

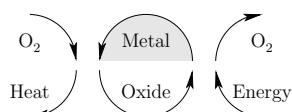
Book of Abstracts

Over the course of the past decade, the idea of using metal powders as recyclable, carbon-neutral energy carriers has gained momentum and research groups all over the world have begun to address open questions, both fundamental and applied, on single particle combustion, dust flames, recycling strategies or practical combustor technologies. This workshop is intended to provide a common forum for these efforts, to support the synthesis of experimental and modelling endeavours and to facilitate thought exchanges on open questions pertaining to the emerging field of an energy economy based on metal fuels. A particular objective of the workshop is to discuss the potential definition of a set of target dust flames for which experimental databases for model calibration and validation can be established and maintained.

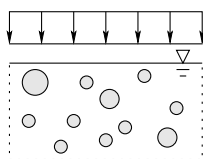
Target flames are characterized by a well-defined burner geometry and flow configuration, including well-controlled and reproducible boundary conditions and fuel properties. Focussing on single phase, non-premixed flames and sooting flames, respectively, target flames have been used in the past by the TNF and ISF workshops to coordinate and guide modelling endeavours. As part of this workshop, we wish to incite and encourage a discussion within the scientific community on potential target flames for metal fuels whose global (*e.g.*, flame speed, fuel conversion degree) and spatially resolved (*e.g.*, gas phase velocity, mean particle velocity, pollutant profiles, temperature) characteristics can be measured using different experimental diagnostic techniques. This may lead to a comprehensive database that supports model validation and provides a common ground for sharing physical submodels.

Graphical summary

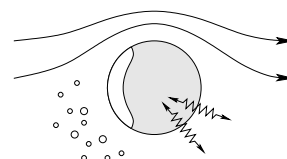
Cycle economy



Metal-water slurry reactors



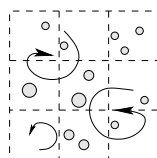
Single particle combustion



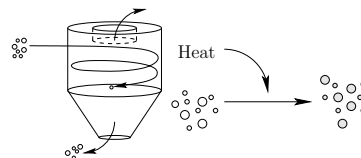
Metal dust flames



Turbulence-particle interactions



Retrieval and reduction



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1 Economy of the metal fuel cycle

Retrofit of district heating plants from biomass-fired combustors into iron redox systems — assessment of the Swedish case

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The energy field in Sweden is transiting to a new scenario characterized by a much stronger competence for biomass and a sharp increase in the volatility of electricity prices. With the district heating sector being currently dominated by biomass-fueled plants, a transition towards systems using electricity as input is envisioned as solution to the limited availability of biomass and the expected need for large-scale long-term energy storage. This work presents a techno-economic assessment of the retrofitting of biomass-fired district heating plants into systems which, using thermochemical energy storage based on an iron redox cycle, produce dispatchable heat and power from electricity of high price volatility. A linear cost optimization model is used to investigate the impact of the electricity price variability on the cost-optimal size and operation of electrified retrofits of current district heating plants. Different technological choices for the retrofit are considered (type of electrolyzer, on-site storage of H₂), and the results are compared to current and competing technologies (*e.g.*, heat pumps). The results also indicate that with the use of the iron as energy carrier (and storage medium) current heat demand curves can be covered at a cost of 55-70 €/MWh, *i.e.*, competitive with the foreseen biomass prices.

Thermodynamic assessment of iron as an energy carrier for carbon-free electricity generation

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Green energy carriers are essential for balancing the temporal and geographic mismatch between renewable energy supply and demand. Along with the necessary growth of renewable energies, metal fuels – especially iron – show great promise as energy carriers for this purpose. Electrical energy from renewable sources can be stored in iron through the thermochemical reduction of iron oxides with green hydrogen. The stored energy can then be converted back into electricity by thermochemical oxidation, for example, in retrofitted coal-fired power plants. Spatial and temporal separation of renewable energy storage and release is made possible by transporting the iron/iron oxide in a closed circle.

Comprehensive thermodynamic models have been developed to assess the oxidation process in retrofitted coal-fired power plants for carbon-free electricity generation, as well as the thermochemical reduction process in shaft furnace plants with green hydrogen for the regeneration of iron oxides. These models are linked through transport and intermediate storage, which may result in losses (partial oxidation of the iron) by themselves. The quantification of individual sub-process efficiencies, overall power-to-power efficiency, and identification of crucial process steps and parameters are carried out through a detailed evaluation of these individual models as well as the overarching interconnected model.

Techno-economic analysis of aluminum, zinc and magnesium as potential clean energy carriers

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Aluminum, zinc and magnesium are among promising metal fuels candidates due to their energy density and ability to be converted back into electricity through high-temperature water oxidation and a combination of heat engines and/or fuel cells. For any metal fuel cycle to be sustainable and cost-competitive, the oxides produced must be collected and reduced back to metal using a carbon-free process. In this work, a techno-economic analysis of the reduction process of various metals was conducted to estimate their recharging cost if used as energy carriers. A review of current industrial production method for all candidates was performed to assess their efficiency, scalability, sustainability, and cost. Results compare the competitiveness of these metals with alternatives such as hydrogen and ammonia over a range of electricity prices and shipping distances, thereby evaluating their potential as long duration energy storage or for decarbonizing remote communities and industries. Overall, this study provides the first step (Power-to-X) required to assess the feasibility of using aluminum, zinc and magnesium as a sustainable and cost-competitive energy carriers.

