

Modelling turbulence interaction and the preferential concentration of reacting iron particles

S.S. Hemamalini^{1,2}, S. Guhathakurta¹, B. Cuenot^{1,3}, J. A. van Oijen¹, X.C. Mi^{*,1,2}

¹ Department of Mechanical Engineering, Eindhoven University of Technology
P.O. Box 513, 5600MB, Eindhoven, The Netherlands

² Eindhoven Institute of Renewable Energy Systems, Eindhoven University of Technology
P.O. Box 513, 5600MB, Eindhoven, The Netherlands

³ CERFACS
42, Avenue G. Coriolis, 31057 Toulouse Cedex 01, France

1 Introduction

To overcome humanity's dependence on fossil fuels, renewable fuels are being developed in an unprecedented speed through the past decade. While most of the alternative fuels such as solar energy and wind energy are viable options, they are geographically scattered and temporally fluctuating. To overcome this problem, the scientific community is in search of a reliable and efficient energy storage alternative. Iron powders have been proposed by a number of scientists as a promising candidate owing to their carbon-free energy cycle, high energy density, and recyclability [4]. A typical iron-based renewable energy cycle is illustrated in Fig. 1.

To realize the illustrated iron-based cycle, efficient combustors of iron particles are required. Iron as a material has a high boiling point, 3135 K, meaning that the particles can remain in the condensed phase throughout the combustion process. Hence, the phenomenon of iron particle combustion is unlike combustion dynamics of other volatile fuels. The non-volatile nature of the combustion process of iron particles results in a unique heterogeneous spatial heat release referred to as spatially discrete flame in literature [7]. As stabilized turbulent flames of iron particles lie at the heart of practical combustors, it is important to understand the interplay between the unique spatially discrete iron particle flames and turbulence.

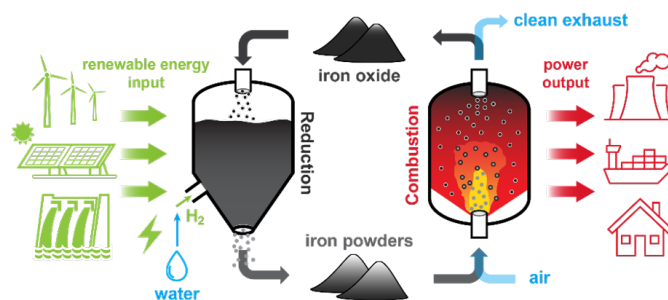


Figure 1: A carbon-free iron-based cycle of renewable energy.

The present work attempts in numerically modelling the kinetics of the iron particles, the interparticle gradients, flow entrainment and their effects on the heat release, oxygen absorption and contribution to the energy spectra of turbulence. Several studies are ongoing to describe the ignition and burning characteristics of isolated iron particles and laminar flames. This proposed study is the first attempt in linking the combustion dynamics of iron particles with particle-laden turbulence.

2 Dimensional analysis: why the interplay between turbulence and the reacting iron particle is unique and important

Since heterogeneously reacting iron particles tend to induce interparticle gradients in gas-phase temperature, oxygen concentration and flow velocity, the mean particle spacing, l_p , is a key length scale anchoring the combustion dynamics of iron particles. Hence, an important analysis would be the comparison of l_p with the length scales of turbulence – the integral length scale L and the Kolmogorov scale l_k . The mean particle spacing l_p can be estimated knowing the initial mean particle size, $d_{p,0}$, and the initial concentration of iron mass, $C_{Fe,0}$. The initial concentrations of iron and oxygen injected into a combustor are related via the equivalence ratio ϕ_{FeO} . For iron particles of $d_{p,0} = 30 \mu\text{m}$, which is a typical size of iron powders used in practical combustors, mixed with air at standard conditions and $\phi_{FeO} = 1$, the mean particle spacing is estimated to be $l_p \approx 0.61 \text{ mm}$. The overall volume fraction of the particles is on the order of 10^{-4} .

