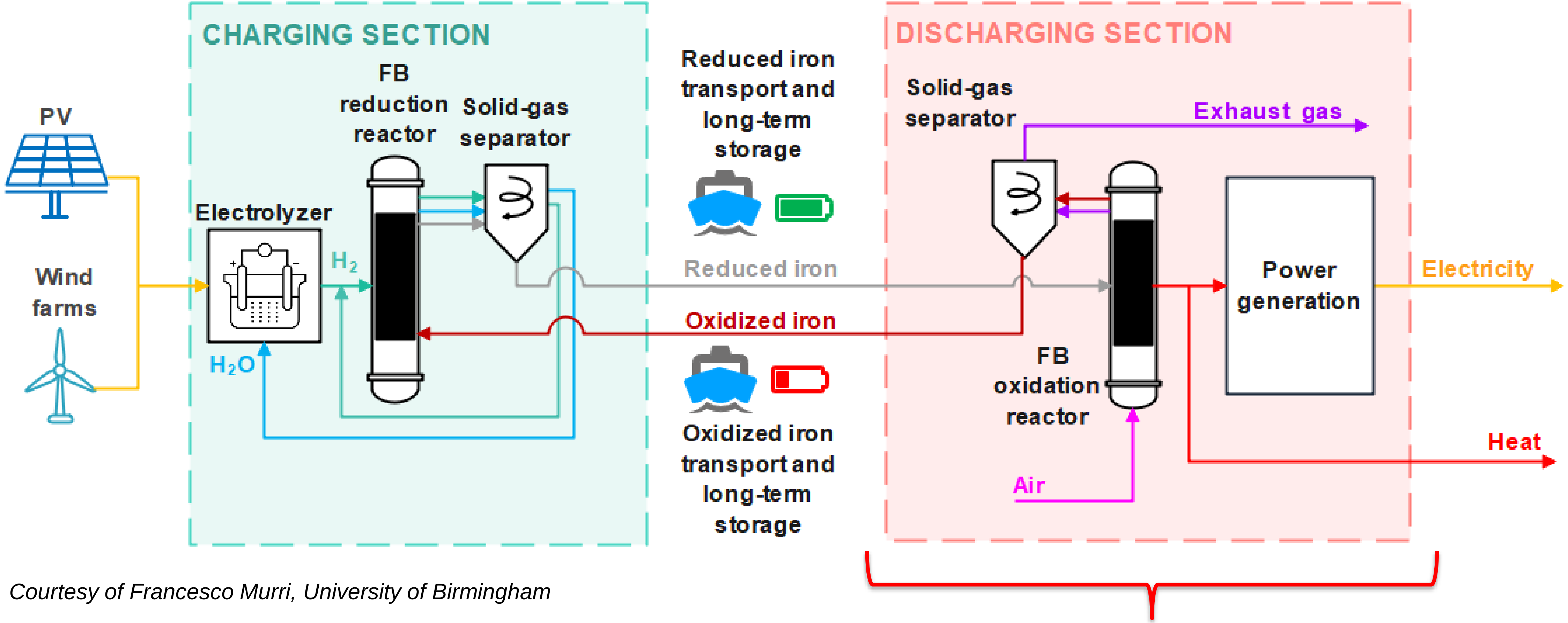


✚ **Technological roadblocks :**

- ☐ Reduction processes: high CapEx/OpEx
- ☐ Combustion processes: particle emissions

Wronski T. & Sciacovelli A., Analysis of the potential of four reactive metals as zero carbon energy carriers for energy storage and conversion, 2024.

The iron-based energy storage & conversion cycle



Courtesy of Francesco Murri, University of Birmingham

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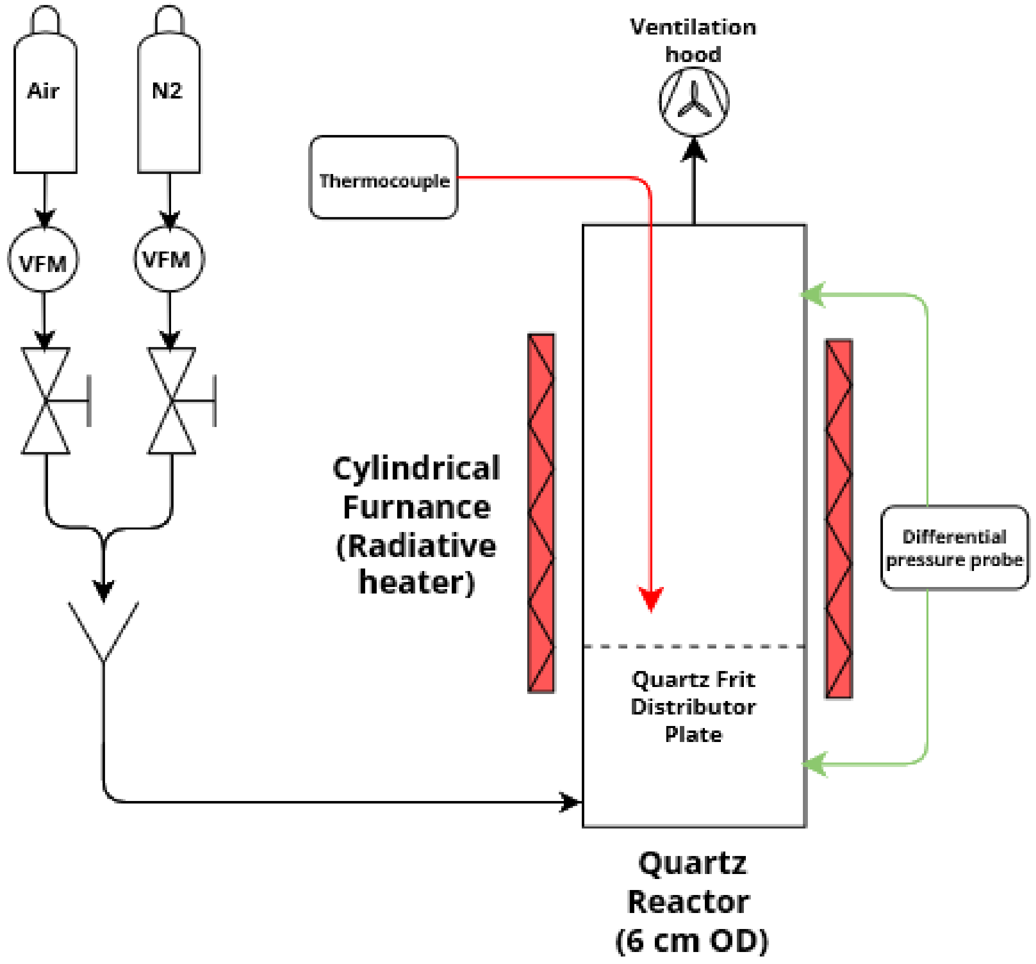
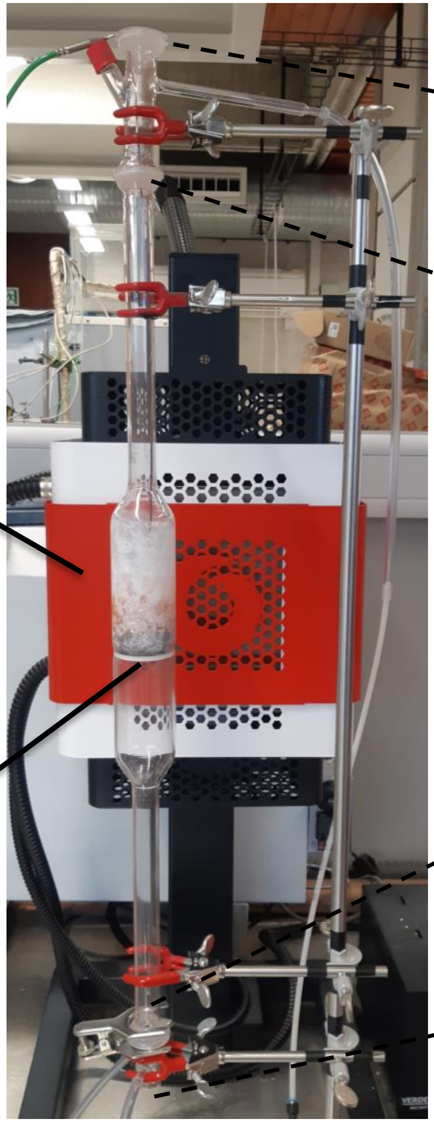
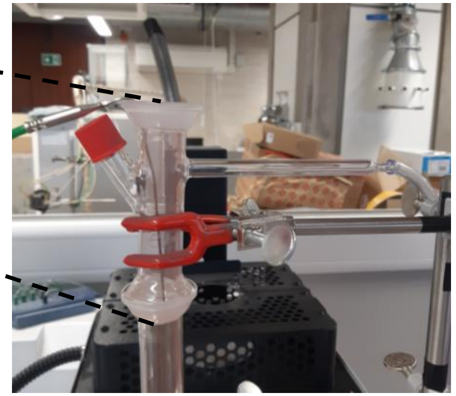
Project MixMOXes