Techno-economic analysis of iron fuel for energy storage and distribution

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Recently, iron has been proposed as a novel carbon-free fuel for both energy storage and distribution. Iron is energy dense, safe and stable, and as a globally traded commodity, it is an ideal energy carrier that can be used to replace current fossil fuel trade with green energy produced from clean resources such as wind, solar and hydropower. Several different metal powered systems are being developed worldwide, however the question of their economic viability in a competitive marketplace remains. Here, a case-study of a Canadian-German iron fuel trade scenario is assessed. The entire iron fuel process is evaluated considering the raw materials, combustion and energy production, fuel recharging methods, storage duration and distribution distance to determine the levelized cost of energy produced from iron fuel. Results show that iron-based systems can be cost competitive with conventional fossil fuel systems and other green solutions such as hydrogen. Iron fuel produced with low-cost green hydroelectricity in Canada can deliver energy to Germany on par with conventional systems below 0.20 \$/kWh. As the storage duration or transport distance increases, the gap between the cost of iron fuel and hydrogen increases drastically, favouring the use of iron over hydrogen as an energy commodity.

2 Metal-water slurries

Investigating the role of particle morphology on the kinetics of the aluminum-water reaction based on a multi-stage shrinking core model

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Hydrogen production through aluminum oxidation with water allows sustainable and emission-free in-situ hydrogen generation. Compared to spherical particles, flake-shaped structures have a larger specific surface area that can lead to higher reaction rates and shorter reaction times; however, most of the existing experimental and theoretical studies are limited to spherical geometries. To investigate the effect of particle shape on the kinetics of the aluminum-water reaction, a two-staged analytical model based on the principles of the shrinking core model was developed for both spherical and flake-like particles. The flake-like morphology of the particle was represented by a flat plate geometry. The first stage of the oxidation reaction, *i.e.*, the induction phase, is assumed to be controlled by the kinetics of hydration of the protective alumina shell to form boehmite. During the next step, the reaction is carried on through the oxidation of the aluminum core which is controlled by the kinetics of the oxidation reaction as well as the diffusion of the oxidizer in the oxide shell. While the first mechanism is dominant at the earlier stages of the reaction, diffusion rate becomes the rate-limiting step as the oxide layer grows. The model predictions are then validated with the heat release in isothermal microcalorimetry for 40 nm and 1 μm spherical as well as 2 μm flake-like particles.

Thermal ignition of micro-aluminum powder and with compressed water

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In this study, micro-aluminum powders and water slurries were reacted in a constant volume batch reactor to examine the effect of pressure on mixture ignition (*i.e.*, thermal runaway). The aluminum-water slurries consisted of 13 mL distilled water and 10 g aluminum powder (99.7% purity). The powders used had nominal sizes of 1, 10, 45 μm (spherical) and a 2 μm flake that corresponded to specific surface areas (SSA) of 7.85, 1.94, 2.21 and 15.42 m^2/g , respectively. A 900 W electrical heating band on the external wall was used to increase the mixture temperature and ignite it. Results showed that for powders with SSA higher than 7.85 m^2/g (1 μm spherical and 2 μm flakes), thermal runaway was achieved while the H₂O oxidizer was still in a liquid state. Larger particles with SSA less than 2.21 m^2/g (10 μm and 45 μm) did not undergo thermal runaway until after the saturation condition (*i.e.*, steam formation) was reached. The results indicate a marked increase in reaction rate as water transitions from liquid to vapour phase, and that thermal runaway of large powders is only achievable in a steam environment. Reaction rate, estimated from temperature data, did not show variation with pressure for reactions occurring in a liquid state, but increased with pressure for reactions occurring in the vapor phase.

Effect of particle size distribution on thermal ignition criteria for aluminum and water batch reactions

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In this study micro aluminum powders marketed as 1, 10 and 45 μm with specific surface area of 7.85, 2.21 and 1.94 m^2/g , respectively, reacted with distilled water in a batch process with back-pressure regulation. The mixture was pre-pressurized by argon gas and a 900 W electric band heater increased its temperature to the water saturation state. Measurements show that particle size distribution and saturated water state are fundamental criteria for thermal ignition (*i.e.*, temperature runaway). The 1 μm Al powders released significant heat in compressed water but required saturation temperatures to ignite, whereas the 10 and 45 μm Al powder released most heat after ignition.

The lognormal particle size distributions, specific surface areas and Arrhenius kinetic parameters in literature were used to develop a batch reactor model based on the core-shell particle geometry. The model is benchmarked with particle oxidation in water at isothermal conditions and predicts induction time as well as conversion ratio in excellent agreement with measurements. Calculated mixture temperature for the batch process is in good agreement with measurements when water is in compressed liquid state. Unreacted aluminum at the water saturation point predicted by the model is correlated to the steam concentration requirement for thermal ignition. The results of this study are useful in reactor design and optimization of the operating conditions required to maximize the aluminum and water reaction yield.

Fundamentals of high temperature liquid water and supercritical metal–water reactions

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Metal–water reactions are a means of producing hydrogen on–demand and in–situ. This has the potential to expand the adoption of hydrogen fuelling strategies across sectors that are still heavily reliant on hydrocarbons. Experiments performed under high–temperature and high–pressure, as well as supercritical, conditions have demonstrated that the full conversion of coarse metal particles is possible. Under these conditions mm–scale pellets of Al, Al alloys, Mg, Zn and scrap aluminum were fully oxidized without the use of catalysts or pre–treatment. In the case of Al, a marked improvement in efficiency is observed at 250 °C. In the case of the scrap aluminum, no hydrogen was produced under sub–critical conditions but full conversion was realized under supercritical conditions. The improvements in hydrogen yield are attributed to the changes in water properties as temperature and pressure increase. Changes in properties such as ionic product, relative permittivity, solubility, and viscosity are thought to improve reactivity. Other metals, which are thermodynamically predicted to react with water, either produced very small quantities of hydrogen (Si) or none at all (Ti, Zr). The current hypothesis is that the governing mechanism of reactivity is the solubility properties of the passivating oxide layer.

