Maximise H2 Enrichment in Direct Reduction Shaft Furnaces

Comprehensive Overview

Deliverable 5.3

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1. Introduction

This document provides a comprehensive overview of the MaxH2DR project, six months after its start.

It describes the technical approach as well as targeted outcomes and impacts in the project. Thus, it is focused on the three “technical” work packages (WPs) in this project:

- WP1: New fundamental knowledge and sub-models
- WP2: Enabling Industrial Demonstration of H_2-enriched Direct Reduction
- WP3: Efficient and flexible steelmaking process chains based on H_2-enriched DR

Each of this work packages contains a specific technical approach, which are fused together in the overall MaxH2DR approach of “hybrid demonstration”. The term “hybrid demonstration” refers to the combination of “physical demonstration” and “digital demonstration”.

Additionally, MaxH2DR consists of two work packages dedicated to Dissemination, Exploitation and Communication (WP4) and Project Management (WP5). Their initial contents are described in dedicated Deliverable reports which were submitted by now. These reports are:

- D4.1 “Development of Website and Project Branding Toolkit”,
- D4.2 “Dissemination and Communication strategy”,
- D4.5 “Data Management Plan”,
- D4.6 “Innovation eco-system and stakeholders map”,
- D5.1 “Quality Assurance Plan”, and
- D5.2 “Project Risk Matrix”.

As these contain the main relevant information for the non-technical approach in MaxH2DR concerning Dissemination, Communication, Exploitation and Project Management, these contents are not explained in the Comprehensive Overview to avoid repetition.

The following section therefore present the technical approach (chapter 2) in a work package specific way (sections 2.1 – 2.3). The document then concludes with the main MaxH2DR outcomes and impact to be expected.

2. Approach

MaxH2DR is structured into three technical work packages. These are structured systematically with increasing scope. It increases from particles (WP1) to DR shaft furnace scale (WP2) and finally to the complete steelmaking process chain scale (WP3). This leads to an intuitive and straightforward line of investigations and flow of information. Each scope builds upon the sound basis of the results of the lower scopes. These deeply integrated investigations facilitate internal feedbacks, e.g., an intelligent selection of boundary conditions for the fundamental investigations from the analysis of different shaft furnace operation states, or a connection between the shaft furnace and the process chain regarding product quality, gas quantities and properties. This methodology ensures that the high-level investigations can fully exploit high detail knowledge gathered within the project to yield accurate final tools and results. In the following, the work package specific approaches are presented.

2.1 WP1: New fundamental knowledge and sub-models

Work package 1 is dedicated to chemical and physical investigations, focusing on the reduction processes in H_2-enriched Direct Reduction and the evolution of chemical and physical properties of material during its descent in the furnace until reaching its final product form, Direct Reduced Iron (DRI). In this work package the systematic increase of scope of the overall project is reflected. As such, the scope in WP1 increases from grain through single pellets to beds of pellets, combining fundamental knowledge of basic sub-processes and of complete reduction behavior under realistic operational conditions.

Main knowledge gaps regarding the reduction processes are:

- the complex effect of temperature on the reduction rates when using hydrogen
- changes in the kinetic regime during the reactions
- the retarding role of the metallic iron phase on the final reaction rate[1]
- the sticking between particles

This successive focus on different scales in WP1 enables understanding the mechanisms, as well as obtaining reliable data for the different types of raw materials usable in DR (pellets, lump ore, sinter).

The knowledge is then transferred into accurate kinetic models. A sophisticated single-pellet reaction model based on the experimental data is built and implemented in the multiparticle reactor models. A unique test rig for determination of physical pellet properties at realistic gas composition, temperature and mechanical load in H_2-enriched DR shaft furnaces is established.

In the following sections, the approach for WP1 in MaxH2DR is explained in detail. First, the approach for the experimental investigations of reaction kinetics in different scales is presented. In this section, the reaction kinetics of sub-pellet scale, single pellet scale, pellets bulk scale as well as for sinter material is described. The next section is presenting the approach for the experimental investigations of physical properties of raw materials, intermediates and products. Then, the development approach for kinetic sub-models is described. This chapter closes with the description of the implementation methods for these new sub-models into the DR shaft process models.

2.1.1 Experimental investigations of reduction kinetics in different scales

The experiments conducted in MaxH2DR involve complementary scales and various raw materials. Starting on the finest, sub-pellet, fines scale and with pure iron oxides, the intrinsic kinetics of the gaseous reduction reactions are investigated in detail. Iron ore charged into DR shafts is typically in the form of pellets, or possibly lumps. Kinetic experiments on this scale are relevant to obtain the kinetics

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[1] Mondal, K., et al., Effect of gas composition on the kinetics of iron oxide reduction in a hydrogen production process, Int. J. Hydrogen Energy, 2005/30, pp. 1543–1554.

corresponding to actual industrial conditions. Compared to grain-scale experiments, inter-grain and intra-pellet diffusion processes are considered. The next relevant scale is that of a bed of pellets. Corresponding reduction and softening tests are conducted in MaxH2DR. Fixed DR gas compositions of increasing H_2 content is used first. Later, the program will be changed to simulate the changing gas evolution in a DR shaft. The whole set of outputs generated in the complementary laboratory tests will be exploited for the development of the kinetic sub-models.

These models are relying on sound data obtained from well-designed experiments (at DR-type conditions, with high hydrogen content, with various DR raw materials), due to the predominant role of the kinetics of the iron ore reduction, which control the productivity of the shaft furnaces. These experiments will strengthen the fundamental knowledge of the basic chemical and physical processes, elucidate unclear features and produce accurate data for modelling under realistic operation conditions. The experimental conditions are selected as representative of the DR process and, for most experiments, will be the same for all the partners involved: temperature 800–1100 °C, pellet size 6–14 mm, 3 gas compositions. The first experiment will consist of 55% H_2, 26.2% CO, 14.1% CO_2 and 4.7% H_2O. The second experiment will consist of 80% H_2, 11.6% CO, 6.3% CO_2 and 2.1% H_2O. The third experiment will consist of 100% H_2.

Reaction kinetics investigation at sub-pellet scale

On sub-pellet scale, the intrinsic kinetics of the gaseous reduction reactions are investigated in detail. Iron oxide samples are reacted in different gas atmospheres in a packed-bed reactor to accurately investigate the intrinsic kinetics without other interfering phenomena. This is followed by identical experiments with crushed and sieved fractions of selected pellets and sinter. Differences in the reduction behaviour is also studied by detailed chemical and structural analysis.

