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# A database for hydrogen and mixed-gas reduction of iron ore pellets: process conditions, pellet properties, and reduction rates

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ABSTRACT

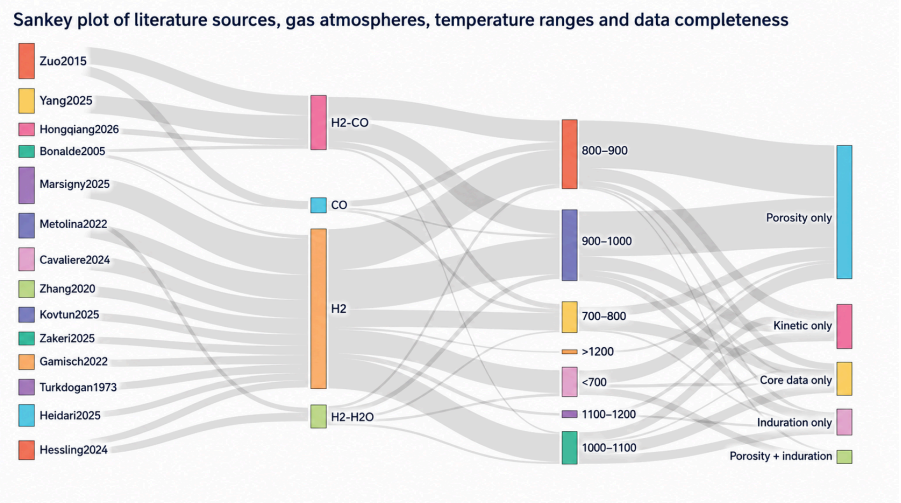
A standardized database of iron ore pellet reduction experiments was prepared from published literature data. The database contains 144 experimental records and 109 structured columns, covering reduction under $H_2$, CO and mixed-gas atmospheres. Each record includes literature metadata, pellet geometry, reduction temperature, gas composition, flow and pressure conditions, pellet chemistry, selected structural parameters, kinetic/model descriptors and standardized conversion–time trajectories. Reduction curves reported only in graphical form were digitized and converted into fixed 40-point α–t trajectories, enabling direct comparison, kinetic fitting and machine-learning analysis.

The database shows good coverage of pellet chemistry, gas composition, flow conditions and reduction curves. However, important descriptors such as induration temperature, holding time, initial and final porosity, pellet structure and directly comparable kinetic parameters are often missing in the original literature. This confirms that the field contains valuable experimental data, but that reporting practices remain fragmented.

The database is intended to support shrinking-core modelling, estimation of effective diffusivity and apparent reaction coefficients, comparison of reduction behavior in different gas atmospheres and development of data-driven models for hydrogen-based ironmaking. The complete dataset is openly available through Zenodo, while the present paper documents its structure, coverage, limitations and recommended reporting standard for future pellet-reduction studies.

*Keywords:* iron ore pellets; hydrogen reduction; direct reduction; pellet reducibility; shrinking-core model; kinetic modelling; machine learning; database; porosity; induration; Zenodo

**Graphical abstract**




Graphical abstract. Sankey visualization of the databas structure, linking literature sources with gas atmosphere temperature ranges and available data-completenes categories.

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## 1. Introduction

The decarbonization of iron and steel production requires major changes in primary ironmaking, where fossil carbon is still used as a reducing agent and an energy source. Among the proposed low-carbon routes, hydrogen-based direct reduction has received particular attention because hydrogen can reduce iron oxides while avoiding direct $CO_2$ formation from the reduction reaction. This route is especially relevant for pellet-based shaft furnace processes, including ENERGIRON/HYL-type systems, where the efficiency of reduction depends on gas composition, temperature, flow conditions, pellet chemistry and internal pore structure.

Iron ore pellets are complex reactive porous bodies. During reduction, hematite, magnetite and wüstite are progressively transformed into metallic iron, while the reaction rate is affected by chemical reaction at the oxide–gas interface, gas diffusion through pores and product layers, heat transfer, swelling, cracking and structural evolution. Earlier and more recent studies have shown that pellet size, porosity, temperature and reducing-gas composition strongly influence reduction kinetics (Bonalde, Henriquez, and Manrique 2005; Zuo et al. 2015; Metolina, Ribeiro, and Guardani 2022). More recent work has expanded this field toward industrial pellets, hydrogen-rich gas mixtures, water-vapour effects, pellet-grade variation and model-based interpretation of reduction curves (Cavaliere et al. 2024; Hessling et al. 2024; Yang et al. 2025; Marsigny et al. 2025).