3 Combustion of single metal particles

Detailed characterization of the combustion of an isolated aluminum particle

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The work that is intended to be presented focuses on the combustion of an isolated aluminum particle. A dedicated facility consisting of an electrodynamic levitator allows the charged particle trapped by electrostatic forces to levitate and burn in a controlled atmosphere. The uniform heating of the particle until its ignition temperature is ensured by a CO₂ laser whose beam is split to hit the particle from both sides and that is stopped when the combustion is initiated. The coupling of this chamber with optical devices yields crucial information in the characterization of aluminum combustion. Characteristic burning times obtained thanks to the signals of the photomultipliers will be presented for varying ambient conditions (pressure and oxidizer). Then a two-colour pyrometry method assembled with photomultipliers combined with visual information of high temporal resolution from a high-speed camera allows the study of ignition’s phenomenology as well as the evaluation of the ignition temperature of the particle for various atmospheres. Measurements of the global temperature (particle and flame) during the combustion process carried out with the same method will be presented. Finally, the ongoing work will also provide spatially and temporally resolved concentration profiles of the condensed-phase combustion products surrounding the burning droplet using a light extinction method.

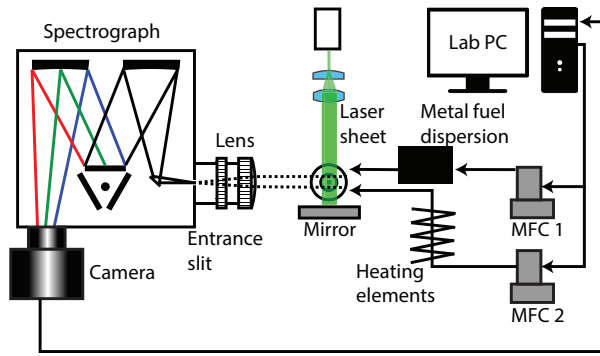


Figure 1 The experimental setup, which consists of a single particle generator, an electrically preheated coflow, an imaging system and some minor components.

Thermogravimetric study of the oxidation of iron particles

by M. Kurnatowska (Michalina.Kurnatowska@dlr.de), Q. Fradet, U. Riedel

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Metals and their oxides can be used in oxidation-reduction cycles for large-scale power generation resulting in CO₂-free energy conversion. The investigation of iron is of particular interest because, unlike other metal fuels, its dry oxidation is associated with limited nanoparticle formation in contrast to other metal fuels. Few studies have addressed the oxidation kinetics of iron powders.

The present work focuses on the kinetics of the thermochemical oxidation of iron particles with air. Experiments are carried out using thermogravimetric analysis (TGA) under isothermal conditions and at linear heating rates. A kinetic model will be developed, that solves for the individual species evolutions, allowing for a direct comparison between experiments and modeling. The model will be able to describe the oxidation of iron up to the ignition point, after which the limiting process is the diffusion of oxygen. Accurate kinetics of the early stages of the particle combustion is essential for reliable CFD simulations of steam generators as it will for example greatly influence the ignition delay times and thus the flame characteristics. The influence of parameters, such as the particle size distribution, the temperature, and the heating rate on the kinetics will be discussed, as well as the sintering that occurs during the TGA experiments.

Acknowledgements: This work was performed within the DLR project IronCircle[®] and the cluster project Clean Circles.

Particle resolved hyperspectral pyrometry measurements of burning iron particles

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The scientific community for metal fuels has been growing for quite some time. As the research into metal fuels expands, the need for accurate diagnostic techniques will also grow. Out of all the flame parameters, temperature might be the most important one. In typical gas flames, the flame temperature is an important indicator for soot and NO_x. In iron flames, soot is not an issue, but evaporation of iron, and the subsequent formation of nano-particles, could be a problem. Multiple experimental studies have been conducted using dual color and three color pyrometry, but these studies do not agree in their results [1, 2].

In this study, a method is presented which enables the measurement of the temperature of burning metal particles using hyperspectral pyrometry. A simple setup was built using a spectrograph and an intensified CCD camera and used for single iron particle combustion in air with the use of an electric preheater. This setup is shown in Figure 1. It is shown that the maximum temperature of iron particles increases slightly with an increasing particle size.

[1] D. Ning, Y. Shoshin, M. van Stiphout, J. van Oijen, G. Finotello, and P. de Goey, Temperature and phase transitions of laser-ignited single iron particle, *Combustion and Flame* 236, 111801, 2022.

[2] A. Panahi, D. Chang, M. Schiemann, A. Fujinawa, X.C. Mi, J. M. Bergthorson, and Y. A. Levendis, Combustion behavior of single iron particles-part I: An experimental study in a drop-tube furnace under high heating rates and high temperatures, *Applications in Energy and Combustion Science* 13, 100097, 2023.

Iron particle ignition in hot coflow

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Understanding the ignition of iron particle combustion in hot environments is critical for harnessing the use of metal fuels in clean energy production.

In this research work, an updated version of a metal particle burner was implemented to disperse and burn iron particles using hot coflow. The burner disperses iron particles through Coulomb forces inside an air-spaced capacitor. A non-oxidizing carrier gas flows through the cloud, dragging a sequence of single particles through a capillary tube towards the downstream of the burner where they are combusted by the hot oxidizer coflow.

The oxidizer coflow is heated up as it passes through a newly designed induction gas burner, which provides efficient heat transfer between the heating element and the coflow gas. Temperature homogeneity was visualized using Schlieren and confirmed by measuring the temperature at the outlet of the coflow tube. Particle ignition and combustion occur in open space, providing excellent conditions for optical diagnostics. Two synchronized high-speed cameras were used to simultaneously determine the particle size using green laser shadowgraphy and detect the status of iron particle ignition.

The results show that the burner was able to provide a uniform coflow temperature field for burning the metal particles up to 6.7 cm above the coflow tube. This allows for the steady combustion of single iron particles in a homogeneous oxidizing atmosphere. It was also observed that at a coflow temperature of 750 °C, 51.3% of the ejected particles were ignited. Detailed information on the particle size distribution and sphericity of the ejected particles is also provided.