For these experiments, an innovative experimental setup applying a Micromeritics Autochem attached to measurement devices is utilized. This equipment includes precise multi-gas composition and flow control at the inlet. It is intended for catalyst characterization, but is extended in MaxH2DR to reduction experiments of iron oxide fines. These are placed in a fixed bed as a single layer or diluted with an inert material, guaranteeing a uniform gas distribution around the particles and eliminating mass transfer resistance from the bulk gas. The gaseous reaction products are accurately analysed with a mass spectrometer and a micro-GC to continuously and quantitatively follow the progress during the experiments. The fines are analysed chemically and morphologically after switching to an inert gas and cooling the reactor. By contrast to studies of larger particles (with diffusion) and fluidised bed setups (where accurate mass balances of the gas phase cannot be used), the MaxH2DR approach will give quantitative information solely related to reaction kinetics. This is used to develop a model of the intrinsic kinetics of iron oxides, including identification of reaction order and estimation of activation energies and pre-exponential factors. Not only iron oxide reduction reductions but also the water-gas shift reaction, which may play a crucial role for the overall reduction rate, are considered. For this, the catalytic functions of iron oxides are studied and modelled. Experiments with pure iron oxides are modelled first, extending the model to the results of fines produced by grinding pellet and sinter particles. Detailed chemical and physical analysis of the unreacted and partly reacted materials are guiding the choice of model structure. The final models of the intrinsic reduction kinetics are used as a basis for the single-pellet model development outlined below.

Reaction kinetics investigation at single pellet scale

Previous studies identified the rate-limiting mechanisms as a function of temperature and conversion. Nevertheless, the occurrence of kinetic slowdowns at 700 and 950 °C (affecting final metallisation), the role of the freshly formed iron layer on morphological evolution and kinetics and on inter-pellet sticking are not clearly identified yet. This will be addressed by conducting dedicated experiments using TGA (Thermo-Gravimetry Analysis) and complementary characterisations. Different pellets types (European and Brazilian pellets, DR grade or BF grade) and one lump ore are being compared. Some pellet reduction tests are being undertaken at changing gas atmosphere and temperature to reproduce the evolution of pellets descending in the shaft, with conditions based on reactor model results. A single pellet will be placed in a thermobalance and its reduction by H_2-CO reducing mixtures is recorded. The temperature and the type of pellet are varied, and lump ore will also be tested. Selected samples are characterised before, in and after the tests by SEM observation, X-ray diffraction, and Mössbauer spectrometry. The system is will utilize improved gas analysis and control systems to vary the gas composition over time.

Reaction kinetics investigation at pellet bulk scale

Further trials are investigating the reaction kinetics in reduction and softening tests at pellet bulk scale. For this, HOSIM and BRASS test equipment is utilized. These tests were originally developed for the BF operating line simulation. Now these are expanded to simulate H_2-enriched DR shaft conditions.

HOSIM ("Hoogovensimulator", blast furnace simulation) tests simulate the conditions in the stack zone of the blast furnace. A 500 g sample is heated according to a predetermined temperature/time profile with corresponding reduction gas composition up to 900 °C. The sample itself controls the gas composition during the test run. The balance between gas composition and reduction degree of the ferrous burden is maintained (O/C vs. O/Fe is fixed), initial process settings can be obtained. HOSIM tests can be interrupted at specified reduction degrees and tumbled subsequent to cooling to determine the disintegration at a function of reduction degree.

The BRASS (Blast furnace Reduction and Softening Simulation) simulates the conditions in the stack and softening zone of the blast furnace. BRASS is based on fixed profiles of temperature and gas composition with given load of 0.8 kg/cm². A 500 g sample is heated according to a predetermined temperature/time profile. The weight loss of the sample, its temperature, the bed height and the pressure drop over the bed are measured. BRASS tests can also be interrupted at specified reduction degrees and tumbled subsequent to cooling to determine the disintegration as a function of reduction degree. Outputs generated from the laboratory tests implemented will be exploited for the evaluation of the reaction kinetics, mechanism in the DR shaft furnace process.

Reaction kinetics investigation of sinter

The possible use of sinter as a feedstock in the DR process is not fully investigated and understood yet. To contribute towards identifying the potential of sinter as a feedstock, the kinetics of the reduction process for different sinter fractions and varying reduction gases are being investigated in MaxH2DR. A pilot-scale sintering pan is being used to produce several types of sinter (industrial as a reference material and with different iron content and using 10-20%wt. biomass as fuel), which will be characterized. To reduce the sinter samples in a hydrogen-containing atmosphere, a specific laboratory installation is designed and built. In this context, the possible use of sinter as a feedstock in the DR process in an atmosphere with 80-100% H_2 is of dedicated interest. The kinetics of the reduction process for different sinter fractions and varying reduction gases are investigated in MaxH2DR. A special stand for testing sinter reduction in a hydrogen-heavy atmosphere is available and will be used. It consists of a high-temperature tubular furnace with an inner diameter of 70 - 100 mm, with accurate temperature control and devices for controlled flow of gases entering the furnace and chemical analysis of the off-gases by mass spectrometer and gas analyzers. The kinetics of sinter reduction is determined in an atmosphere of different hydrogen contents and temperatures ranging around 1000 °C. Experiments are carried out for different grain sizes of sinter such as 3-6 mm, 6-9 mm, 9-12 mm, 12-15 mm. The kinetics of the reduction process is determined based on measurements of the amount of process gases leaving the reactor. Approximately 30 reducibility tests (with a minimum of 2-3 replicates each) are performed. After the reduction process, analyses of the phase and chemical composition of the reduced sinter as well as studies of the microstructure, strength and thermoplastic properties (softening) are carried out. The chemical composition, macro- and microstructure of the reacted sinter is being determined. This finally leads to guidelines for optimal sinter reduction parameters in hydrogen-rich gas.

Based on the experimental results at different scales, a new and accurate kinetic model of a single pellet is being developed. This considers the composition and structural changes of the particle under the reaction process. It is an essential building-block in the models of the DR furnace developed in WP2 and provides the required information that is needed to accurately predict the performance of the reduction process in the shaft furnace, including mixtures of pellets and sinter.

2.1.2 Experimental investigations of physical properties of raw materials, intermediates and products

Besides investigating the chemical properties of the reduction process (e.g. in terms of reaction kinetics), determining the physical properties of raw materials, intermediates and products is of highest relevance. In this context, the characterization of the main relevant physical properties of the raw materials and the reduced products, as well as the changes they undergo along with the reduction, are being investigated.