To the authors' knowledge, laboratory-scale, swirl-stabilized turbulent combustors of iron powders have been independently developed at both McGill University [5] and the Eindhoven University of Technology [1]. Up to the time this abstract was written, the turbulent flow parameters of these combustors had not been revealed in detail. Hence, it is reasonable to assume that turbulent flow conditions created in these combustors are similar to those in laboratory-scale, swirl-stabilized coal combustors. Thus, the turbulent conditions of the Cambridge Coal combustor 1 (CCB1) [2] are considered in this analysis. In CCB1, the integral and Kolmogorov length scales are estimated to be $l = 6.08 \text{ mm}$ and $l_k = 0.11 \text{ mm}$, respectively [2].

Knowing the key length scales, the interaction between turbulence and particles can be characterized as follows:

- (1) For particle volume fractions on the order of 10^{-4} , the two-way coupling between the particle and gas-phase dynamics is expected. For a particle volume fraction less than 0.4%, particle-particle interaction is negligible [11].
- (2) Typical particle sizes (e.g., $30 \mu\text{m}$) are comparable to or smaller than the Kolmogorov length scale, so that the viscous drag of the particles tends to dissipate the turbulent kinetic energy.
- (3) Typical values of mean particle spacing are on the orders of 0.1–1 mm, falling between the integral and Kolmogorov length scales of the turbulence. The spatially discrete energy release from the particles likely enhances the production of turbulent kinetic energy.
- (4) The Stokes numbers of iron particles of sizes $30 \mu\text{m}$ are in the range of $St_k = [1, 10]$, resulting in similar particle and flow timescales. In this case, the particles are entrained by large flow structures, leading to preferential concentration as highlighted by Fig. 2.

The phenomenon of preferential concentration of reacting iron particles is unique compared to volatile solid fuels such as aluminium or biomass. This effect is hypothesized to play an important role in the dynamics of iron combustion systems. In such systems, the clustering of particles occurs in the scale of

large eddies, which approximately correspond to the integral length scale L . This scale is characterized by the production of turbulent kinetic energy. The particle sizes are smaller than the smallest structures of turbulence, corresponding to the Kolmogorov length scale l_k . This scale is characterized by viscous dissipation of turbulent kinetic energy. The mean particle spacing l_p , which is significant in determining interparticle gradients, lies in the inertial subrange where the majority of the energy transfer takes place. Thus, for a typical turbulent iron combustion process, all three characteristic scales of turbulence are equally important and hence, resolved simulations are indispensable to gain insights into the interplay between reacting iron particles and turbulence.

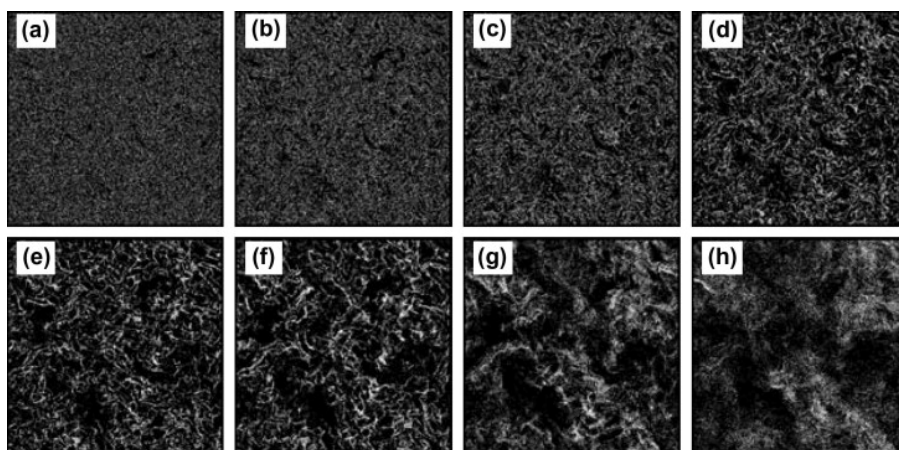


Figure 2: Distribution of particles in a 2D turbulent flow profile with Stokes numbers $Stk = 0.05$ (a), 0.1 (b), 0.2 (c), 0.5 (d), 1 (e), 2 (f), 5 (g), 10 (h). Preferential concentration can be observed in cases (e), (f) and (g) where the distribution of particles directly corresponds to the flow profile. Simulation from Yoshimoto and Goto *et al.* [16]