Solid-phase oxidation time of single iron particle combustion in a hot laminar flow

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The present poster reports the in-situ optical diagnostics of single iron particle combustion in a laminar flow reactor (LFR). The LFR composes a near-adiabatic flat flame burner and a fused silica chimney, which provides well-defined boundary conditions and optical access. Iron particles are ejected into the LFR through a 1mm-inner-diameter tube located at the center of the flat flame burner. Multiple parameters including particle size, burn duration, and particle temperature are measured non-intrusively and simultaneously. The particle size is measured using diffuse backlight illumination (DBI) with high temporal and spatial resolution. Besides, the particle combustion duration is determined by tracking the luminosity of burning particles until the peak radiation intensity. The current synchronized multi-parameter measurement resolves multiple stages of iron particle behavior, including the particle preheating, ignition, solid-state oxidation, melting, and liquid-state combustion. This enables to quantify a series of time scales (ignition delay time, solid-state combustion time, and liquid-state burning duration) as a function of the particle diameter.

Comparing nanosecond and picosecond excitation for laser induced breakdown spectroscopy to determine the oxidation state of iron particles

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Energy storage using chemical energy carriers is highly relevant due to the expansion of renewable energies, and the need to import energy for countries such as Germany. Within the Clean Circles project, iron is being investigated as a chemical energy carrier. Experimental data are needed to develop a better understanding of the detailed processes during reduction and oxidation of the iron. For this purpose, the atomic composition of iron and iron oxide particles will be investigated in situ, by means of laser induced breakdown spectroscopy, in order to determine their oxidation state.

To develop the measurement technique for a quantitative analysis for this application, a parameter study was performed, to analyze the various factors influencing the measured spectra. A time-resolved plasma analysis has been performed, to find an ideal delay time between the excitation of the plasma by the laser pulse and the start of the recording of the plasma spectrum for a ns-pulse and a ps-pulse laser. This

delay time is required to separate the initial continuum radiation from the later element-specific plasma radiation to be detected. The pulse length of the excitation laser is also decisive for the amount of the gas phase surrounding the particle, which is also partly transferred into the plasma.

The results of the parameter study show that for the ns-pulse laser the delay times for the detection of the iron and oxygen signal are in the time range of microseconds, whereas for the ps-pulse laser they are in the ns-range. Excitation with the ps-pulse laser shows a significant reduction in continuum radiation compared to the ns-pulse laser and a significant reduction of the gaseous phase surrounding the particle that is transferred into the plasma. This is decisive for a quantitative measurement of particle compositions to determine the oxidation state.

Towards iron-based alloy combustion: a parametric analysis

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In the quest of improving the understanding of pure iron particle combustion, several numerical and experimental single-particle studies have been conducted. Nevertheless, the current global pure iron production (1.9 Gt/year) is not sufficient to apply the metal-fuel concept at the level it might reach for long-term renewable energy storage (between 5 and 10 Gt/year). Also, purifying iron is costly and associated with CO₂ emissions. This justifies the need in using recycled and/or non-purified iron powder which might contain other elements, called impurities.

To understand the influence of impurities on combustion, I conducted a parametric analysis using a single-particle model coupled with the use of molecular dynamics simulations. This work shows that the ion diffusion coefficients in the solid state are significantly influencing the degree of oxidation. An appropriate alloying element, and an optimal concentration, could be found to maximize it. The heat of oxidation and the specific heat impact the peak temperature and therefore the production of nanoparticles. The model also allows identifying unvalorized impure/recycled iron powders to use in the metal-fuel cycle. The next step is to extend this study to a multi-particle scale to include the collective effects of burning simultaneously thousands of alloyed particles.

On the surface chemisorption of oxidizing fine iron particles: insights gained from molecular dynamics simulations

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Molecular dynamics (MD) simulations are performed to investigate the thermal and mass accommodation coefficients (TAC and MAC, respectively) for the combination of iron(-oxide) and air. The obtained values of TAC and MAC are then used in a point-particle Knudsen model to investigate the effect of chemisorption and the Knudsen transition regime on the combustion behavior of (fine) iron particles. The thermal accommodation for the interactions of Fe with N₂ and Fe_xO_y with O₂ is investigated for different surface temperatures, while the mass accommodation coefficient for iron(-oxide) with oxygen is investigated for different initial oxidation stages Z_O , which represents the molar ratio of O / (O + Fe), and different surface temperatures. The MAC decreases fast from unity to 0.03 as Z_O increases from 0 to 0.5 and then diminishes as Z_O further increases to 0.57. By incorporating the MD-informed accommodation coefficients into the single iron particle combustion model, the oxidation beyond $Z_O = 0.5$ (from stoichiometric FeO to Fe₃O₄) is modeled. A new temperature evolution for single iron particles is observed compared to results obtained with previously developed continuum models. Specifically, results of the present simulations show that the oxidation process continues after the particle reaching the peak temperature, while previous models predicted that the maximum temperature was attained when the particle is oxidized to $Z_O = 0.5$. Since the rate of oxidation slows down as the MAC decreases with an increasing oxidation stage, the rate of heat loss exceeds the rate of heat release upon reaching the maximum temperature, while the particle is not yet oxidized to $Z_O = 0.5$. Finally, the effect of transition-regime heat and mass transfer on the combustion behavior of fine iron particles is investigated and discussed.

A contactless method for *operando* electrical conductivity measurements

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Measuring electrical conductivity of powdered materials is challenging, especially due to contact effects. We present a contactless method, adapted for *operando* use, based on the microwave cavity perturbation technique, as developed by Eichelbaum et al. [1] In this technique, the electrical conductivity of the studied material is determined from the changes in the quality factor of the cavity. As a cavity method, the technique is very sensitive, but limited to study at field frequencies dictated by the cavity size.

The method has been recently adapted for continuous use by reducing the need for calibrations [2] and allows for the study of semi-conductors and their powders in various atmospheres, between room temperature and 850 K, at atmospheric pressure. The study of more conductive samples, such as metals, is possible, but the interpretation of the response as electrical conductivity is complicated by the skin effects in such materials. However, as it is an *operando* measurement technique, it may be of interest for the metal fuels community.