The first part consists of different physical characterizations of the samples, i.e., SEM observation, X-ray diffraction, Mössbauer spectrometry and chemical analysis, including raw materials (pellets, ore, sinter), intermediates, and products. Additionally, metallurgical quality tests are being performed on the direct reduced iron to determine the degree of metallisation, mechanical strength, softening, porosity, etc.

The second part analyses the rolling friction and the sticking behaviour of iron ore pellets at process conditions. A unique new Hot Shear Cell operated at high temperature under hydrogen atmosphere is being built in MaxH2DR. Experiments are being performed at different vertical and shear stresses, evaluating the sensitivity of the mechanical stresses. The temperature (up to 1000 °C) and the partial pressure of the gases is varied and sensors measure the normal force, the torque and the tangential force. After the reduction experiment, the sticking ratio, strength of the pellet bonds by sticking and the bulk density is being determined. The data will be subsequently used for the modelling tasks in MaxH2DR.

Complementing the kinetic investigations at the pellet bulk scale, measurements of physical properties of a constrained bed of pellet as a function of operating parameters bring additional information. As such, the possible influence of the changed solid composition with H_2 enrichment (missing cementite) on the mechanical properties is being investigated. The experimental set-up provides the required information for the development of the mechanical model of the particle adopted in DEM simulations to describe the particle cohesion under the process conditions (temperature up to 1000 °C, stresses up to 8000 kPa and reaction with pure hydrogen). Flow properties of samples of granular material made of primary particles and of pellets with a size up to about 1.5 mm are measured. The system is a cell made of two pistons and a hinged lateral wall, where the upper piston moves vertically and the lower rotates. Sensors measure the normal and tangential force. After loading small pellets in the apparatus, the system is placed in an oven. The gas atmosphere around the pellets, temperature, and the mechanical loading can be controlled by this setup.

2.1.3 Development of kinetic sub-models for H_2-enriched DR

The experimental findings are being used to develop new, validated mathematical models of the reduction kinetics at the scale of a single pellet or sinter particle as a function of the operating conditions.

First, a mechanistic-based model of the intrinsic kinetics of reduction of pure iron oxides in hydrogen-rich gas atmospheres at different temperatures is being developed. It is based on the reduction experiments with iron oxide fines. Reaction orders, activation energies and pre-exponential factors in the domain of intrinsic kinetics are being determined accurately. The catalytic functions of the different iron oxides, mainly related to the forward or reverse water-gas-shift reaction, are incorporated, as they can be either beneficial or detrimental for the iron oxide reduction. Possible adsorption/desorption phenomena involved in the reduction reactions are being considered. The models developed for pure iron oxides and their mixtures serves as the basis for the modelling of ground commercial pellets and sinters.

Second, these models of the intrinsic reduction kinetics will be implemented in the single-pellet model developed by UL. This model, for which a first version already exists, is based on the law of additive reaction times and a multi-scale geometrical representation of a pellet made of small grains, possibly sub-divided into crystallites. The model will be further improved to considering the more detailed intrinsic chemical kinetics, the ability to differentiate between different types of pellets, a better description of the end of the reaction with the reduction slowdowns at 700 and 950 °C. It will be assessed and validated by comparison with the experiments of Task 1.1. The resulting model will be much more sophisticated and faster than traditional (e.g., shrinking core at the level of a pellet) models, and specifically developed for DR conditions.

2.1.4 Implementation of new kinetic sub-models into DR shaft process

The single-pellet kinetic model is then perfectly suited for implementation in multi-particle reactor models. To ensure compatibility of the results of the project partners, the single-pellet sub-model is being implemented as a subroutine in the reactor-scale models.

The Reductor model of UL simulates the direct reduction shaft furnaces by solving mass, heat, and momentum balance equations of the solid and gas phases using the finite volume method. The new single-pellet kinetic model is being incorporated to provide the reduction reaction rates that are source terms in these equations, yielding a more accurate prediction of the chemical transformations and final metallisation degree. The FEM-based process model of BFI was originally developed as a BF stack model and was recently verified for online application. In MaxH2DR, the reaction kinetics of the model are modified to H_2-enriched reduction by incorporating the new single-pellet sub-model. The coupled DEM/CFD model of RUB is being utilised for studying the DR process, also incorporating the same kinetic single-pellet sub-model. However, as computing times often become critical for the DEM/CFD simulations of large-scale systems, simplified reduction models may be used and compared with the rigorous UL model. The coupling of the DEM-code to openFOAM (CFD) is being adapted to the present process. As for inter-particle interactions, an existing cohesion model is adapted to account for adhesive forces between particles under DR conditions. Furthermore, contact force models for cohesive particles available in literature are being evaluated. The adhesive forces are then described as a function of reduction degree and local contact temperature between particles based on the hot shear cell experiments. Further force model parameters will be iteratively adapted by using the (DEM-based) digital twin of the physical test rig. The three improved process models (Reductor, FEM, DEM/CFD) will subsequently be used in the process simulations of WP2.

2.2 WP2: Enabling Industrial Demonstration of H_2-enriched Direct Reduction

Work package 2 is dedicated to physical and digital demonstration of the DR furnace, combined to the hybrid approach which is a major feature of the MaxH2DR methodology. Its first step is the physical investigation of permeability at counter-flow conditions in demonstration scale. The results will be combined with WP1 results and implemented into a world-first DEM/CFD DR shaft furnace model, forming a hybrid demonstrator.

H_2 enrichment in DR is affecting the reduction processes, the mineral phases and physical properties of the DRI product and of the partly reduced pellets inside the furnace. Currently no quantification is possible yet and no knowledge exists to which extent this will affect the operation of industrial plants. However, also due to endothermic nature of reduction by H_2 and lower gas heat capacity, the temperatures and flow characteristics expected to differ significantly. This major challenge is tackled by the MaxH2DR methodology: the material properties and their change along the passage through the reactor are identified. These data and the physical demonstration of the coupled solid and gas flow are fused into digital tools to provide a “Hybrid demonstrator”.