The available literature is therefore rich in experimental results, but its quantitative reuse remains limited. Many studies report conversion–time curves, final reduction degrees or fitted kinetic parameters, while essential experimental metadata are absent, incomplete or expressed in different forms. Reliable comparison between datasets requires clear information on pellet diameter or radius, sample mass, initial and final porosity, chemical composition, induration temperature and holding time, gas composition, gas flow rate, total pressure, partial pressures and reactor conditions. Without these parameters, reduction curves can be reproduced for individual cases, but comparison across studies becomes uncertain.

This problem is particularly important for mechanistic modelling. Shrinking-core models, grain models and related kinetic approaches require physically meaningful structural and process parameters to distinguish chemical-reaction control, internal diffusion control and mixed-control regimes. For example, pellet porosity and particle size directly affect the interpretation of kinetic constants and effective diffusivity (Bonalde, Henriquez, and Manrique 2005; Zuo et al. 2015). Induration conditions are also important because they define the initial mineralogy, strength, pore network and reducibility of the pellet. However, these parameters are frequently missing or reported without sufficient detail.

The same limitation affects data-driven modelling. Machine-learning models require structured and comparable input variables, especially when the objective is to predict reduction routes, apparent kinetic parameters or process performance under new conditions. If variables such as pellet porosity, induration parameters, gas partial pressures or chemical composition are missing, the model may capture statistical trends but its physical interpretation and extrapolation capability remain weak. A standardized database is therefore needed as a connection between experimental data, kinetic modelling and machine-learning analysis.

In this work, a literature-based database of iron ore pellet reduction experiments was collected in a standardized, machine-readable format. The database includes experimental metadata, pellet geometry, gas composition, reduction conditions, pellet chemistry, selected structural parameters, kinetic/model parameters and conversion–time trajectories. The complete public version of the dataset has been deposited in Zenodo (Manojlović 2026). The main objective of this paper is to document the dataset and provide a reusable basis for kinetic analysis, shrinking-core modelling and machine-learning applications. A second objective is to identify the most frequent gaps in the published literature and to propose practical recommendations for future experimental reporting, with emphasis on induration conditions, porosity, pellet geometry, gas-flow conditions and full numerical reduction curves.

## 2. Database description and data coverage

The database was prepared as a structured Excel dataset in which each row represents one reduction experiment and each column represents one experimental, material, kinetic or trajectory variable. The current public version, deposited as a Zenodo dataset (Manojlović 2026), contains 144 experimental records and 109 columns. The variables were arranged into several logical groups in order to make the dataset suitable for direct use in kinetic analysis, shrinking-core modelling and machine-learning workflows.

The first group contains basic metadata. These columns include the experiment identifier exp_id, the literature source code ref and the original reference or figure/table identifier ref_id. This structure allows each experimental record to be traced back to the original publication and to the specific source from which the numerical data were extracted.

The second group describes pellet geometry and reduction conditions. The pellet radius is given as r_i_mm, while the reduction temperature is given as T_K. Gas composition is represented through individual gas-fraction columns, including H2, CO, CO2, CH4, H2O, He and N2. The gas-flow conditions are described by the total gas flow rate Q_gas_L_min, together with specific flow rates for hydrogen and carbon monoxide where available, Q_H2_L_min and Q_CO_L_min. The pressure conditions are described by the total pressure p_total_Pa and the hydrogen partial pressure p_H2_Pa. Other partial pressures can be calculated from the total pressure and gas-composition fields when required.

The third group contains the main chemical composition of the pellets. The selected variables include total iron content Fe_tot_wt and the major gangue or fluxing oxides: SiO2_wt, CaO_wt, Al2O3_wt and MgO_wt. These variables were included because pellet chemistry affects reducibility, slag-forming tendency, basicity, pore evolution and the interpretation of reduction kinetics.