[1] M. Eichelbaum, R. Stößer, A. Karpov, C.-K. Dobner, F. Rosowski, A. Trunschke, and R. Schlögl, The microwave cavity perturbation technique for contact-free and in situ electrical conductivity measurements in catalysis and materials science, *Physical Chemistry Chemical Physics* 14(3), 1302–1312, 2012.

[2] P. Kraus, E.H. Wolf, C. Prinz, G. Bellini, A. Trunschke, and R. Schlögl, Towards automation of *operando* experiments: a case study in contactless conductivity measurements, *Digital Discovery* 1(3), 241–254, 2022.

Modelling of aluminum combustion in homogeneous reactors

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Within the scope of the metal fuel cycle, metal powders serve as recyclable and carbon-neutral energy carriers. Focusing on the size distribution characterizing the oxide smoke that is formed during the combustion of aluminum, we present two spatially homogeneous model formulations as a first step towards a detailed understanding of the localized oxide smoke dynamics. On the one hand, the perfectly stirred reactor with a reactive surface constitutes the spatially homogeneous counterpart of a finite volume cell at the surface of a burning aluminum particle in a laminar flow simulation. The size-resolved droplet formation dynamics are modeled using a population balance approach synthesizing nucleation, growth/dissociation, coagulation and deposition. A particular novelty is the calibration of coagulation enhancement factors for viscous retardation and van der Waals attraction. The partially stirred reactor, on the other hand, features heterogeneity on the smallest scales as incited in turbulent flames, for instance, and permits an analysis of how micro-mixing influences key observables such as temperature, the mean droplet size and the produced NO_x concentration. A novel *pdf* formulation is presented that accounts for the presence of a reactive surface and includes advective stirring as a mechanism for altering the association of surface and dispersion elements. The perfectly stirred and partially stirred reactor models are instrumented to identify the key processes that shape the droplet size distribution in gas phase aluminum combustion.

Aluminum particle combustion: A combined PBE-CFD approach

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Metal particles have recently been identified as recyclable energy carriers that may not only replace hydrocarbon-based fuels, but are also compatible with a sustainable, cyclic energy economy. The efficacy of the metal fuel cycle is strongly tied to the ability to separate the polysized oxide particles which form during the combustion of metal powders from the exhaust fumes. Here, we present a comprehensive model for the combustion of a single, spatially resolved aluminum particle that permits an analysis of the size-resolved smoke dynamics and may provide answers to open questions on the separability of oxide smoke fines. In our model, the oxide smoke droplets are described in a purely Eulerian fashion in terms of a droplet size distribution that evolves according to the spatially inhomogeneous population balance equation (PBE). The PBE is kinetically driven by nucleation, growth/dissociation and coagulation. Furthermore, droplet radiation and deposition on the reactive surface of a metal fuel particle are taken

into account. The PBE is embedded into a framework of balance equations for the gas phase species as well as the temperature, mass and momentum of the gas-droplet dispersion, allowing for a consistent description of gas-droplet equilibration in terms of temperature and bulk velocity. The governing equations are complemented by flux-matching boundary conditions at the interface separating the aluminum particle from the gas-droplet dispersion. Physically, these boundary conditions correspond to mass and enthalpy balances that yield the gas composition, temperature and Stefan flow velocity at the reactive surface of the burning aluminum particle. Finally, the developed model is validated by comparison with available experimental measurements of radial profiles of the AlO and Al₂O₃(l) concentration as well as temperature and employed to predict the smoke size distribution in a spatially resolved way.

4 Metal dust flames

4.1 Experimental analyses of laminar dust flames

Development of spectroscopic techniques to determine particle and gas-phase temperatures in premixed aluminum dust flames

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Aluminum burns, after particle ignition, with micro-diffusion flames surrounding the particles which burn at the adiabatic flame temperature of the stoichiometric mixture. The surrounding bulk gas is heated, through the flame front, to another temperature, that is close to the adiabatic flame temperature of the actual fuel-oxidizer mixture, due to heat transfer rate between particles. The particle surface is at yet another temperature, typically at the boiling point of the metal, which differs from both the bulk gas and micro-diffusion flame temperature. The combustion of aluminum also results in the formation of nanometric particles of aluminum oxide that may be at another temperature. In order to understand these temperatures and the combustion behaviour of aluminum dust, absorption and emission spectroscopy techniques are employed. The absorption of nitric oxide (NO), a gas-phase species, is measured through laser absorption spectroscopy (LAS) to determine bulk gas temperature. This measurement is done in the post-flame region above the tip of the aluminum Bunsen flames. 1D dual-range emission spectroscopy is used to record the continuous blackbody radiation and the electronic-vibrational AlO spectrum simultaneously across the flame. Based on Planck's law, the blackbody radiation is used to derive a temperature related to the fuel particle/droplet and oxide-product temperatures. AlO is an intermediate combustion product; therefore, the AlO temperature is considered to be the temperature representing that of the diffusion micro-flame. These measurements will help in understanding the complex physics of aluminum combustion.

Experimental investigation of the laminar reaction front speed of Fe-N₂/O₂ mixtures in a tube burner

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For the investigations on iron dust-air flames, an optimized air-knife-seeder combined with a tube burner was developed, which minimizes fluctuations of the seeding density. This setup enables to investigate laminar iron dust-air flames in a wide range of conditions and even without air preheating. A carbonyl iron powder with a Sauter diameter of about 13 μm was used in the experiments, and the iron dust-air ratio was varied. After ignition, a cone-shaped flame stabilized at the tube exit. The flame was visualized by camera recordings and Abel transformed images were used to determine the position of the flame front. In addition, the velocity profiles of the gas phase and the iron particles were measured using PIV (Particle Image Velocimetry). Both pieces of information were used to determine the local reaction front speed. The global laminar reaction front speed was then extracted from the flame region, which is not subject to curvature or stretching. The measured reaction front speed corresponds well to the results of experiments carried out in microgravity. The laminar reaction front speed is independent of the fuel equivalence ratio for the investigated conditions.