2.2.1 Physical demonstration of coupled solid and gas flow in DR shaft furnace

The physical demonstration of coupled solid and gas flow is utilizing an existing demonstration shaft furnace test rig: a quasi-2-dimensional shaft furnace with variable side walls and an optically transparent front wall. This construction is built to analyse the interaction of bulk and gas flow (bulk and gas in counter-flow and locally (near side wall gas inlet) in crossflow). This set-up allows usage of real materials (in particular ore pellets) and optical tracking of the particles by cameras directed through the transparent acrylic front wall. The test rig will be further adapted towards reflecting real direct reduction furnace geometries. It is being used to investigate particle movement and permeability of iron ore pellets, sinter and coke bulks in a BF geometry. The experimental rig has a height of 2800 mm, a width of 1200 mm and a depth of 300 mm. The particle movement is trackable through the acrylic front plate and the sidewall angles are changeable for different experimental conditions. The setup has inlets for the airflow in the middle under the construction and two smaller at the left and the right side, with the air outlet at the top. The solids enter at the top and exit through two outlets at the left and right bottom side. Pressures are measured for different sections and material flows are recorded optically and by weighing. The results can be effectively extrapolated to other conditions by the DEM/CFD model. The mass flow of solids and volume flow of air can be adjusted. For the DR shaft furnace the funnel flow in the lower part is expected to be more influential than the shaft flow in the upper flow, so the geometry is being adapted to analyze the critical region. Approximately 1200-1500 kg of pellets or other materials are required for each experiment. In MaxH2DR, original material from industry is being used to identify the permeability of real bulk materials since the particle characteristics significantly influences the permeability.[2] For instance, the effect of sticking changes the gas and solid flow characteristics and induce irregularities.[3] To realistically represent solid flow, particles with different sticking tendency, friction and hardness are studied by shear tests and the DEM/CFD model.

First steps of the experimental series are measurements of the stationary bulk properties (as non-moving particles): pressure drop, porosity, permeability and gas velocity profile above the bulk. The permeability is determined by the share of void spaces between the particles, which are detected optically though the acrylic front wall and mathematically corrected by the known wall effects. In a second step, the flow behaviour of pellets is analysed. This series will use material of different strength and surface friction, adapted to the physical properties of pellets in the reaction zone of H_2-enriched DR, as supplied by WP1. Additional trials are performed to mimic the effect of particle agglomerates generated by adhesive forces. Therefore, larger clustered objects are being charged with the pellet bulk. The influence on local pellet movement and integral permeability field is analysed. All experimental series will include a variation of mass flow of solids and volume flows of gas (in cross- and counterflow). The data allows assessing the influence of physical particle properties (e.g., a friction coefficient), particle size distribution and particle agglomeration (mimicked by clustered particles) on the permeability field in a DR reactor. Vice versa, it determines the local gas flow rates and hence is decisive for overall system behaviour. Additionally, the data is used for DEM/CFD simulation validation.

2.2.2 Digital demonstration of H_2-enriched DR

The digital side of the “hybrid demonstrator” approach is based on three states-of-the-art models with different strengths. Currently the best available model for the DR process is the model ‘Reductor’ of UL, which simulates the main internal processes and conditions in a fine-tuned manner and serves as a

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[2] K. Vollmari et. Al. Experimental and numerical study of fluidization and pressure drop of spherical and non-spherical particles in a model scale fluidized bed, Powder Technology, 2016/291, pp. 506-521

[3] Yi, L. et. al., “Sticking of iron ore pellets during reduction with hydrogen and carbon monoxide mixtures: Behavior and mechanism", Powder Technology 235, 2013, pp. 1001-1007

sound starting point. Reductor, which has been validated against Midrex plant data[4], is a 2D, 2-phase, 3-zone, 10-reaction, finite volume method-based CFD model specifically developed for DR shaft furnaces. Its distinctive asset is a sophisticated description of the physicochemical and thermal phenomena involved. The model in being improved in MaxH2DR based on the new results obtained concerning kinetics and solid flow. The adjustment towards H_2-enriched operation is achieved by the implementation of WP1 kinetic sub-models.

A fast (calculation time less than 1 hour) and flexible FEM model of the BF process in two or three dimensions has been developed by BFI. The permeability field can be flexibly tuned according to the BF charging models (regarding the burden layer structure). Due to process similarity, the relevant phenomena for the DR shaft are already implemented, but need tuning to incorporate the MaxH2DR results with respect to kinetics, burden rheology and permeability field. This model is validated in online application at a BF plant. It is directly connected to the operational data (burden charging, blast & off gas, wall pressures, etc.) processing system and tunes its own internal model parameters (cohesive zone shape, permeability) to the current operational state. With this approach, MaxH2DR exploits the benefits of digital models for process monitoring and control in ironmaking.

It is an essential step on the pathway to impact for MaxH2DR to achieve this also for H_2-enriched DR. Since the full methodology of online application is already available in the BF model and due to its computational efficiency and flexibility, this FEM model is being used within MaxH2DR for optimization and scale-up investigations after adaptation to the H_2-DR process.

Additionally. DEM/CFD technology will be used in MaxH2DR. The main limitation of existing models is the missing description of particle behaviour and the resulting local permeability distribution in the shaft furnace, which is essential to describe operational limitations and non-ideal states which are in the focus of operational monitoring and control. A major step forward in this direction is the DEM/CFD technology. The DEM/CFD approach so far was not applied for complete DR shaft furnaces. However, several applications exist, e.g., the blast furnace DEM/CFD model at RUB.[5] One major feature of the MaxH2DR methodology is to transfer this sound experiences and tools from the blast furnace to the DR process. This is creating major synergies and enabling starting at a high level of detail.

However, this sophisticated technology still has shortcomings which limit its applicability and exploitation. These are mainly the extremely high computational effort and the missing information regarding physical particle properties of real materials in industrial environment (restitution coefficient, friction parameters, etc.). In order to reduce the computational effort, the particle shape is usually simplified to be spherical. This simplification is reasonable for DR since the fresh pellets coarsely resembles spheres. Nevertheless, the material properties must be known to describe the solid flow pattern (and thus the permeability) in the shaft correctly. During conversion and reduction, the strength of the material is expected to diminish with temperature and the occurrence of pure iron on the surface will induce increasing friction and adhesion.

Cohesion among the particles can drastically change the overall behaviour of the flowing bulk material and the resulting gas distribution if it raises to the so-called “sticking” which is well known as an industrial issue of DR furnaces.[6] Depending on the local stickiness, in counterflow reactors the effect of “channelling” may be induced (also known as a typical issue in industrial shaft furnaces). Channelling severely interferes with the transport of the reacting agent and heat to the pellets resulting in instable fluid and loss of process efficiency and product quality. In severe cases the particles may even form clusters of objects moving together and thus disturbing the solid flow.