3 Model description

An Euler-Lagrange framework similar to the model formulated by Hazenberg & van Oijen [8] is used to simulate the particle-laden flow and kinetics of iron particles. The reaction model proposed by Soo *et al.* [12] is used to model the oxidation of iron (Fe) to ferrous oxide (FeO). Other products of oxidation of iron are not currently considered. An Arrhenius-type equation is used to model the reaction rate, with gas phase properties interpolated at the location of each particle. A better physics-informed model [9,13–15] is under development to be incorporated into the current framework. The gas phase is modelled using non-dimensional forms of the continuity, momentum, energy, and mass conservation equations using the compressible DNS flow solver NTMIX-CHEMKIN developed by CERFACS [3,6].

4 Simulations of iron particle combustion in a turbulent mixing layer

Simulations of a turbulent mixing layer offers several computational advantages in modelling particle-laden turbulent flows with reacting particles. The domain can be adequately small in the streamwise direction, as periodic boundaries can be used. The extents of the domain can be scaled to multiples of the integral length scale, and the domain resolution can be scaled with the Kolmogorov length scale. The heat diffusion at the mixing layer provides a spatially and temporally smooth ignition process of the iron particles. Hence, the present work focusses on the simulations of interaction between reacting iron particles and particle-laden turbulence in a turbulent mixing layer.

4.1 Case Setup

The case setup in the present work is similar to work done by Rieth *et al.* [10] in their simulations of pulverized coal particle combustion. A monodisperse powder of iron, with particle size $d_p = 10 \mu\text{m}$, is fed through a mixing layer of air at a relative velocity of $U = 20 \text{ m/s}$. The initial flow profile is characterized by two streams – a hot stream with a mean velocity in the flow direction $v_{\text{hot}} = -17.6 \text{ m/s}$ at a temperature of $T_{\text{hot},0} = 1693 \text{ K}$ and a cold stream with a mean velocity $v_{\text{cold}} = 2.4 \text{ m/s}$ at a temperature of $T_{\text{cold},0} = 600 \text{ K}$. The particles are released onto the cold stream, preheated to $T_{\text{ptcl},0} = 600 \text{ K}$. The flow corresponds to a Reynolds number of $\text{Re} = 110$.

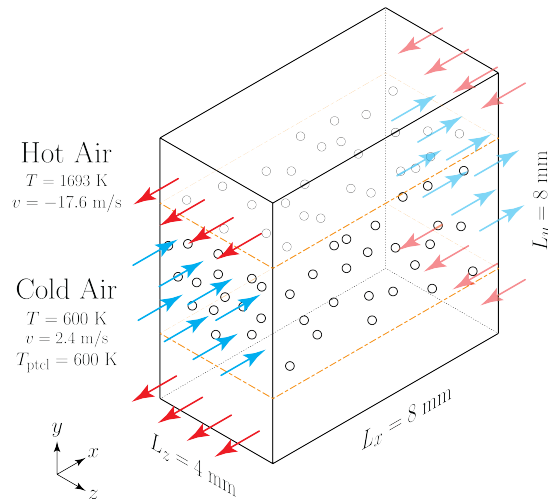


Figure 3: Case setup for 3D turbulent mixing layer simulations

Both 2D and 3D simulations are carried out with the same flow profile. The domain spans $L_x = L_y = 8 \text{ mm}$, approximately equal to the integral length scale L of the flow. The span in the z -direction is set at $L_z = 4 \text{ mm}$ for 3D simulations. In the case of 2D simulations, L_z is set to the length of mean interparticle spacing, l_p such that $L_z = l_p = 102.59 \mu\text{m}$. The particles are initialized. The number of the particles in the domain are set using stoichiometric analysis assuming an equivalence ratio $\phi = 1$ for the volume of the cold stream. Periodic boundaries are used on all the three axes. The case setup is illustrated in Fig. 3.