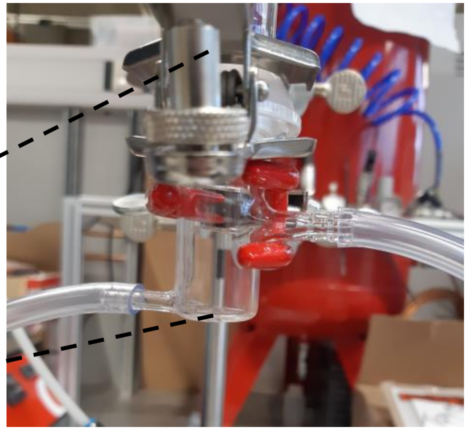
Rig setup







Thermocouple & pressure tap (atmospheric)



Gas inlet & pressure tap

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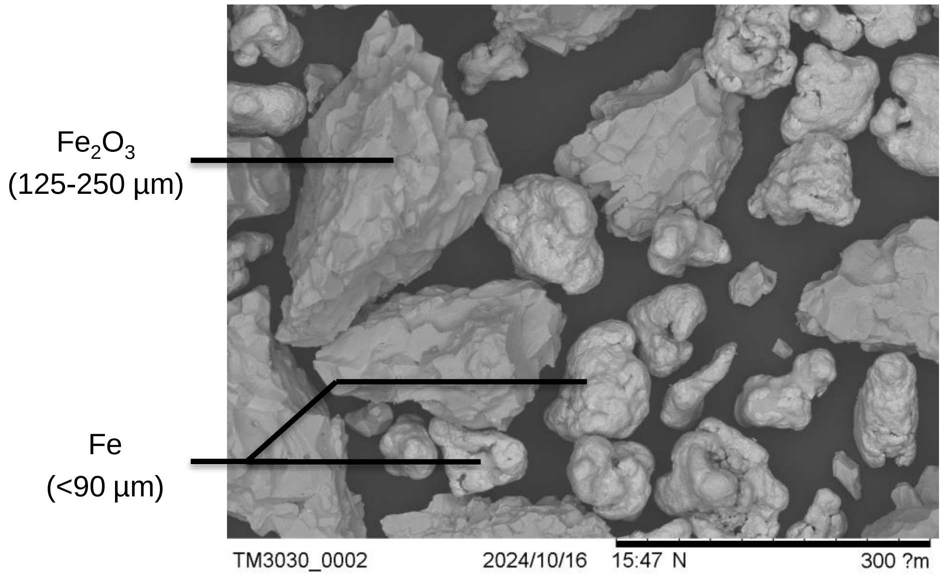
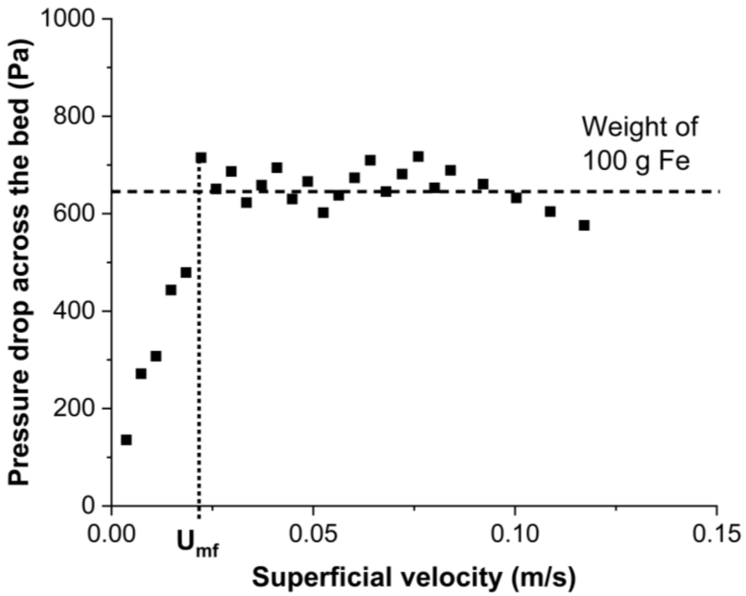
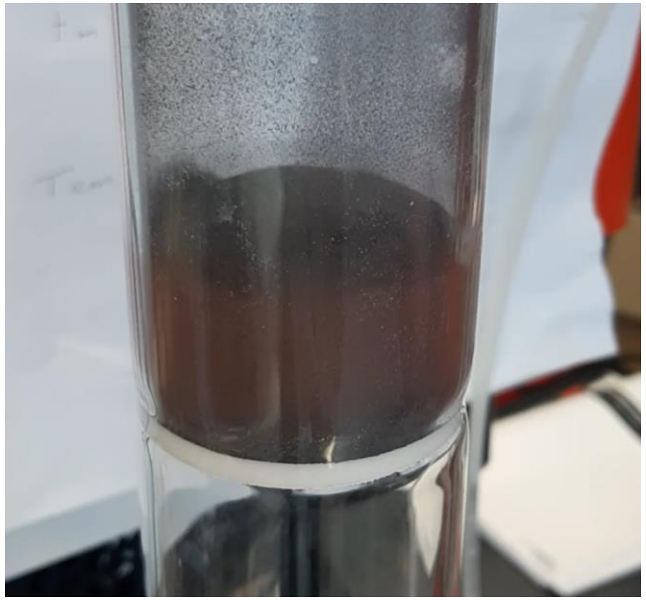
Fluidization