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[4] F. Patisson, Detailed Modeling of the Direct Reduction of Iron Ore in a Shaft Furnace, Materials, 2018

[5] F. Bambauer, Transient DEM-CFD simulation of solid and fluid flow in a three dimensional blast furnace model, Powder Technology, Volume 334, 2018, pp 53-64

[6] Helle, H., et al., Nonlinear optimization of steel production using traditional and novel BF operation strategies, Chemical Engineering Science 2011/66, pp. 6470-6481

The DEM/CFD model currently state-of-the-art for detailed offline simulation of blast furnaces is being adapted towards DR shaft furnaces in MaxH2DR. A calibration of this model is realised based on hot shear cell experimental data. After calibration, the DEM/CFD model will be validated against the physical demonstrator. Based on these, the permeability field as well as the solid and gas flow is optimised. Finally, also data of DR plants in demonstration and/or industrial scale are being used for validation.

As the computational effort of the DEM/CFD reference model is too high for further utilisation in extensive studies, its strength in most detailed calculation of solid flow and permeability fields is exploited by transferring these as input parameters into the fast and flexible FEM model. This is then used for DR process optimisation in terms of different scale-up steps and gas conditions to be investigated. These investigations are closely coordinated with the gas preparation modelling part in WP3, to which the calculated values are exported.

2.2.3 Coupled DEM/CFD simulation of particle movement and permeability in DR shaft furnaces

A comprehensive simulation study based on the demonstration shaft furnace test rig is conducted to validate the DEM/CFD approach against experiments in terms of correct representation of particle movement and gas pressure field. Therefore, a ‘digital twin’ of the test rig is set up. The spatially distributed morphology, i.e., the permeability field, of the particle assembly and the associated blocking of the fluid pathway and/or formation of passages are modelled based on the materials input data from Task 2.1 (size, friction coefficient, shape). To guarantee quantitative data at affordable computing costs, the spatial resolution of the simulation domain is adapted to local conditions. This leads to an intermediate resolution (particles represented as a porous medium in the fluid domain) for the regions of low fluid velocity and a higher resolution (locally resolved representation of particle shape) in regions of high gas phase velocity gradients as e.g., gas injection locations. Results are compared to the measured particle trajectories and pressure loss. The local gas velocity field obtained by DEM/CFD simulation is complementary to the measurements in Task 2.1. It is expected to be decisive for the correct representation of associated gas phase reactions and pressure loss. The quasi-2D test rig might incorporate specific 3D effects, which are possibly difficult to be quantified as only data from the test rig front wall are available. These 3D effects (e.g., segregation in lateral direction) are analysed by DEM/CFD as it provides data from the whole cross section of the test rig.

An important quantitative output is the porosity distribution and solid flow velocities, resulting from the actual particle shapes and positions obtained by DEM. This is transferred as spatial permeability field to the FEM model and implemented. Furthermore, the DEM/CFD tool is validated against measurements and thus, becoming ready for “reactive simulations”.

2.2.4 Development of validated hybrid demonstrator by synergetic combination of models with physical demonstration

Main target is to convert the finite element method (FEM) based process model into an overall process model for DR shaft furnace reactors. The DEM/CFD model allows for the analysis on the smallest length scales and includes direct description of local permeability and particle movement. The finite volume method (FVM) based Reductor model serves as a reference for the current state-of-the-art.

The benchmarking of models on common reference cases enables a multi-feature validation and identification of pros and cons of each model. In order to realise this, the geometries are adapted to a selected DR demonstration scale plant and the kinetic sub-models are included according to the results obtained. Since the FEM model and Reductor model do not solve the details of particle mechanics, pre-computed solid flow and permeability field provided from the DEM/CFD simulations by RUB are used in these cases. In that context, a rheological model can be tuned for the solid flow field and the permeability field can be expressed as a function of the space and state variables. The simulations are coupling all main physical and chemical phenomena for a DR shaft furnace. Utilising the selected DR reference plant, two reference cases are assessed: One reference case according to current NG-based industrial operating conditions and a second reference case based on hydrogen. The results will be analysed with respect to process conditions (e.g., gas temperature and composition, flow, local and global pressure drop) and product quality. Concluding this task, the FEM model is supposed to serve as the work horse for process optimisation and for dynamic DR process calculation.

2.2.5 Scale-up towards digital demonstration of industrial DR shaft furnace reactors

Specific problems of industrial DR shaft furnace reactors are investigated in MaxH2DR. The influence of reactor dimensions (and the ratio of reactor dimension/pellet size) to the solid phase movement and the gas distribution in the shaft (limited penetration depth of the injected gas) is studied using the process models. Furthermore, potential countermeasures (as fuel lances or pellet charging strategies) are examined in detail. The increasing shaft height is not only affecting the inter-particle forces to a certain extent (depending on the diameter/height ratio, shearing angle) but also the reaction rates (with varying pressure). Another scale-up issue is the substantial knowledge gap of the internal high temperature processes, regarding the softening process and solid/gas flows. The permeability, which controls the gas flow and process reactions, can only be roughly estimated because of this knowledge gap. All these mentioned effects are assessed to achieve an efficient and stable DR shaft furnace operation for high product quality.

The large number of particles is critical for DEM/CFD computing time for the industrial scale. Hence, the proven method of coarse graining (large particles representing multiple elements of actual size) and periodic boundary conditions (allowing a reduction of the simulation domain to a cylindrical sector segment of e.g., 60° or 90°) as well as locally varied spatial resolution is employed. Various promising operational states are studied with intensive parameter and sensitivity analyses mainly by the FEM based process model. The results are evaluated with respect to process efficiency, stability, and product quality (e.g. metallisation degree, carbon content) for different degrees of H_2 enrichment. Promising states are analysed in parallel with the other models to ensure consistency and validity of results. The conclusions of this task will be exploited for recommendations and guidelines regarding the scale-up process.

2.2.6 Process optimisation for industrial scale DR shaft furnace reactors

First step in this task is the definition of the validation strategy aiming to exploit further data of demonstration and/or industrial plants as final but crucial validation step. The intermediate results of WP1 and WP2 and consultations of Advisory Board and stakeholders are concluded to identify critical parameters and aspects for validation (e.g. risk of sticking due to load, temperature and particle properties, carbonisation). Depending on these conclusions it can be assessed if (detailed) data of demonstration scale plants with high H_2 enrichment are more appropriate or rather data of industrial plants with realistic dimensions and mechanical loads. This is helping to select the priorities of validation and of process optimisation as well as to acquire/select additional data. In this context, an IPR/compliance check will be performed, and appropriate non-disclosure contracts are prepared if required. Parameter sensitivity analyses and case studies are performed with the process models to identify possible overall process optimisations for optimal temperature distribution and flow conditions after deciding the priorities based on the intermediate results and stakeholder consultations. Important aspects are e.g., the variation of the reduction gas properties (H_2 enrichment), the variation of the gas injection technology (additional or adjusted injection points), or the variation of material properties and charging. The influences of these aspects on the main quality parameters of the DRI (metallisation degree, carbon content) is studied. DEM/CFD simulations of local effects will support the FEM simulation model for selected optimised DR shaft furnace geometries. Such details could be e.g., design of burner lances, identification of channelling or gas flow maldistribution.