The essential role of reduced-gravity environment for the study of flames in fuel suspensions

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Microgravity plays a crucial role in the study of flames in metallic suspensions. For larger particles intended for practical combustors (tens of microns), the combination of particle sedimentation and low burning velocity usually prevents the stabilization of laminar flames on the ground. As for flames propagating in tubes, the added effect of buoyant convection leads to recirculation cells which distort the flames and strongly affect their propagation. Thus, reduced gravity often presents the only way to produce benchmark experimental results that can be used to provide clean parametric studies. The importance of microgravity research has been demonstrated by the PERWAVES project, which studies flames in iron suspensions in oxygen/xenon gas in tubes. The effect of gravity was demonstrated by high-speed videos performed at normal gravity on the ground, at $\sim 10\text{-}2\text{g}$ aboard parabolic flights, and at $\sim 10\text{-}5\text{g}$ aboard sounding rockets. For the same mixture, the flames showed speeds of tens of cm/s, 5–7 cm/s, and 1 cm/s, in the three platforms respectively. Only the low speeds and stability of the flame aboard sounding rockets allowed a detailed study of the discrete regime of combustion which has otherwise been suspected to affect flame behaviour in previous ground-based experiments in flames in fuel-lean suspensions observed in tubes, balloons, and counter-flow burners.

In-situ optical investigations of metal powder oxidation on different combustion scales

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Within the Cluster Project Clean Circles, the oxidation properties of iron particles in several environmental conditions are investigated on different scales, starting from single particle combustion in a laminar flow reactor, continuing to stabilized iron dust flames in a laminar jet, and ending with an optically accessible laboratory-scale swirl combustor. Hereby, non-intrusive optical measurement techniques are employed, enabling an investigation of oxidation phenomena like nanoparticle formation with minimal influence on the combustion behavior. In this work, an overview of results on the mentioned scales is provided. At the single particle level, nano-oxide formation during oxidation of iron particles in a hot gas environment is investigated using Diffuse Backlight Illumination (DBI) measurements. Furthermore, stages of single particle combustion are evaluated using DBI and Particle Luminescence Imaging. For laminar iron dust flames, the reaction front speed of a laminar lifted iron dust flame is investigated using particle imaging velocimetry (PIV). In the turbulent swirl combustion chamber, a swirled gas-assisted iron dust flame is stabilized, allowing the investigation of complex turbulent flow interaction. The measurements of combustion phenomena on different scales allow for the investigation of single sensitive parameters on the oxidation behavior as well as the coupled effects of these parameters on the reaction and transport processes. These investigations aim to deepen our knowledge, provide validation data for numerical simulations from a single particle level up to a turbulent swirling combustor and pave the way for future applications of metal fuels in a decarbonized energy economy.

The heat flux method adapted for hybrid iron-methane-air flames

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Since the proposition of the metal fuel cycle, much research, both numerically and experimentally has been conducted. However, a lot still remains unclear about the burning velocities and effects of stretch and strain on iron dust flames. Therefore, the heat flux method was adapted for hybrid iron-methane-air flames. This method uses a heated perforated burnerplate to create a flat flame and uses thermocouples to measure the heat flux from and to the burner plate. This way the adiabatic burning velocity of flat hybrid iron-methane-air flames is measured. Results of this method for hybrid flames are presented as a proof of system, and adaptations from the classical heat flux burner are described. An in-house developed dispersion system was used to create a steady iron mass flow in the range of 1 to 30 mg/s. To ensure that the terminal velocity of the powders did not exceed the burning velocity, powder with a D50 of 7 μm was used. Addition of this iron powder to a stoichiometric CH_4 -flame shows clear reduction of laminar burning velocity in the order of several cm/s. These results show good agreement with recent simulations.

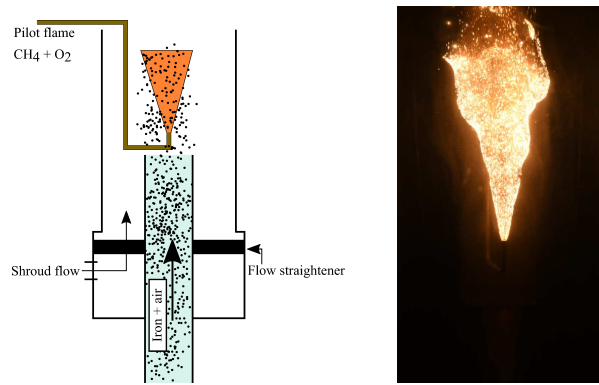


Figure 2 Left: schematic of the burner. Right: an image of the resulting flame showing the sharp flame front.

Characterising iron powder combustion using a v-shaped flame

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We present a v-flame burner, built to characterise various parameters of iron powder combustion (Figure 2). We also present the results of experiments performed by this burner, including an initial burning velocity value. The v-shaped flame is similar to a traditional Bunsen flame, however the flame is inverted – it begins at a point (stabilised with a pilot flame) and expands outwards, rather than the traditional Bunsen burner which starts from a ring and converges to a point. The flame front is clear and sharp which allows for a more accurate calculation of the flame surface area, and thus of the burning velocity, compared to the more diffuse flame front of a traditional Bunsen flame. The inverted burner also provides better conditions for optical diagnostics of the thermal structure of the flame, as the preheat zone is not blocked by the highly-radiating combustion zone and by combustion products which may contain highly scattering nano-oxides.

Minimum explosive concentration of micron-sized aluminum-silicon powder mixtures

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Aluminum and silicon are abundant elements in lunar regolith that show promise as solid rocket propellant. Leveraging lunar regolith for aluminum and silicon as rocket fuel can offer significant benefits for lunar exploration and future space missions. This approach eliminates the need to transport these materials from earth, leading to cost reductions and overcoming logistical challenges associated with space travel. Moreover, utilizing lunar resources paves the way for sustained lunar exploration and serves as a stepping stone for deeper space ventures.