	Oxide (125-250 µm)	Iron (90-150 µm)
Minimum fluidization velocity (m/s)	0.037	0.022
First bubble (m/s)	0.064	0.030
Turbulent transition (m/s)	0.163	0.084

Coherent with analytical predictions (Wen and Yu equation)

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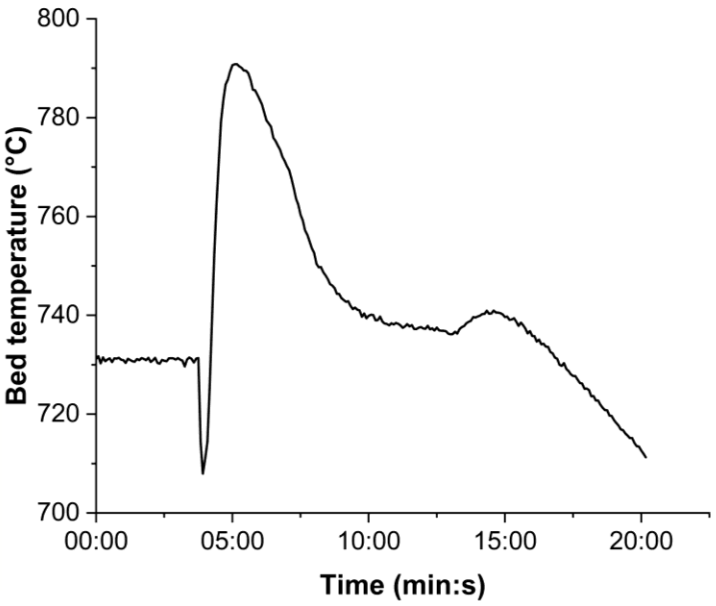
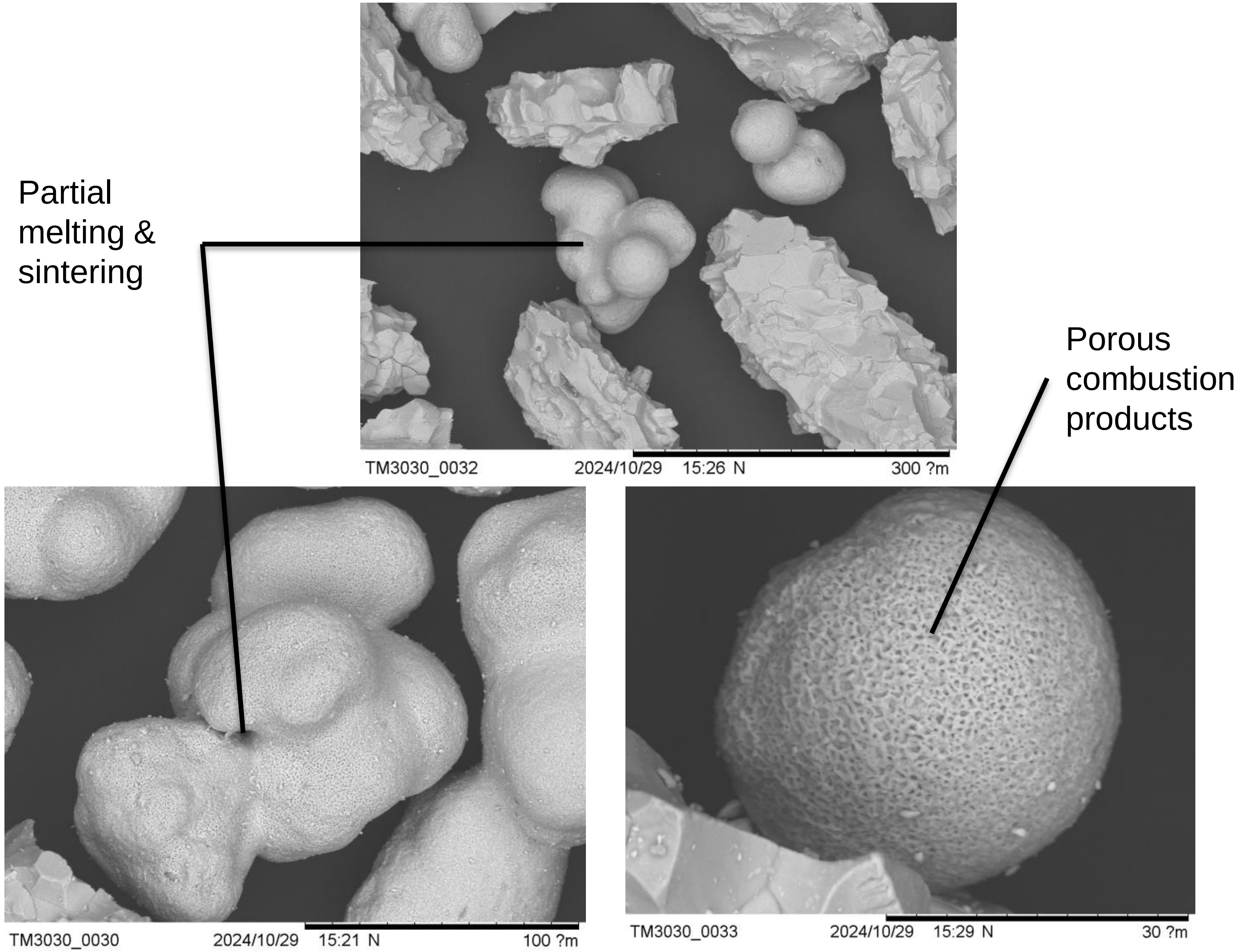
Oxidation case - example:

Initial oxide mass	90	g
Oxide particle size range	125-250	µm
Initial iron mass	10	g
Iron particle size range	< 90	µm
Initial bed temperature	730	°C
O_2 fraction during combustion	9.8	%
Superficial velocity	0.37	m/s





First observations:

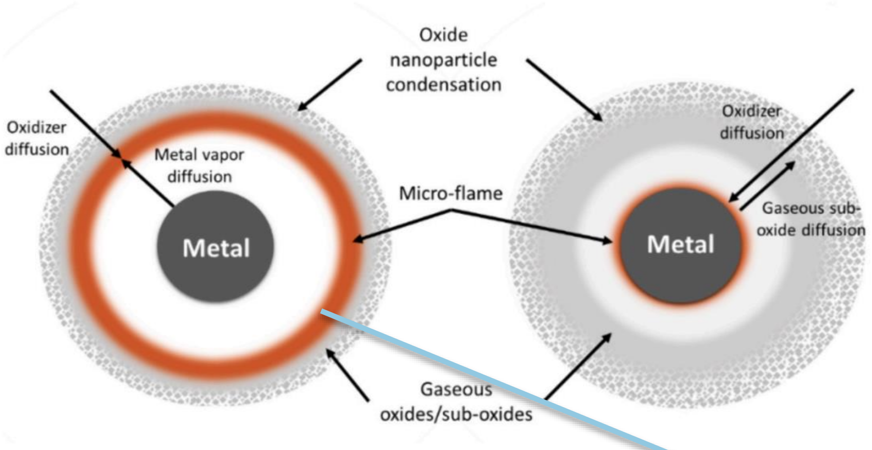
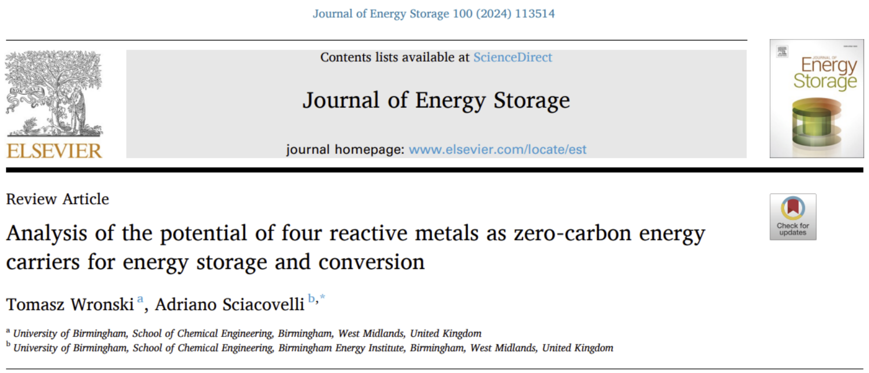


Fig. 4. Schematic of the three combustion modes of a metal particle. Adapted from Bergthorson et al. [26].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Review Article

Analysis of the potential of four reactive metals as zero-carbon energy carriers for energy storage and conversion

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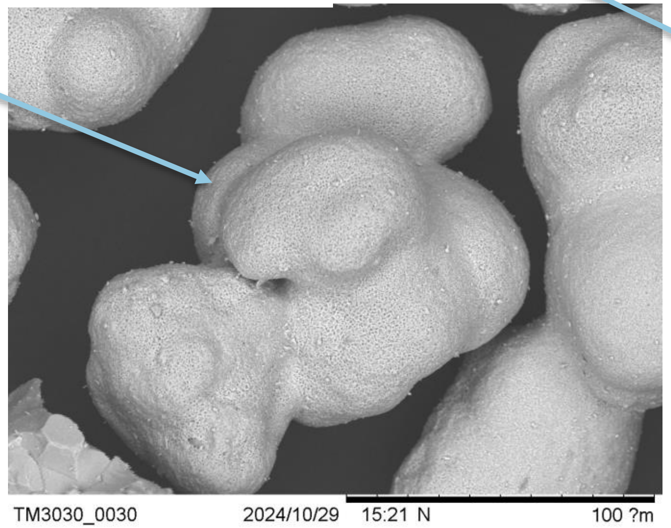

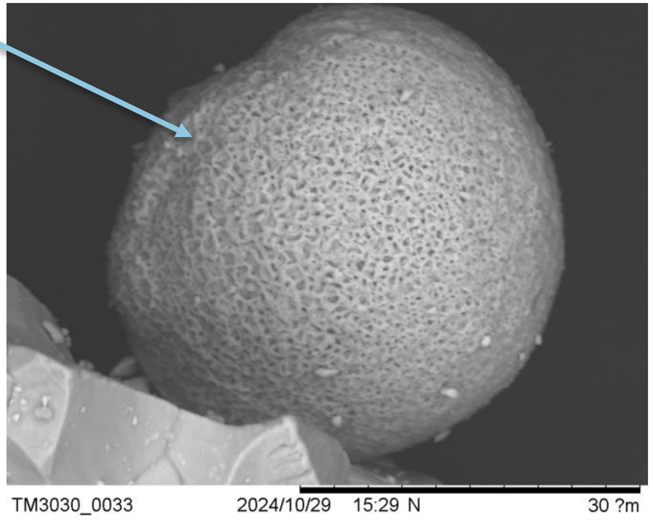

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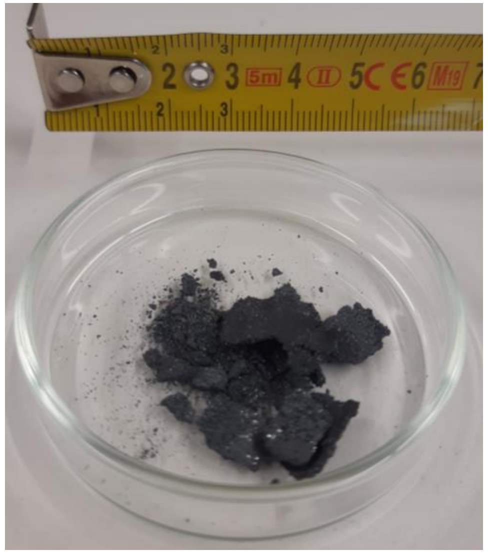
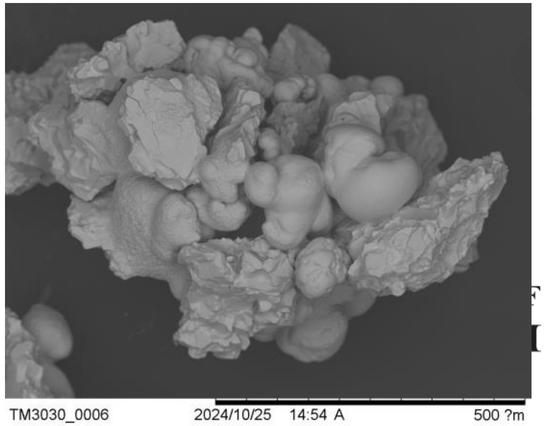
First observations:

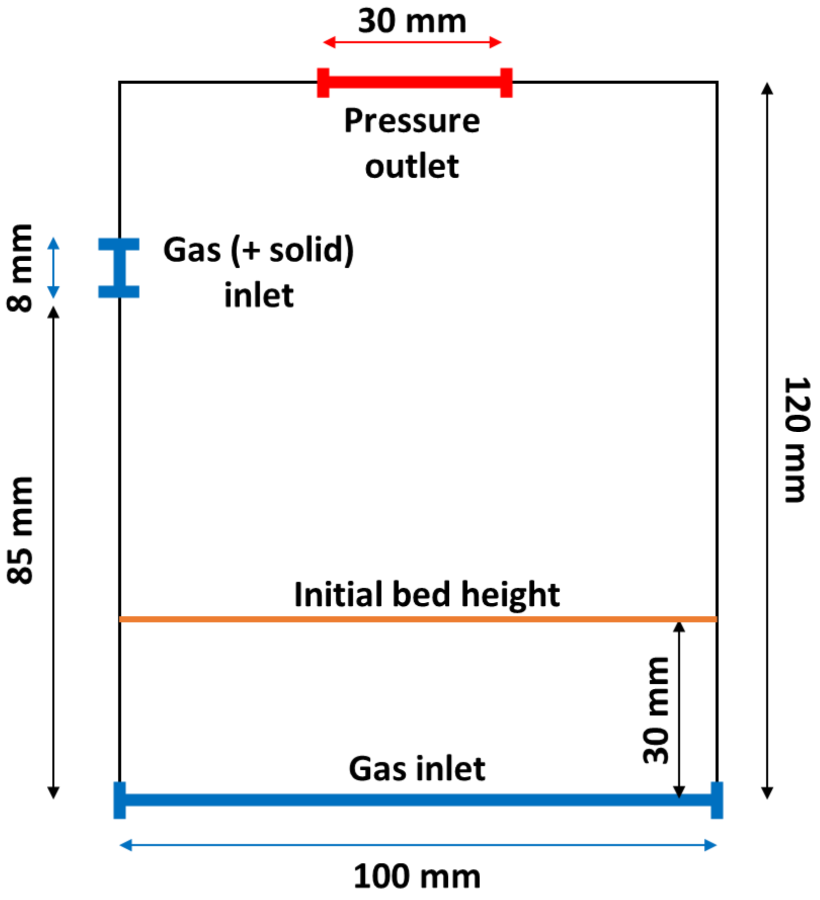


Aggregates formed between inert and combusting particles.



- Melting/sintering of iron leads to formation of aggregates and to partial defluidization at lower gas velocities.
- Aggregation is heavily reduced by increasing gas velocity and bed turbulence.
- Reaction rate difficult to measure, but seems consistent with single particle combustion rates.
- Phase-level heat dissipation seems consistent with CFD model.

Boundary and initial conditions



Initial & boundary conditions:

- Transient, 3D, circular
- Initial oxide bed at 1100 K
- Iron injection at 300 K

Numerical model:

- Eulerian multiphase model: 3 phases represented by their volume fractions

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Conservation equations:

- Mass:

$$\frac{1}{\rho_{rq}}\left(\frac{\partial}{\partial t}(\alpha_q\rho_q) + \nabla.(\alpha_q\rho_q\vec{v}_q) = \sum_{p=1}^{n}\dot{m}_{pq}\right)$$

- Momentum:

$$\frac{\partial}{\partial t}(\alpha_q\rho_q\vec{v}_q) + \nabla.(\alpha_q\rho_q\vec{v}_q\vec{v}_q) = -\alpha_q\nabla p + \nabla.\bar{\bar{\tau}}_q + \alpha_q\rho_q\vec{g} + \sum_{p=1}^{n}K_{pq}(\vec{v}_p - \vec{v}_q) + \dot{m}_{pq}\vec{v}_{pq} + \vec{F}_{td,q}$$

- Energy:

$$\frac{\partial}{\partial t}\left(\alpha_q\rho_q\left(e_q + \frac{\vec{v}_q^{\,2}}{2}\right)\right) + \nabla\cdot\left(\alpha_q\rho_q\vec{v}_q\left(h_q + \frac{\vec{v}_q^{\,2}}{2}\right)\right)$$
$$= \nabla\cdot\left(\alpha_q k_{eff,q}\nabla T_q - \sum_j h_{j,q}\vec{J}_{j,q} + \bar{\bar{\tau}}_{eff,q}\,.\,\vec{v}_q\right) + \sum_{p=1}^{n}(Q_{pq} + \dot{m}_{pq}h_{pq}) + p\frac{\partial\alpha_q}{\partial t} + S_q$$

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Chemical species conservation and reaction rate formulation

$$\frac{\partial}{\partial t}\left(\rho^q \alpha^q Y_i^q\right) + \nabla \cdot \left(\rho^q \alpha^q \vec{v}^q Y_i^q\right) = -\nabla \cdot \alpha^q \vec{J}_i^q + R \cdot M_i$$

- Burn time of a single iron particle in air[1]: $t_b = 0.000079 * {d_p}^{1.65}$

- User Defined Function:

$$\mathrm{R} = \frac{\rho_{Fe}\alpha_{Fe}}{t_b * MW_{Fe}} * \frac{1}{1 + \exp\left(-100 * \left(Y_{O_2} - 0.05\right)\right)} \qquad (\mathrm{kmol.m^{-3}.s^{-1}})$$