The results are assessed regarding product properties (e.g., metallisation degree and carbon content) and process efficiency (e.g., productivity, energy consumption) and converted for use in the process chain simulations in WP3. Additionally, appropriate ranges of reduction gas properties are provided by the flowsheet tool assessment in WP3 (Aspen Plus simulations). The conclusions of this task are exploited for recommendations and guidelines regarding process optimisation.

2.3 WP3: Efficient and flexible steelmaking process chains based on H_2-enriched DR

This WP is focused on steelmaking process chain simulations for maximising H_2-enriched DR utilisation and demand-response flexible operation to incorporate intermittent RES availability. Three existing process chain simulation tools with individual strengths are adapted and jointly exploited in a multipurpose simulation toolkit for maximum synergy and reliability. An AML-based tool is exploring novel low emission and low-cost plant concepts for feasibility. IRMA is used for optimisation studies focused on metallurgical aspects and effects on up/downstream units. Aspen Plus is used focusing on gas and energy handling, considering RES intermittency. LCA, LCC and social impact analyses conclude the WP.

Main target of this WP is optimising the integration of the H_2-enriched DR process into existing steelworks to digitally demonstrate and assess promising complete process chains. The transition towards a novel integrated steelmaking process employing H_2-enriched DR furnaces has fundamental impact on the operation of up- and downstream processes, with respect to metallurgical aspects, material and energy flows, as well as recycling of residues. For instance, the replacement of a BF with a H_2-enriched DR combined with an EAF leads to less blast furnace and coke oven gas with consequent decrease of internal electricity production but instead a higher power demand. The most efficient operation states of integrated steelworks with H_2-enriched DR units are still unknown and vary depending on the individual boundary conditions. Furthermore, there are several options on how to operate and integrate DR units in the process chain. The major target is to mitigate CO_2 emissions, but other impact on the environment is considered by Life-Cycle Assessment (LCA). Furthermore, costs and social impacts must be considered to achieve sustainable future steel plants.

The holistic studies of MaxH2DR combine three different tools to a multipurpose simulation toolkit by specifically exploiting their individual strengths and avoiding their weaknesses. An algebraic model-based steelmaking chain superstructure with highly simplified unit models is provided, including tools for multi-objective optimisation. The optimisation will provide rough estimates of promising plant states and layouts, which are further analysed with special focus on gas and energy networks by an Aspen+ based tool and on critical metallurgical aspects by the Iron Making model (IRMA). A multifunction toolkit is made available for holistic investigations of new steelmaking plants that will evolve. The environmental impact of the future plant concepts developed and studied in the analyses is subjected to a detailed LCA, and for some of the promising alternatives also Life Cycle Cost will be studied.

Holistic studies of all the main effects start from the structure of an integrated BF-BOF steelworks with two BFs and investigate different (structural and operating) transition stages to a configuration mainly based on the application of H_2-enriched DR. These investigations will determine the best pathway and provide guidelines to be followed for maintaining desired metallurgical performance, product quality and achieving a compromise between CO_2 emission, energy demand and costs efficiency in all the transition steps.

An AML-based (Automation Markup Language e.g., in GAMS or AMPL) steelmaking chain superstructure that includes simplified unit models but also tools for multi-objective optimisation[7] of CO_2 emissions

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[7] Mencarelli, L., et al., Grossmann, I.E.; "A review on superstructure optimization approaches in process system engineering", Computers and Chemical Engineering, 2020/136, p.106808.

and costs, as applied in studies of other novel ironmaking technologies, is provided.[8,9] The DR furnace model of WP2 is incorporated in the AML model in a simplified form, which is applied to find promising plant layouts and operation regimes. This narrows down the space to further explore, allowing deeper analysis and feasibility checks by more complex models.

The IRMA model, which was used and validated in the ULCOS project for comparing different iron and steel making processes, is exploited in MaxH2DR. The standardised reference steel plant forms an ideal starting point for the analyses. IRMA is based on energy and mass balances complemented by a mix of thermodynamic equilibria (using the ChemApp library) and empirical relations. IRMA model was extensively validated: for a Rotary Hearth Furnace combined with EAF (as reported in ULCOS), and in an adaption for the Tata Steel IJmuiden site.

As most building blocks are already implemented, IRMA is ideal for accurate assessment of the metallurgical performance of the production units and plant entity. It is complemented by models of the new unit processes and the accurate G&E management of the Aspen Plus model to rigorously simulate the complete future steelmaking production chains. IRMA is receiving reducing gas-related data from the Aspen Plus model, makes its detailed metallurgical evaluations and provides the Aspen plus model by refined information on process off-gases (POGs) in an iterative manner until a static state is reached. Further expertise and models related to gas handling and treatment, and energy conversion, processing and management is exploited in WP3.

The available models are both stationary and dynamic. Models of electrolyser units for hydrogen production[10], steam methane reforming process and scrubbers developed in Aspen+ in earlier projects are combined with new unit models (e.g., separators, heat exchanger systems, compressors, gas enrichment or CCS/U units, power plant) that are being developed based on information in literature and domain expertise.

The underlying rigorous and extensive thermodynamic database of Aspen Plus and its well-established unit operation models, makes the flowsheet model reliable and accurate for estimating G&E flows in the plant. The necessary information is passed iteratively to IRMA as outlined above. By this, the stationary scenario analyses are appropriately considering the G&E flows together with the metallurgical performance of the units obtained through IRMA. This multipurpose simulation toolkit approach combines the strengths of both tools and clearly raises the quality of the prognostic analyses compared to any state-of-the-art tool. The results of the analysis are concluded into the key performance indicators (KPIs) computation to reveal the feasibility of the studied scenarios and generate the information required in the LCA analysis. In addition, results related to the appropriate ranges of reducing gas properties are also obtained to be exploited for optimizing DR shaft furnace operation. The FEM model and the results are used in WP 3 to improve the model of reduction gas properties and get a higher gas utilisation and product quality in the DR process.