The fourth group describes porosity and structural properties. The initial porosity is given as eps0, while the final porosity after reduction is given as eps_f when available. These variables are important for diffusion-controlled and mixed-control reduction regimes, because the pore structure influences gas transport inside the pellet and through the reduced iron layer. In the present database, porosity values were retained as reported in the original sources whenever possible.

The fifth group contains induration parameters. The induration temperature is given as T_sint_K, and the holding time is given as t_sint_min. These variables are included because induration conditions define the initial pellet structure, mineralogical state, strength, porosity and reducibility. Their inclusion also makes it possible to connect pellet preparation with subsequent reduction behaviour.

The sixth group contains kinetic and model-related parameters. The effective diffusivity is given as Deff_m2_s, while the apparent surface reaction coefficient is given as k_reac_m_s. These parameters are intended for mechanistic interpretation.

The final and largest group contains the reduction trajectory. Graphical reduction curves were digitized using the online WebPlotDigitizer application, which enabled the extraction of numerical conversion–time data from published figures for curve fitting and standardization (Rohatgi 2024). Each reduction curve is represented by paired conversion–time columns, from alpha_1/t_1 to alpha_40/t_40. The variable alpha represents the fractional degree of reduction, while t gives the corresponding time value. The use of 40 paired points gives a common structure for curves taken from different publications. This format is useful because it allows direct comparison of reduction trajectories, fitting of kinetic models, calculation of curve descriptors

and application of machine-learning methods without requiring each user to re-digitize or restructure the original data.

A summarized view of the database organization is given in Table 1.

**Table 1.** Main groups of variables in the pellet reduction database

| Variable group | Main fields and purpose |
|---|---|
| Metadata | exp_id, ref, ref_id; identification of each experiment and link to the original literature source. |
| Pellet geometry and reduction conditions | r_i_mm, T_K, gas fractions, gas-flow rates and pressure fields; description of pellet size, temperature, reducing atmosphere, flow rate and pressure conditions. |
| Pellet chemistry | Fe_tot_wt, SiO2_wt, CaO_wt, Al2O3_wt, MgO_wt; main chemical composition of the pellet. |
| Porosity and structure | eps0, eps_f; initial and final porosity, where available. |
| Induration parameters | T_sint_K, t_sint_min; thermal preparation conditions before reduction. |
| Kinetic/model parameters | Deff_m2_s, k_reac_m_s; effective diffusivity and apparent reaction-rate parameter. |
| Reduction trajectory | alpha_1/t_1 to alpha_40/t_40; standardized conversion-time data for each reduction curve. |

The database contains 144 reduction experiments. The most complete part of the dataset is related to pellet chemistry and reduction conditions. Chemical composition is available for all 144 experiments, including total iron and the main oxide components. Gas composition, gas flow rate and pressure conditions are also available for all experiments, which allows comparison of reduction behavior under different $H_2$, CO and mixed-gas atmospheres.

The coverage is lower for structural and preparation-related variables. Initial porosity eps0 is available for 87 experiments, while final porosity after reduction eps_f is reported for only 20 experiments (Table 2). Induration temperature T_sint_K and holding time t_sint_min are available for 19 experiments. This is an important limitation because pellet induration directly affects strength, pore structure and reducibility.

Kinetic and model parameters are also available for a limited number of records. The effective diffusivity Deff_m2_s is available for 21 experiments, while the apparent reaction coefficient k_reac_m_s is available for 24 experiments.

**Table 2.** Coverage of key variables

| Variable group | Available records | Total records | Coverage |
|---|---|---|---|
| Chemical composition | 144 | 144 | 100% |
| Gas composition, flow and pressure | 144 | 144 | 100% |
| Initial porosity eps0 | 87 | 144 | 60.4% |
| Final porosity eps_f | 20 | 144 | 13.9% |
| Induration temperature/time | 19 | 144 | 13.2% |
| Effective diffusivity Deff_m2_s | 21 | 144 | 14.6% |
| Reaction coefficient k_reac_m_s | 24 | 144 | 16.7% |
| Standardized α–t trajectory | 144 | 144 | 100% |

Direct kinetic interpretation is shown in Figure 1, where the characteristic time required to reach 80% reduction, $t_{80}$, is plotted as a function of reduction temperature. The logarithmic scale emphasizes the wide range of reduction times reported in the literature. In general, higher temperatures tend to reduce $t_{80}$, but the scatter remains significant. This scatter reflects the combined influence of gas atmosphere, pellet radius, chemical composition, porosity, induration history and differences in experimental procedure. The figure also shows that the database covers several common experimental temperature levels, especially around 800–1000 °C, while lower and higher temperature ranges are less uniformly populated.