4.2 Preliminary Results

At the start of the simulation, the particles and the hot air are separated. As the simulation progresses, the development of a mixing zone between the two streams can be observed. This development results in entrainment of particles into the hot stream. Gradual heating of the particles results in ignition and, subsequently, completion of the oxidation reaction and heat release. The particles closer to the mixing layer start to react with oxygen at $t = 1 \text{ ms}$ corresponding to a gradual increase in temperature until ignition. The gas expansion and the temperature gradients caused by the exothermic combustion of iron particles induces turbulence in the mixing layer. The onset of turbulence can be seen in Fig. 4. The heat release from the combustion enhances heat diffusion in the mixing layer, further accelerating reaction of particles in the vicinity.

For 3D simulations, the timescale for the completion of the oxidation reaction is of the order 0.2 ms . For the chosen 3D flow configuration, the characteristic large eddy turnover time can be estimated to be

$\tau_L = L/U = 0.4$ ms. The timescale of the smaller eddies is estimated to be $\tau_l = \tau_L/\text{Re}^{1/2} = 0.04$ ms. Assuming the dynamic viscosity of air at $T = 1200$ K to be $\mu_g = 0.04626$ mPa.s, an estimate for the particle timescale is calculated as $\tau_p = 0.9$ ms. Thus, the Stokes number for the flow is approximated to be in the range $\text{Stk} \approx 1-10$.

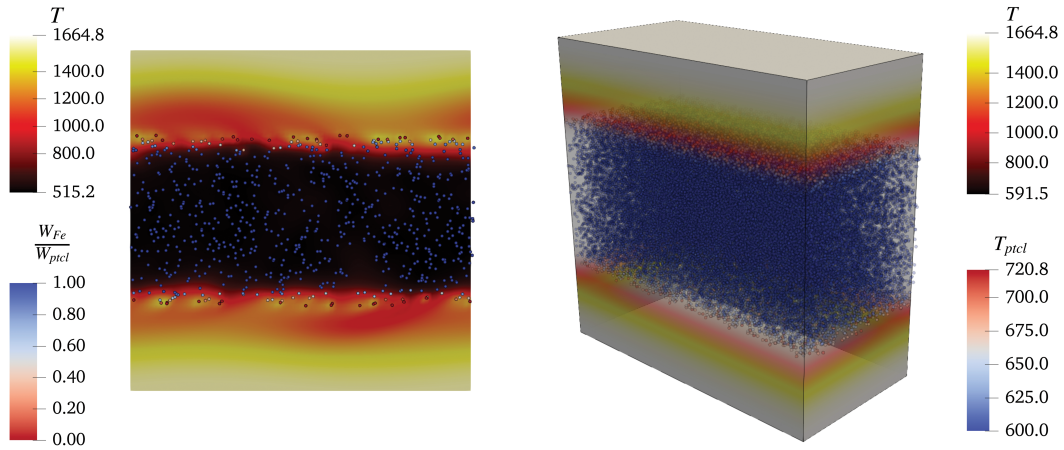


Figure 4: Left: Gas phase temperatures and particle Fe mass fraction for a 2D turbulent mixing layer simulation at a flow time of $t = 1.29$ ms, Right: Gas phase and particle temperatures for a 3D turbulent mixing layer simulation at a flow time of $t = 0.66$ ms. Temperatures are in [K].

5 Summary

The present work is the first study in numerically simulating reacting iron particles in a turbulent flow regime. The interplay between the combustion dynamics of iron particles and particle-laden turbulence is an essential milestone in understanding complex turbulent flames of iron particles. A turbulent mixing layer is simulated using a DNS flow solver NTMIX-CHEMKIN and the combustion reaction of iron is modelled using the reaction model proposed by Hazenberg and van Oijen [8]. A similar case setup as Reith *et al.* [10] is used to model the turbulent mixing layer. Preliminary results show the gradual ignition of iron particles as they are entrained by the mixing layer. Heat release from the exothermic reaction induces turbulence in the mixing layer. For particles of size $d_p = 10$ μm , the Stokes number is estimated to be $\text{Stk} \approx [1, 10]$. Therefore, prolonged simulations are expected to show preferential concentration of iron particles as they are entrained by the mixing layer. A more substantial set of simulation data and in-depth analysis will be presented at the Colloquium.