The WP3 activities also include dynamic investigations to simulate novel steelmaking concepts based on H_2-enriched DR under conditions of high RES exploitation. A management of the process is studied to ensure the energy supply under RES volatility: dynamic and joint minimisation of economic and environmental costs are researched by optimizing resources dispatching and purchase, production allocation as well as hydrogen production and storage or H_2 enrichment of the reducing gas. The stationary Aspen Plus model is converted to consider dynamics, developing a RES volatility model and

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[8] Helle, H., et al., Nonlinear optimization of steel production using traditional and novel BF operation strategies, Chemical Engineering Science 2011/66, pp. 6470-6481

[9] Ghanbari, H., et al., Optimal Design and Operation of a Steel Plant Integrated with a Polygeneration System, AIChE Journal, 2013/59, pp. 3659-3670

[10] Zaccara, A., et al., Renewable hydrogen production processes for the off-gas valorization in integrated steelworks through hydrogen intensified methane and methanol syntheses. Metals, 2020/10(11), p. 1535

a dynamic one for DR-shaft furnace starting from the WP2 results and found kinetics, configuring a dispatch controller and coupling them with available models simulating the process offgases.[11,12]

In order to complete the investigation, environmental and social impact assessment based on the results of the scenario analyses are carried out. The unique interplay between the AML-based superstructure and detailed flowsheet models in a multipurpose simulation toolkit, the possibilities of carrying out both stationary and dynamic investigations, LCA, LCC and social impact analyses make it possible to systematically evaluate the conditions and requirements for the transfer of new H_2-DR shaft furnace technology in European steelmaking industry.

2.3.1. Adaptation and extension of available models and interconnection development

Subtasks are provided to adapt and link existing tools and to model missing units for completing the multipurpose simulation toolkit. An integrated BF-BOF steelworks with two BFs is exploited for benchmarking. A Communication database is being developed. In this context, Input/output streams among the tools are defined. AML model is providing configurations and operation regimes to IRMA and Aspen Plus models, which exchange data regarding reducing gas and POGs. An interconnection database is being developed and deployed on a server.

Adaptations and improvements of stationary models and reference-case simulation are identified. In a first step, industrial knowledge, literature information and data are collected. A holistic steel plant model basis for explorative investigation is written in AML and includes reduced models of main production units and G&E network. The superstructure is updated and new unit models (e.g., H_2-DR furnace, EAF) and related links are being included. Based on WP2 findings and an 1D DR shaft model, a surrogate DR model is being developed and refined. In this way, new alternative plant configurations can be explored. The IRMA-based model library includes all the main production units and stockyards, mixing and distribution sections. The tool is being updated in MaxH2DR. DR IRMA model (0-D/1-D) is being adapted for H_2 operation with literature data and then refined with WP1 & WP2 results. An IRMA EAF model is being built. Earlier ULCOS models can be taken as reference depending on the relevance of the generated EAF operating scenarios. A stationary detailed G&E network model is being developed in Aspen Plus including both sections related to reducing gas production and POGs handling. Already available unit models are being adapted (e.g., steam and/or autothermal reforming for processing methane/POGs blends) and new ones will be configured (e.g., power plant). Stationary flowsheet include several G&E dispatching possibilities for allowing different distribution scenarios, preparing the model to include dynamics. Treatment and processing of a wide range of POGs, produced under different conditions, are extensively tested through models developed in ENCOP. Adapted tools are interconnected by means of the developed database. A reference case is simulated to benchmark AML-based model with the coupling of IRMA and Aspen Plus models. Consistency and robustness is being verified. Excel-based ULCOS steel mill model with 4 Mt HRC per annum capacity act as reference for site configuration and main material and energy flow rates. Model changes are carried out to obtain results in mutual agreement.

Further, there will be progress in dynamic model development. A dynamic site model for investigations of flexible operation with respect on G&E use, considering RES intermittency and DR shaft furnace behaviour, is being developed. Stationary G&E networks model will be converted to a dynamic counterpart by including storage units and required equipment. Available Echo State Neural Network models to forecast POGs are adapted with industrial data and coupled with the network model. An H_2-DR furnace dynamic model is being developed through AI/hybrid methods and using WP2 results and

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[11] Matino, I., et al., Machine Learning-Based Models for Supporting Optimal Exploitation of Process Off-Gases in Integrated Steelworks. Impact and Opportunities of Artificial Intelligence Techniques in the Steel Industry: Ongoing Applications, Perspectives and Future Trends, 2021, pp. 1338

[12] Dettori, S., et al., A Deep Learning-based approach for forecasting off-gas production and consumption in the blast furnace. Neural Computing and Applications, 2021, pp. 1-13

the found kinetics. The reducing gas properties are optimized through adjustment between the models. The gas utilization of the of the DR process is being optimised. RES volatility is modelled, and steelworks internal G&E demands are estimated. A dispatch controller (DC) will be configured with an Economic Model Predictive Control (EMPC) approach to optimize, e.g., G&E distribution, H_2 and DRI productions, reducing gas H_2/CH_4 ratio, by considering RES availability and process operation (particularly the DR shaft furnace).

2.3.2 Stationary scenario analyses for transitional pathways

For scenario analyses to study gradual transition stages from the reference integrated steelmaking route towards novel routes with H2-enriched DR, a stationary toolkit part is used. Transition plant setups are explored from different points of view by the three tools. The following modifications are analysed first:

- replacement of one BF with H_2-DR furnace and DRI exploitation in the remaining BF, BOF or EAF
- replacement of both BFs with H_2-DR shaft furnaces and DRI usage in BOF or in EAFs

These configurations have strong implications for the plant state in terms of metallurgical performance, product quality, raw material demand, but also effects on operation of up/downstream processes as well as on emissions, G&E handling and operating costs. Depending on the configuration, changes in main process parameters affect the plant performance differently. Thus, simulations with the following ranges are undertaken: H_2 share in the reducing gas 60-100%, DRI C-content 0-4%, inlet reducing gas temperature 750-950 °C, DRI usage in the different production units (0-100% of the charge depending on the unit), ratio of POGs used for heat, power generation, reducing gas/hydrogen production 0-100% (for each usage). These are having specific effects on CO_2 emissions, POGs availability, material and energy demand, residuals in steel, slag features, etc. For each of the listed transition plant configurations and considering the whole process parameters range of interest, optimal plant operation regimes with respect to emissions and operation costs are investigated preliminarily under pertinent constraints by AML superstructure. This is enabled by its low computational burden, followed by a multi-objective MILNP approach yielding Pareto fronts with sets of alternative solutions. Deeper explorations on the reduced exploration space are done by using IRMA and Aspen Plus tools jointly. By this, consistency checks and an accurate estimate of metallurgical performances, product quality, raw material demand, CO_2 reduction, effect on up/downstream processes and on G&E handling are undertaken. In particular, the effects on the defined KPIs are evaluated. Modifications refining the preliminary optimized plant configurations and regimes are studied next to find the best feasible solution for each transition step. In the AML tool investigations, unconventional and unexpected, but still promising solutions are also expected to be found. In this case, these are scrutinized with the other two tools in the same way already explained.