The standardized 40-point reduction trajectories were analyzed using PCA to compare curve shapes in a common numerical space. Each point in Figure 2 represents one experiment. PC1 and PC2 are mathematical axes that summarize the main differences between reduction curves. PC1 mainly reflects the overall progression of reduction, while PC2 captures secondary differences in curve shape, such as early acceleration or late-stage slowing. The partial separation of $H_2$, CO, $H_2$–CO and $H_2$–$H_2O$ experiments suggests that gas atmosphere affects the reduction trajectory. However, the overlap between groups shows that temperature, pellet size, chemistry, porosity and experimental methodology also influence the curve shape.

## 3. Database use cases and limitations

The database was designed for quantitative analysis of iron ore pellet reduction under $H_2$, CO and mixed-gas atmospheres. Its main advantage

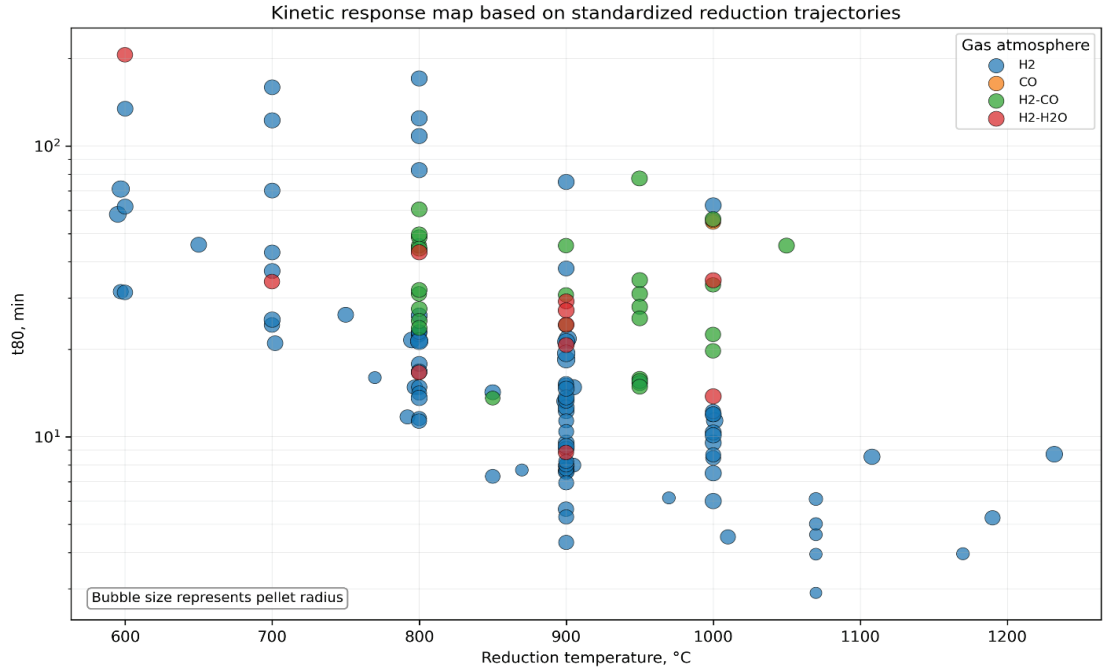


**Fig. 1.** Kinetic response map based on standardized reduction trajectories: the characteristic time $t_{80}$ was calculated from each α–t curve and plotted against reduction temperature; bubble size represents pellet radius.

