Advanced Simulation of Iron Oxide Reduction Using Hydrogen: CFD-DEM and USCM Integration

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The reduction of iron ores is a core process for the iron and steel-making industries. In addition, the large rate of fossil fuels/reductants needed makes pyrometallurgical processes very intensive regarding CO2 emissions. Accordingly, to make the steel industry more CO2-neutral and achieve the zero-waste goal, new circular economy solutions (using H2 as a reductant) must be developed and validated before their industrial implementation. Understanding the methods to obtain iron ores is crucial to optimizing and decarbonizing these industries. In these processes, a hot gas (reductant agent) is injected into the furnace and filled with ores. The gas heats the particles (in the form of stones, briquettes, and pellets) and may move them (as in fluidized beds). As the ores heat up, the reduction occurs inside each stone according to its exposition to temperature and reductant agent. Thanks to the advancement of software and hardware, it is possible to perform physics-based simulations that give rich details of complex processes [1]. A simulation gives access to information that cannot be obtained in the laboratory due to physical limitations. Hence, this work presents a computational framework for simulating the Direct Reduction Iron (DRI) by combining Computational Fluid Dynamics (CFD, Discrete Element Method (DEM) and the Unreacted Shrinking Core Model (USCM) to simulate the complex physicochemical phenomena occurring in DRI furnaces analyzing the fluid-particle interactions, heat transfer direct reduction evolution.

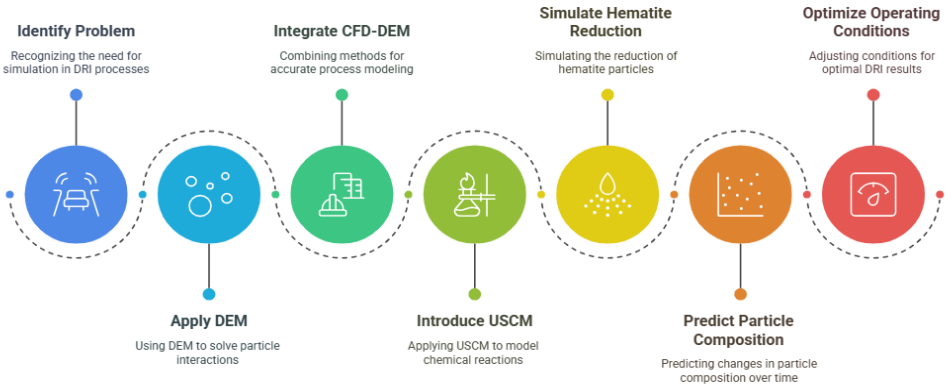

Figure 1 Framework of simulation of DRI process.

Computational Fluid Dynamics (CFD) has long been used in the industry as a standard method for simulating fluid flow and heat transfer. This method, however, cannot handle discrete particles (solids) like the ones we find in the DRI furnace once is used for fluid. Hence, the discrete element method (DEM) has been used as a new standard in the industry for solving coupled solid-fluid problems such as DRI furnaces. This way, the forces acting on the particles, including their mutual interaction, can be solved by directly integrating the Newton equation. For an application to DRI, it is ideal to combine both methods to obtain an accurate picture of the processes and interactions taking place between gas and particles. With this, the temperature of each particle and its exposure to the reductant agent (hot gas), can be determined by the particle position in the furnace. The use of a coupled CDF-DEM model provides the time-dependent composition of each particle.

However, another problem must be solved: the chemical process of Iron reduction. The unreacted shrinking core model (USCM) has been largely applied to calculate the reduction. In this work, it is applied to a particle of hematite. When the temperature is appropriate, the exposed surface of hematite reacts with the hydrogen and transforms into magnetite. As the reaction happens, the magnetite layer grows thicker, and the hematite core shrinks. When the right conditions are reached, the magnetite reacts with hydrogen to produce wustite, and, in turn, this will react to produce iron. At any given time, the particle will consist of a hematite core and layers of magnetite, wustite and iron. Hence, the full Direct Reduction Iron (DRI) simulation comprises three different

coupled methods: CFD, DEM and USCM. With this three-couple method, the time-dependent composition of the particles is obtained as a function of the gas conditions.