The results of these scenario analyses are the bases for the next tasks and will provide useful information to activities concerning the proper ranges of reducing gas features; in effect the gas properties obtained are used for process optimizing the industrial scale DR furnace operation.

2.3.3 Dynamic investigations for flexible operation of new integrated steelworks with H_2-enriched DR for high RES integration

Dynamic models and DC is configured for recreating the previous found optimal configurations. Simulations are carried out to study the real operation of steelworks with H_2-enriched DR in the case of high RES use. Considering the objective of minimizing economic and emission costs by allowing the satisfaction of process energy demand considering RES volatility, the DC allows flexible and smooth operation of these new steelmaking routes by focusing especially on the DR shaft furnace operation. Optimization is carried out for G&E distribution or external purchase from different sources, H_2 production/storage, reducing gas H_2/CH_4 ratio, production allocation. The final goal is to demonstrate flexible demand-response operation with an efficient integration of RES in future steelworks with H_2-enriched DR. The results are used in the Life Cycle Assessment.

2.3.4. Life Cycle Assessment and Cost

Life Cycle Assessment (LCA) is a key tool for studying environmental impact and sustainability of a process (or a part of it), product or service through its whole life length from raw materials to the final deposit or recycling, according to the ISO 14040:2006 standard. Since the process chains studied and evolved in this WP are novel and have not been applied before in industrial production, their impacts on the environment are not defined yet. But these are central for the development towards sustainable steelmaking. Main scenarios for future steelmaking will be evaluated and selected promising ones from cradle to gate. LCA software SimaPro using Ecoinvent and other databases is applied as the basis for the analysis to calculate process environmental impact using the IMPACT 2002+ method. Life cycle impact is calculated around 15 midpoint categories, which are summarized into four damage categories: Human Health, Ecosystem Quality, Climate Change and Resource Depletion. For some of the studied plant concepts, LCA is extended to Lifecycle Cost Analysis (LCC).

2.3.5. Social impact assessments

Social impact assessments of the implementation of different configurations of new integrated steelworks with H_2-enriched DR consider two dimensions:

1. Impacts within companies (employees and organisation);
2. Impacts on a societal level outside the companies (infrastructure, CO_2 reduction, stakeholder involvement).

The study is based on written outputs, employee/partner survey and interviews of relevant stakeholders for social key performance indicators (SKPIs) estimation. Some potential SKPIs to be evaluated are as follows:

a. skill matching of affected job roles and current employees;
b. steel company people awareness on their decarbonization contribution and climate protection;
c. appropriateness of new solutions for daily operation based on experience of affected employees;
d. job satisfaction of employees with affected job roles (needs to be better or equal to status quo);
e. degree of knowledge of potential occupational safety and health risks, and of required training and safety certification/regulations.

On the societal level outside the companies, potential Social Regional level Key Performance Indicators are:

- impact on climate protection in terms of CO_2 emission when H2-DR is fully implemented in the steelworks;
- key stakeholders' (government, companies, research, civil society) involvement level in the process;
- degree of reporting of additional requirements for the implementation of new integrated steelworks with H_2-DR that affect other stakeholders than the company itself (e.g., additional infrastructure requirements, RE production sites, raw material supply, by-product storage or transport in the area);
- affected stakeholders' information level on needs and possibility to voice their views and concerns;
- scenario developers' degree of addressing voiced opportunities, risks and concerns;
- key stakeholders' acceptance level of the proposed solutions.

3. Outcomes and Impact

MaxH2DR is providing digital toolkits enabling the demonstration of plants incorporating Carbon Direct Avoidance measures. The gained knowledge regarding H_2-enriched Direct Reduction is significantly supporting the scale-up and investment planning and decision making. This is leading to plant suppliers and steel producers selling and implementing more new H_2-enriched Direct Reduction processes. Additionally, existing plants are being modified by steel producers so that the hydrogen content in Direct Reduction will be increased more quickly and stronger. Overall, MaxH2DR is contributing towards shifting the focus of steel producers from carbon-based blast furnace to hydrogen-based direct reduction processes. This is expected to lead to decrease CO_2 emissions from ironmaking in 2030 by Mt/a and much more after 2030, due to faster industrial implementation and hydrogen enrichment in direct reduction processes. By that, the sustainability of the whole European industry is profiting due to being supplied with “green” CO_2-free steel for carbon neutral end user products.

The operation of existing or newly built direct reduction shafts gains more flexibility by MaxH2DR. Dependent on the hydrogen availability, a more flexible switch or composition adjustment of hydrogen and natural gas is established. MaxH2DR is providing validated simulation models. This improved model validation is increasing overall industrial digitization and its acceptance, particularly for the energy intensive ironmaking. Furthermore, the models are developed for online application which is improving process monitoring and control operations. The innovation potential of energy intensive process industries is raised by exploiting the digital technologies and validation strategies for practical industrial use. Overall, society is profiting from this innovation potential, emission mitigation and prevention of job losses. The social acceptance of steel industry as sustainable and innovative part of European economy raise. Ultimately, the improvements in digital optimization, monitoring and control are improving efficiency, safety and sustainability in the steel industry.

The financial impact for steel producers is estimated to be 1.8 bn €/a in 2030 by saving expenditures for CO_2 emission certificates only. This is significantly increasing the international competitiveness of the European steel industry.

List of Acronyms and Abbreviations

Acronym	Full Name
AI	Artificial Intelligence
AML	Automation Markup Language
BF	Blast Furnace
BFI	VDEh-Betriebsforschungsinstitut GmbH
BOF	Basic Oxygen Furnace
BRASS	Blast furnace Reduction and Softening Simulation
CCS/U	Carbon Capture and Storage or Utilisation
CFD	Computational Fluid Dynamics
DEM	Discrete Element Method
DR	Direct Reduction
DRI	Direct Reduced Iron
EAF	Electric Arc Furnace
EMPC	Economic Model Predictive Control
FEM	Finite Element Method
FVM	Finite Volume Method
HOSIM	“Hoogovensimulator”, blast furnace simulation
IRMA	Iron Making Model
KPI	Key Performance Indicator
LCA	Life Cycle Analysis
LCC	Life Cycle Cost Analysis
RES	Renewable Energy Sources
RUB	Ruhr-Universität Bochum / Ruhr-University Bochum
SKPI	Social Key Performance Indicator
POGs	Process off-gases
WP	Work Package