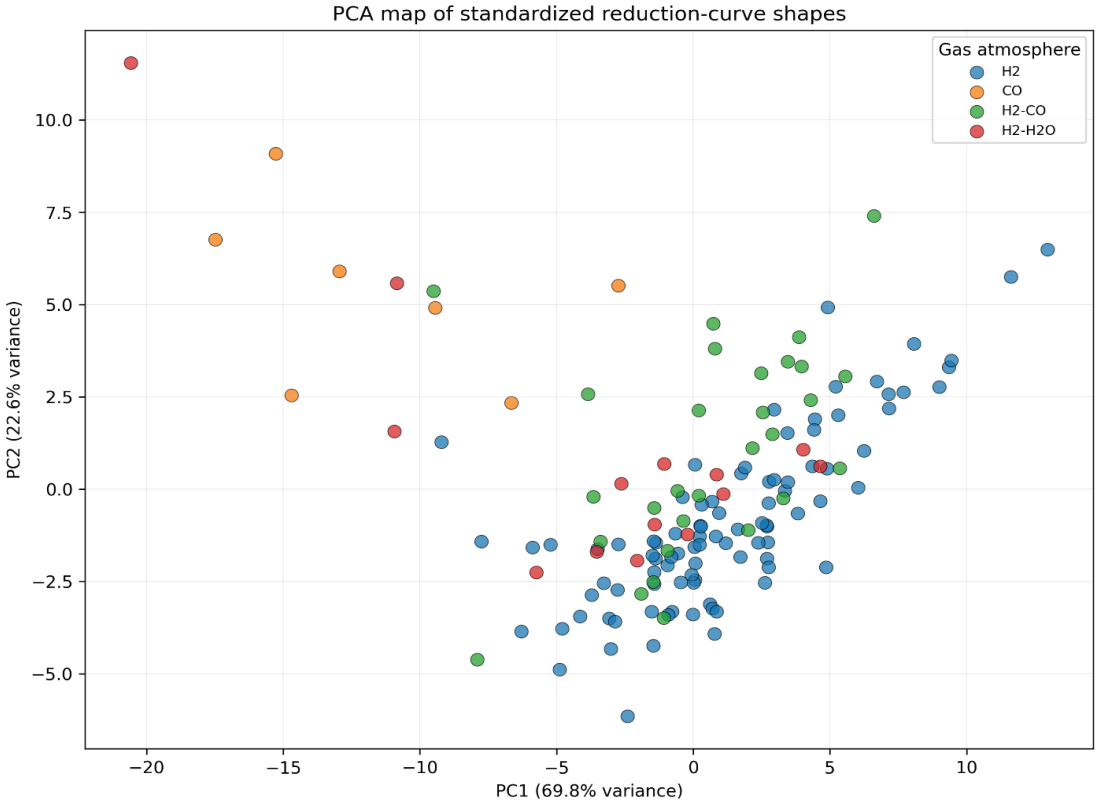


**Fig. 2.** PCA map of standardized reduction-curve shapes. Each point represents one experiment described by a 40-point α–t trajectory. PC1 and PC2 summarize the main mathematical differences between curve shapes and enable exploratory comparison of reduction behavior.

is that it combines three types of information in one structure: reduction conditions, pellet properties and standardized reduction trajectories.

The database can be used for the development and validation of shrinking-core models and related kinetic descriptions. It also enables estimation and comparison of effective diffusivity and apparent surface reaction coefficients under different temperatures, gas compositions and pellet properties. Since the reduction curves are standardized into 40 conversion–time points, the dataset is suitable for curve fitting, calculation of kinetic descriptors and direct comparison between experiments from different sources.

Another important application is machine-learning modelling. The database can be used to train models for predicting reduction curves, characteristic reduction times, apparent kinetic parameters or the influence of process variables such as temperature, pellet radius, gas composition, chemical composition and porosity.

At the same time, the dataset has several limitations. The public database retains all 144 records for transparency; for specific modelling tasks, users may apply additional reliability screening and exclude selected records when metadata quality or curve consistency is insufficient. The data were collected from different literature sources, so pellet preparation methods, reactor types and experimental procedures are not fully uniform. Porosity is not always reported, and in some cases, it is given as a fraction, while in others it is given as a percentage. In many studies, it is also unclear whether the reported porosity represents total porosity, open porosity, initial porosity or porosity after reduction.