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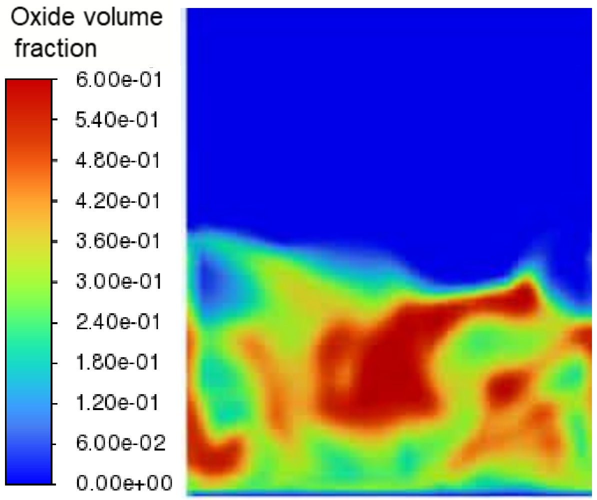
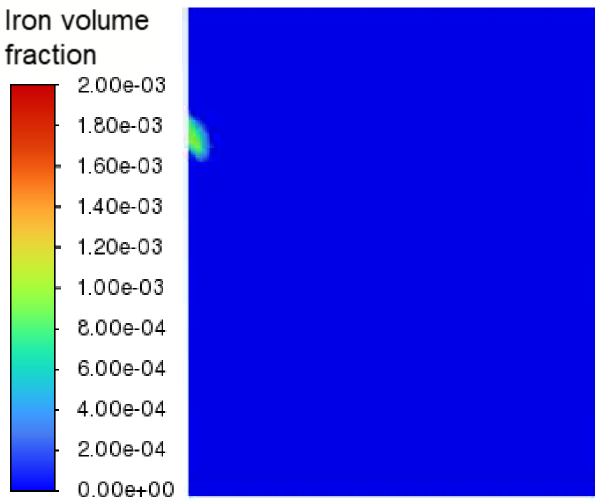
[1] *Ning et al., Burn time and combustion regime of laser-ignited single iron particle, 2021*

Qualitative analysis for stoichiometric mixture

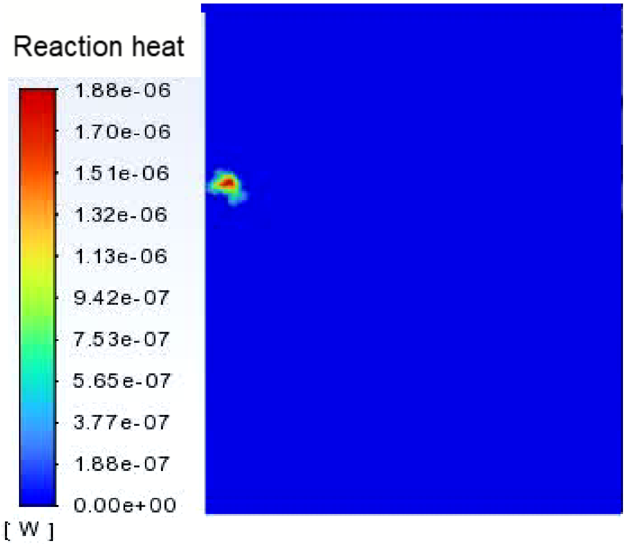
- Iron injection: 1 kg/h
- Fluidizing velocity: 0.2 m/s
- Nominal heat output: 2 kW



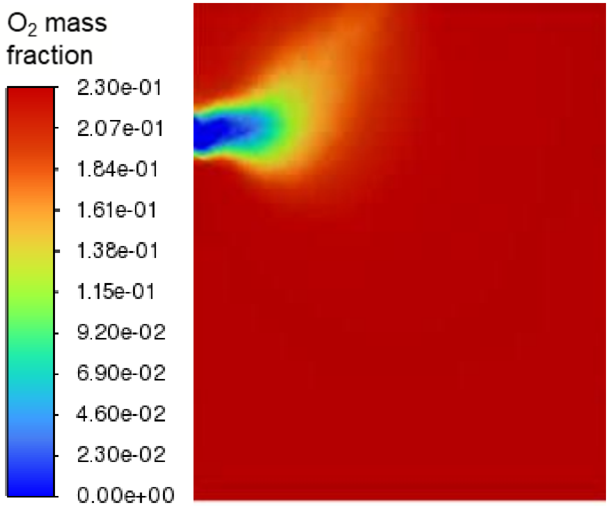
Oxide volume fraction



Iron volume fraction



Heat of reaction (W)



Oxygen mass fraction

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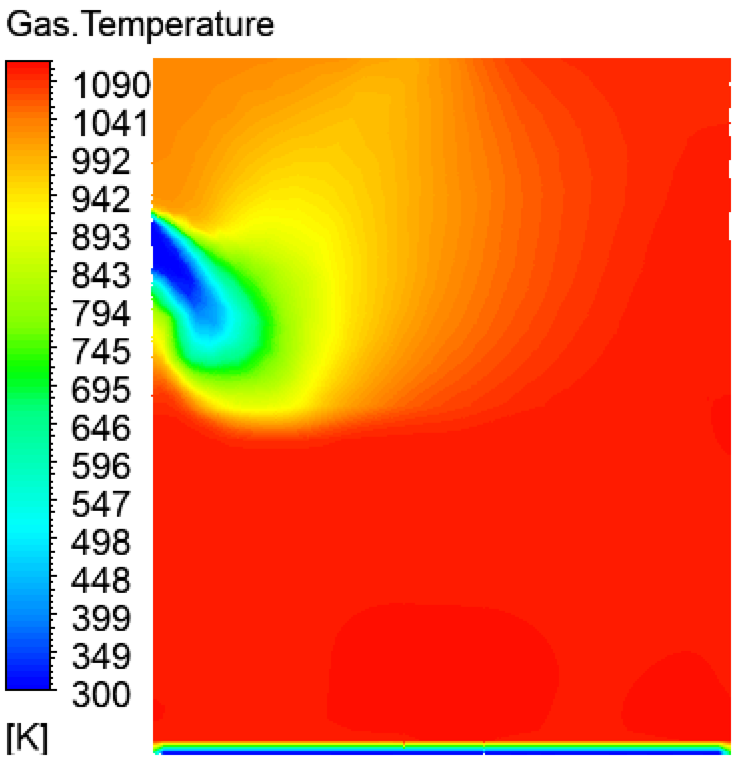
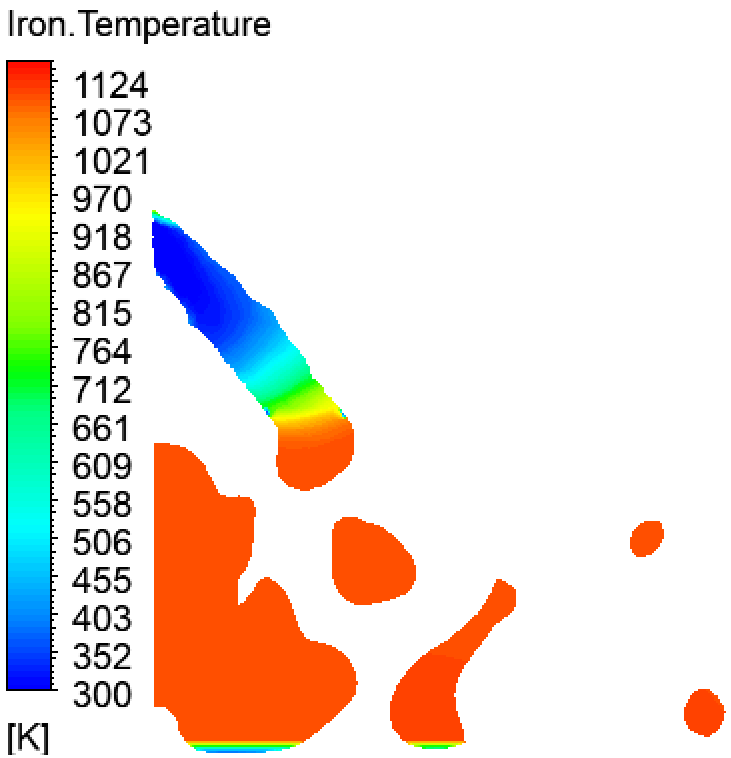
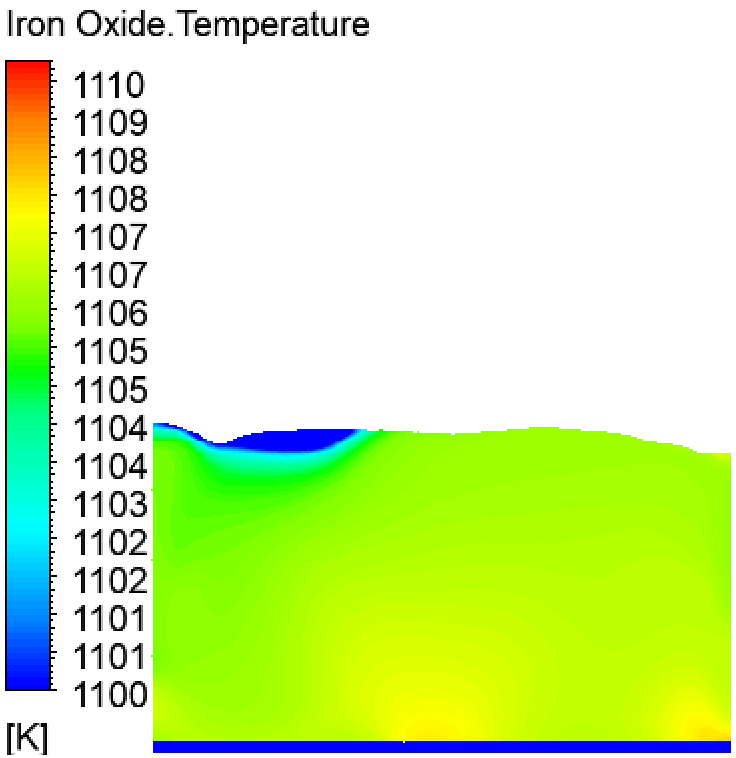