The practical implementation of using lunar regolith as rocket fuel requires careful consideration of technical and engineering aspects. To this end, experimental research with aluminum-silicon mixtures of various weight ratios has been conducted to investigate the effect of dust cloud mixture composition on the minimum explosive concentration (MEC). The study examined mixtures with particle sizes ranging from 10–70 μm . The experimental results revealed that as the proportion of silicon increases, the MEC also increases. Furthermore it was found that for aluminum the MEC is not very particle size dependent, whereas with increasing silicon weight fraction the MEC becomes more particle size dependent. This highlights the importance of improving the understanding of aluminum-silicon mixture combustion and optimizing the mixture for safe and efficient propulsion.

4.2 Modelling of laminar dust flames

Nitrogen oxide emissions in iron dust flames

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Metal fuels are intensively researched as promising carbon-free energy carrier. As a carbon-free energy carrier, the emissions of soot, unburned hydrocarbon and carbon dioxide are of no concern. However, emissions of oxides of nitrogen (NO_x) are still a concern. The flame temperature of an iron flame is very similar to that of a hydrocarbon flame. As such, the temperature is sufficiently high to activate Zeldovich's mechanism for NO_x formation. In this contribution, we will explore the nitrogen oxide emissions in iron flames. Both the emissions in the bulk gas and the impact of the particle boundary layer will be discussed.

Numerical determination of laminar flame speeds with the counterflow twin-flame technique for dispersed fuels

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Currently a lot of research is performed to investigate the possibility of metal powders as a zero-carbon fuel. For the development of practical iron fuel-burning set-ups a thorough fundamental understanding on iron combustion characteristics is required. A key parameter for fundamental and practical purposes is the laminar burning velocity, S_L .

For gaseous flames it is well known that laminar flame speeds can be substantially modified by stretch effects such as flow non-uniformity, flame curvature, and flame/flow unsteadiness. These effects must be taken into consideration for an accurate prediction of the flame speed. For that reason, Wu and Law [1] proposed the development of the counterflow twin-flame technique for the determination of S_L . For dispersed flames, stretch effects are also at play and additional complexity is expected due to the inertia of the particles.

In this work, a quasi 1D counterflow twin-flame model is developed based on the model of Hazenberg and van Oijen [2]. With this model, the impact of stretch on the burning rate is investigated. Furthermore, extrapolation to zero stretch (*e.g.*, [1]) is performed to obtain the unstretched laminar burning velocity.

[1] C. Wu and C. Law, On the determination of laminar flame speeds from stretched flames, Twentieth Symposium (International) on Combustion 20(1), 1941--1949, 1985.

[2] T. Hazenberg and J. Van Oijen, Structures and burning velocities of flames in iron aerosols, Proceedings of the Combustion Institute 38(3), 4383--4390, 2021.

Numerical simulation of iron-air suspensions: reaction zone structures and reaction front speed

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The combination of numerical simulations and laboratory-scale experiments can provide fundamental insights into the inherent processes and mechanisms of iron-air flames. The characteristics of iron-air flames are determined by the interactions between the iron particles and the flow field. In this study, a laminar iron-air Bunsen flame is simulated using a multiphase CFD framework based on OpenFOAM[®]. The iron particles are modeled using a state-of-the-art single-particle model and tracked using a Lagrangian approach, while the gas phase is treated as a Eulerian phase. The particle model accounts for the formation of FeO and Fe₃O₄ and includes the melting of iron and its oxides, while the particles' oxidation rate can be either diffusion-limited or kinetically controlled. Additionally, radiative heat transfer between particles is considered. The aim of this study is to analyze the influences on the reaction front speed and structure in multi-dimensional iron dust flames. Furthermore, the relationship between particle flow, flame topology, and flame stability is investigated. This includes time dependent particle size distributions and particle loadings. The results are compared to recent experimental data and serve as a reference case for developing a better understanding of iron-air flames.

Numerical studies on flame propagation through iron dust suspensions in confinement

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The flame structure and speed of iron dust flames in confinement are investigated numerically. An Euler-Lagrange simulation framework is employed, where the gas-phase is described by the compressible

Navier-Stokes equations for an O_2 - N_2 mixture, and the particle-phase is described by individually tracked Lagrangian particles with a point-particle model. Despite gas pressurization via constant volume heating, it is found that no significant preheating of the gas and particles ahead of the flame front occurs. Instead, the density gradient of the gas due to O_2 consumption drives a flow field compressing the unburnt gas and eventually the reaction zone, preventing discernible temperature increase by virtue of the ideal gas equation of state. The flame speed in a stoichiometric mixture of iron dust and air in confinement is shown to be approximately twice as fast as that of the same mixture in a semi-open isobaric channel. The increased gas density due to closed-vessel gas dynamics results in a significantly lower ignition delay time predicted by the oxidation model with a first order dependence on surface O_2 concentration.

A population balance model for describing laminar aluminum dust flames

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In order to support the design of metal dust combustors with a view towards an efficient oxide recovery, we present a fully Eulerian modeling and solution approach for laminar dust flames that provides quantitative insights into the flame structure and permits an assessment of the exhaust’s pollutant charge. Focusing on aluminum, the combustible fuel particles are locally characterized in terms of a property distribution that quantifies the particles’ polydispersity. The spatial and temporal evolution of the property distribution is governed by a population balance equation (PBE) and kinetically driven by the rates at which the properties of any single particle change due to mass, momentum and heat exchanges with the carrier gas. A particular feature of our formulation is the limitation to three thermochemical particle properties that are taken as the particle temperature, mass and oxide mass fraction, aiding computational economy. Phase changes due to melting and solidification are taken into account by regularizing the thermodynamic properties of aluminum and its oxide in the solid and liquid aggregate states. The thermochemical properties are complemented by the particle velocity, expressing the inertial nature of the fuel particles. The PBE is solved with the aid of a Eulerian Monte Carlo method whose discrete formulation relies on a kinetic finite volume scheme. Finally, we apply the Eulerian modeling and simulation technique to an aluminum dust counterflow flame, validating predictions of the mean particle centerline velocity with available experimental measurements and assessing both the pollutant emissions and the oxide residue size distribution.