Induration conditions are another important limitation. Induration temperature and holding time are frequently missing, although they strongly affect pellet strength, mineralogy, pore structure and reducibility. Some publications also do not provide complete information on gas flow rate, pellet geometry, total pressure or partial pressures. Finally, kinetic parameters reported in the literature are not always directly comparable because they depend on the selected kinetic model, fitting range and assumptions used by the authors.

## 4. Recommendations for future research

Future studies on iron ore pellet reduction with hydrogen and gas mixtures should report a minimum set of experimental and material parameters in a standardized form. This would improve comparison between different studies and make the data more useful for kinetic modelling.

The recommended minimum dataset should include pellet geometry, such as diameter or radius, sample mass and size distribution. The chemical composition should include total iron, main iron oxide phases where possible, and the main gangue or fluxing oxides, especially $SiO_2$, $Al_2O_3$, CaO and MgO.

Induration conditions should be reported in more detail. This includes induration temperature, holding time, heating rate, atmosphere and cooling conditions. These parameters are important because they define the initial pellet structure, strength, mineralogy, porosity and reducibility.

Structural properties should include initial porosity, and, where possible, open and closed porosity, pore-size distribution and tortuosity. Final porosity after reduction is also valuable because it describes structural evolution during the reaction. Mechanical properties, especially cold compressive strength before reduction and after reduction, should be included when available.

Reduction conditions should be fully described. The required parameters are reduction temperature, gas composition, total gas flow rate, total pressure, partial pressures, sample mass and reactor geometry.

For kinetic interpretation, authors should clearly state the model assumptions, fitting range, fitted parameters and quality of fit. This is necessary because kinetic parameters depend strongly on the selected model and cannot be compared directly without knowing the underlying assumptions.

Finally, future publications should include numerical data tables as supplementary material. Providing full datasets, rather than only graphical curves, would significantly improve data reuse, model validation and the development of reliable kinetic models for hydrogen-based iron ore pellet reduction.

**Table 3.** Recommended minimum reporting standard

| Category | Recommended data |
|---|---|
| Pellet geometry | Diameter/radius, mass, size distribution |
| Chemistry | Fe total, FeO/$Fe_2O_3$/$Fe_3O_4$ if possible, $SiO_2$, $Al_2O_3$, CaO, MgO, basicity |
| Induration | Temperature, holding time, heating rate, atmosphere, cooling conditions |
| Structure | Initial porosity, open/closed porosity, pore-size distribution, tortuosity |
| Mechanical properties | Cold compressive strength before and after reduction |
| Reduction conditions | Temperature, gas composition, flow rate, pressure, partial pressures, sample mass, reactor geometry |
| Reduction data | Full numerical α–t curve (supplementary material) |
| Kinetic interpretation | Model assumptions, fitting range, fitted parameters, fit quality |
| Data availability | Numerical tables in supplementary material |

## 5. Conclusion

This work presents a standardized and machine-readable database of iron ore pellet reduction experiments under $H_2$, CO and mixed-gas atmospheres. The database integrates literature metadata, pellet geometry, chemical composition, reduction conditions, selected structural parameters, kinetic descriptors and standardized 40-point conversion–time trajectories.

The main value of the database is that it connects process conditions, pellet properties and full reduction curves in a single structure. This enables direct comparison of experimental results, fitting and validation of kinetic models, SCM-based interpretation and the development of machine-learning models for predicting reduction behavior.

The analysis also shows that the published literature remains fragmented in several important aspects. Chemical composition, gas atmosphere and reduction curves are generally well reported, while induration conditions, porosity, pellet structure and kinetic parameters are often missing or reported in non-standardized forms. These missing data limit the transferability of kinetic parameters and reduce the reliability of comparative modelling.

Future studies on pellet reduction should provide more complete numerical datasets, including pellet geometry, induration parameters, porosity, gas-flow conditions, partial pressures and full conversion–time curves. Such reporting would improve data reuse and support more reliable mechanistic and data-driven modelling in hydrogen-based ironmaking.

## Data availability

The complete dataset described in this paper is available through Zenodo: https://doi.org/10.5281/zenodo.20603367 (Manojlović 2026). The repository contains the Excel database in its first public release, v1.0.0, with 144 standardized records. Users should cite both the Zenodo dataset and this descriptive paper when using the data.

### Conflict of Interest

The author declares no conflict of interest.

### Acknowledgments

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