Gas temperature

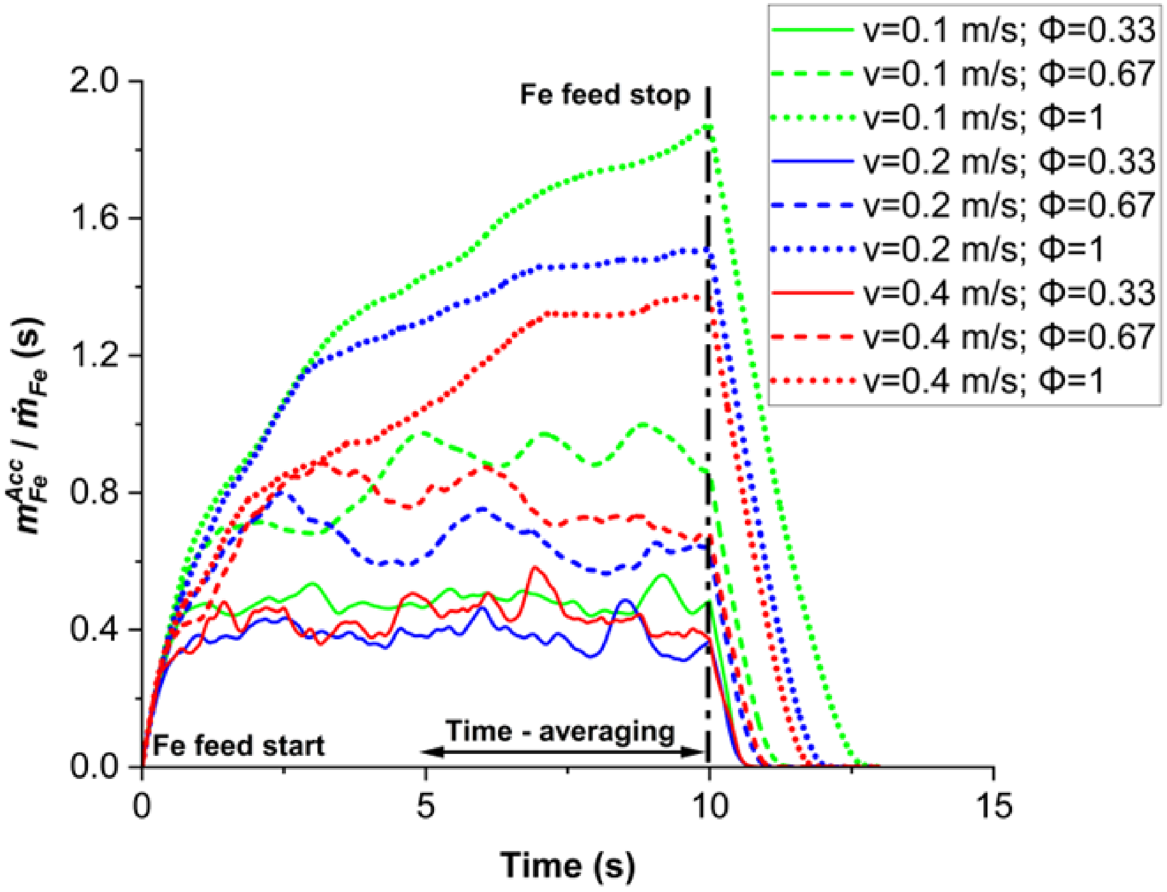


Iron temperature



Oxide temperature

Quantitative comparison: 9 cases



- Time to stabilization and iron buildup in the reactor increase with mixture fraction and decrease with turbulence.
- “Surplus time” to be compared with particle residence time.
- Effects on combustion efficiency.