4.3 Modelling of turbulent dust flames

Modelling turbulence interaction and the preferential concentration of reacting iron particles

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In the midst of energy transition, iron powders have been proposed by a number of scientists as a promising energy storage alternative owing to their carbon-free energy cycle, high energy density, and recyclability [1]. 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 [2]. 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.

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.

In the present work, 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 Mi et al. [3]. A

similar case setup as Rieth et al. [4] 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 $d_p = 10 \mu\text{m}$, the Stokes number is estimated to be $St \approx [1, 10]$. 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 workshop.

[1] J.M. Bergthorson, Recyclable metal fuels for clean and compact zero-carbon power, *Progress in Energy and Combustion Science* 68, 169–196, 2018.

[2] S. Goroshin, J. Palecka, J.M. Bergthorson, Some fundamental aspects of laminar flames in nonvolatile solid fuel suspensions, *Progress in Energy and Combustion Science* 91, 100994, 2022.

[3] X.C. Mi, A. Fujinawa, J.M. Bergthorson, A quantitative analysis of the ignition characteristics of fine iron particles, *Combustion and Flame* 240, 112011, 2022.

[4] M. Rieth, A.M. Kempf, A. Kronenburg, O.T. Stein, Carrier-phase DNS of pulverized coal particle ignition and volatile burning in a turbulent mixing layer, *Fuel* 212, 364–374, 2018.

Slow combustion of spherical magnesium particles in a fluidized bed reactor: experiments and simulations

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Slow combustion experiments were performed on spherical magnesium particles in a fluidized bed reactor, under isothermal temperatures of 530, 550 and 570 °C. Approximately, 200 mg of magnesium particles were injected in the reactor, then fluidized with a mixture of helium and oxygen (80:20) injected from the bottom of the reactor under the appropriate flow of 10 NL/h. The temperature was first increased under a temperature ramp of 50 °C/min until the desired isothermal temperature, to reduce the conversion occurring during this non-isothermal phase. The oxygen fraction was continuously measured at the exhaust of the reactor with a catharometer, then converted in magnesium to magnesia conversion. For comparison, combustion experiments were also performed in a thermobalance with approximately 6 mg of magnesium particles and under the same temperature increase. The sample mass was here measured during the experiment. Comparisons between these sets of combustion experiments will be presented, together with simulations performed with either a single reaction involving the Avrami-Erofeev function of order two or Mampel-Delmon model.

MgO and NO_x emissions from a swirled-stabilized Mg flame

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Among the new sources of alternative and clean energy, magnesium (Mg) is a very promising metal fuel. The present contribution focuses on the nitrogen oxides (NO_x) and magnesium oxide (MgO) emissions produced by a swirled-stabilized Mg flame delivering a power ranging from 4 to 25 kW. A poly-dispersed aerosol of pure Mg was injected in the combustion chamber. The influence of Mg particle size (20–50 μm, 50–70 μm, 70–100 μm), equivalence ratio (from 0.2 to 1) and the swirl level (geometrical swirl numbers of 0.7 and 7.3) were considered. Emission levels of NO_x never exceeded 7 g_{NO_x}/kWh, which is lower than the maximal value of NO_x emissions from a gasoline engine. A multi-cyclone system is implemented downflow the combustion chamber to trap the particles of MgO. More than 89 wt-% of MgO was trapped with a significant positive effect of the presence of two cyclones in cascade. The emitted aerosol was characterized by an Electrical Low Pressure Impactor (ELPI). The uncollected particles of MgO are mainly PM₁ with a maximum of particles observed in the range 320–760 nm. The structure of MgO was analyzed by transmission electron microscope (TEM). Cubic and rounded crystals of MgO were observed.

5 Metal oxide recycling and reduction

Enhanced Size Prediction of Reduction Reactors in a Metal Fuel Cycle

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In the scope of a metal fuel circular economy, multiple sub-systems are to be integrated into a holistic overall model to enable economic and environmental assessment and optimization. Considering iron as recyclable energy carrier [1], the present contribution deals with reactor design for the iron oxide reduction step. Novel flash reactors seem a promising choice for the reduction of iron oxide due to energy savings and compatibility within the cycle [2]. One important factor in the economic assessment is the reactor size needed for optimal cycling conditions, hence for achieving the highest possible reduction degree. An accurate prediction of the reduction degree depends on modeling factors like kinetics, residence time distribution and mixing. By using the well-known axial dispersion model [3], we establish a feasible model of the reactor, which can cover any mixing model between complete mixing and the plug flow limit. We consider the influence of the mixing model on the economic assessment of the reactor and use the concept of Taylor-Aris dispersion [4] to determine an accurate dispersion coefficient for reactors from the literature [2]. This way we use synergies from the fields of chemical engineering and technical thermodynamics and we efficiently combine modeling approaches on the global and local scale.

[1] P. Debiagi, R. Rocha, A. Scholtissek, J. Janicka, and C. Hasse, Iron as a sustainable chemical carrier of renewable energy: Analysis of opportunities and challenges for retrofitting coal-fired power plants, *Renewable and Sustainable Energy Reviews* 165, 112579, 2022.

[2] X. Wang, G. Fu, W. Li, and M. Zhu, Numerical simulation of effect of operating conditions on flash reduction behaviour of magnetite under H₂ atmosphere, *International Journal of Hydrogen Energy* 44, pp. 26261–26270, 2019.

[3] O. Levenspiel, *Chemical Reaction Engineering*, 3rd ed., John Wiley & Sons, New York, 1998.

[4] B. D. Wood, Taylor-Aris dispersion: An explicit example for understanding multiscale analysis via volume averaging, *Chemical Engineering Education* 43(1), pp. 29–38, 2009.