References

- [1] Baigmohammadi, M., Prasadha, W., Stevens, N., Shoshin, Y. L., Spee, T., & de Goey, P. (2023). Towards Utilization of Iron Powders For Heating and Power. Applications in Energy and Combustion Science, 100116.
- [2] Balusamy, S., Schmidt, A., Hochgreb, S. (2013). Flow field measurements of pulverized coal combustion using optical diagnostic techniques. Exp. Fluids. 54: 1–14.

- [3] Baum, M., Poinso, T. J., Haworth, D. C., & Darabiha, N. (1994) Direct numerical simulation of H₂/O₂/N₂ flames with complex chemistry in two-dimensional turbulent flows. *J. Fluid Mech.* 281: 1–32.
- [4] Bergthorson, J. M. (2018). Recyclable metal fuels for clean and compact zero-carbon power. *Prog. Energy Combust. Sci.* 68: 169-196.
- [5] Bergthorson, J. M. (2022), “Burning metals for carbon-free power” the Combustion Webinar, May 28th, 2022, <https://youtu.be/ImJqyxcOeI8>
- [6] Brouzet, D., Talei, M., Brear, M. J., & Cuenot, B. (2021) The impact of chemical modeling on turbulent premixed flame acoustics. *J. Fluid Mech.* 915: A3.
- [7] Goroshin, S., Palecka, J., Bergthorson, J. M. (2022). Some fundamental aspects of laminar flames in nonvolatile solid fuel suspensions. *Prog. Energy Combust. Sci.* 91: 100994.
- [8] Hazenberg, T. & van Oijen, J. A. (2021). Structures and burning velocities of flames in iron aerosols. *Proc. Combust. Inst.* 38: 4383–4390.
- [9] Mi, X., Fujinawa, A., & Bergthorson, J. M. (2022). A quantitative analysis of the ignition characteristics of fine iron particles. *Combustion and Flame*, 240: 112011.
- [10] Rieth, M., Kempf, A. M., Kronenburg, A., & Stein, O. T. (2018). Carrier-phase DNS of pulverized coal particle ignition and volatile burning in a turbulent mixing layer. *Fuel*, 212: 364-374.
- [11] Rizk, M. A., Elghobashi, S. E. (1989). A two-equation turbulence model for dispersed dilute confined two-phase flows. *Int. J. Multiph. Flow.* 15: 119–133.
- [12] Soo, M., Mi, X., Goroshin, S., Higgins, A. J., & Bergthorson, J. M. (2018) Combustion of particles, agglomerates, and suspensions — A basic thermophysical analysis. *Combust. Flame.* 192: 384–400.
- [13] Thijs, L. C., van Gool, C. E. A. G., Ramaekers, W. J. S., van Oijen, J. A., & de Goey, L. P. H. (2022). Resolved simulations of single iron particle combustion and the release of nano-particles. *Proceedings of the Combustion Institute.*
- [14] Thijs, L. C., van Gool, C. G., Ramaekers, W. J. S., Kuerten, J. G. M., van Oijen, J. A., & de Goey, L. P. H. (2022). Improvement of heat-and mass transfer modeling for single iron particles combustion using resolved simulations. *Combustion Science and Technology*, 1-17.
- [15] Thijs, L. C., Kritikos, E., Giusti, A., Ramaekers, W. J., van Oijen, J. A., de Goey, L. P., & Mi, X. C. (2022). On the combustion of fine iron particles beyond FeO stoichiometry: Insights gained from molecular dynamics simulations. *arXiv preprint arXiv:2212.06432.*
- [16] Yoshimoto, H., & Goto, S. (2007). Self-similar clustering of inertial particles in homogeneous turbulence. *Journal of Fluid Mechanics*, 577: 275-286.