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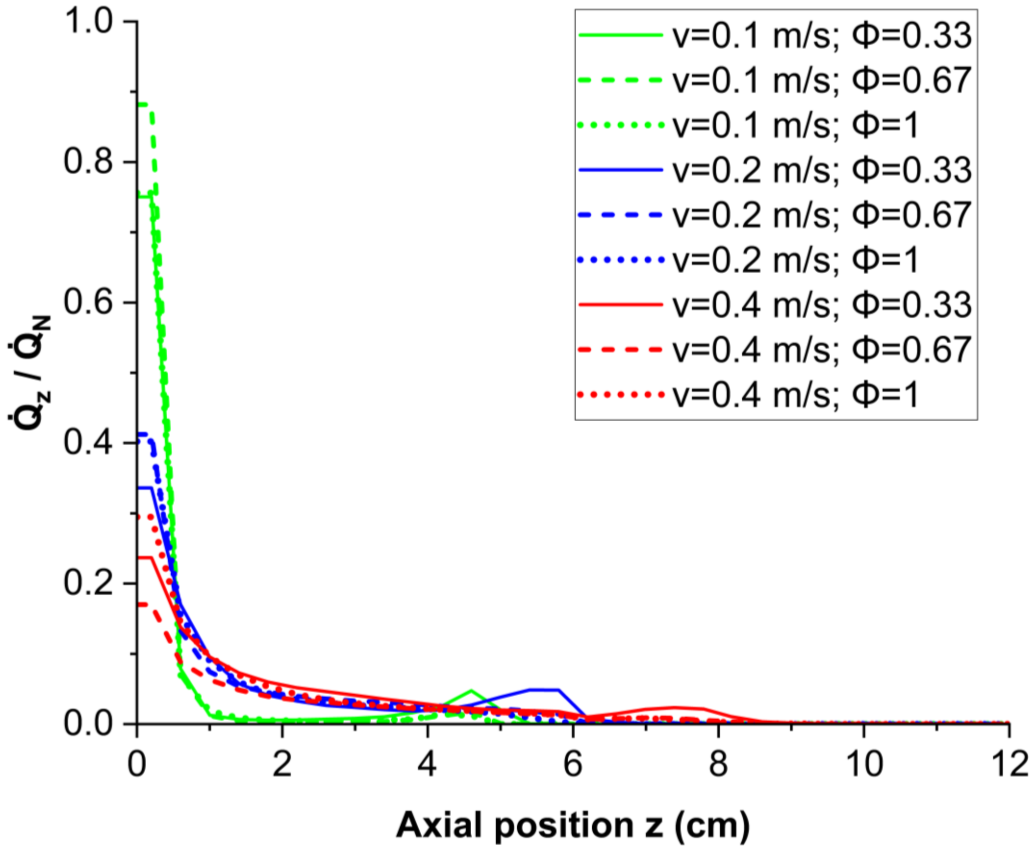
Time-averaged heat generation rate



- Reaction occurs mainly at the bottom (and surface) of the bed.
- Higher velocity: higher power density, taller bed, and increased mixing.
- Higher mixture fraction: shifts reaction towards the bottom.

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Conclusions

CFD EXP
- Similar fluidization behaviour for metal and oxide particles, removing the need for a third inert material. Remains to be tested with actual product particles.

CFD
- Limits of Euler-Euler approach: need to account for particle-level reaction rates and temperature increase (→ vaporization ?).

EXP
- Partial melting, mitigated by higher turbulence and smaller particle size.

EXP
- Near future: assessment of combustion efficiency and product analysis.

EXP
- Limits of batch experiments: much higher fraction of iron in the bed compared to continuous operation → impact on aggregation and local oxygen fraction.

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MIX-MOXes - Mixed Metal Oxides Energy Stations for zero-carbon thermal energy generation with integrated heat storage (EP/X000249/1)

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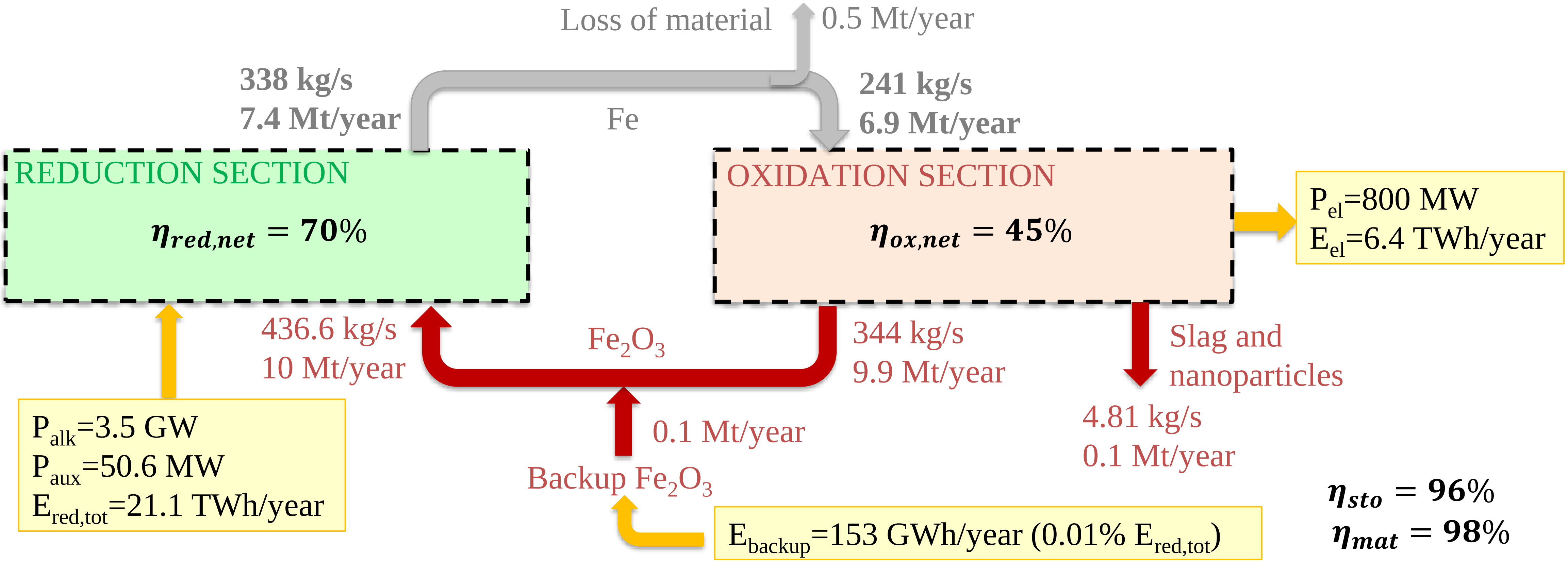
Thermodynamic Analysis



$\eta_{sto} = 96\%$
$\eta_{mat} = 98\%$
$\eta_{backup} \approx 100\%$

Transport Distance	Short	Medium	Long	Very long
η_{tra} [%]	98.3	96.4	95.7	90.7
η_{cyc} [%]	28.5	28	27.8	26.3