In this simulation, the circulation of the gas is determined by the porosity of the particle bed. Different parts of the reactor can be subjected to different conditions, making the reduction process time-space dependent. The Fluent (CFD) package simulates the fluid coupled with Rocky (DEM). The USCM is implemented as a separate C code and fed to the CFD simulation. When this is started, the three modules continuously exchange information about all the variables. With this, Fig.1(left) shows the evolution of the composition of a particle, which is pure hematite, at the beginning of the process. The amount of hematite is reduced while that of magnetite, wustite, and iron increases. Since magnetite and wustite are reactants as well as products, their quantities start to decrease after period of time. The Fig1. (right) shows the evolution of the overall reduction (a function of the masses of the oxides), which reaches nearly 90% after one hour.

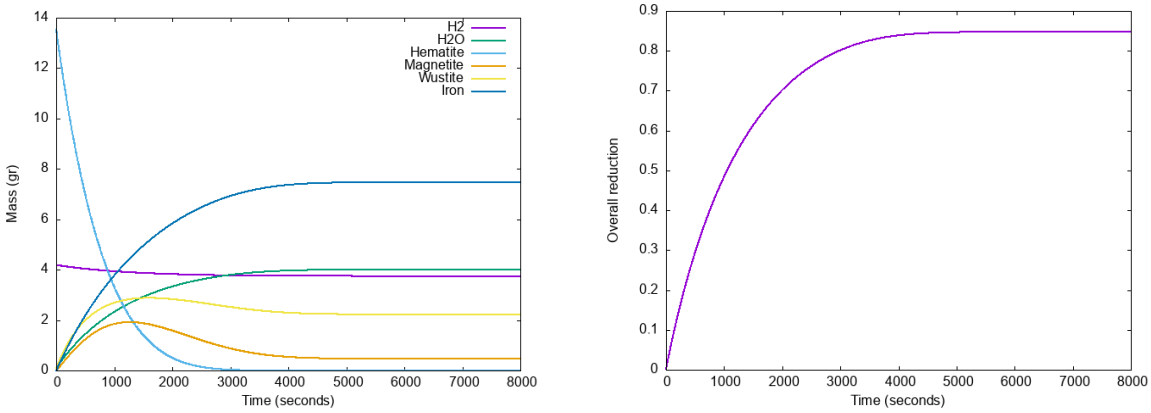

Figure 1. Left: mass composition vs. time of a particle as predicted by the USCM. Right: Overall reduction of the particle.

Fig.2 (left) shows the interaction of particles and gas. At an early stage of the process, the particles on top of the bed increase the temperature due to their exposition to the gas (T=900K). The gas temperature also changes upon contact with the particles due to heat transfer. Fig 2 (right) shows that the flow velocity is high at the injection point and slows down in the bed of particles. Then, it accelerates again in the narrow exit tube.

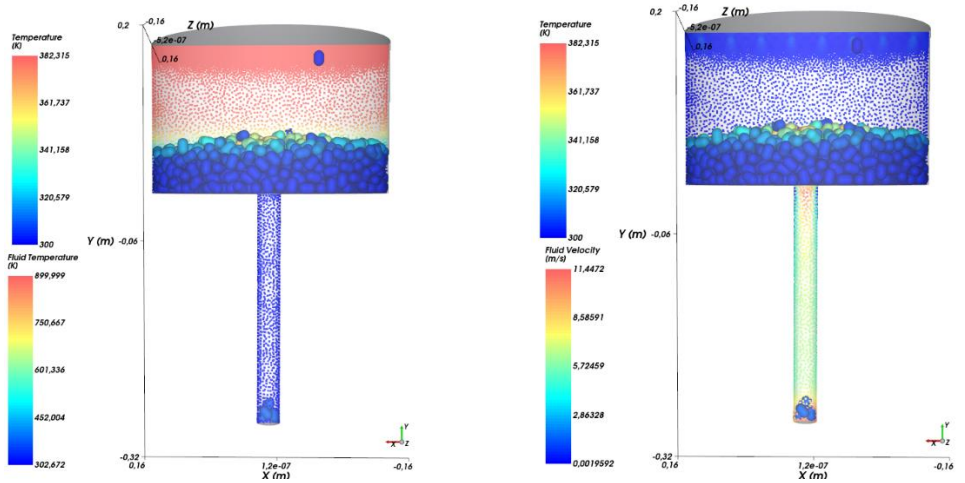

Figure 2. Left: The temperature of the particles and the gas interior of the DRI bucket. Right: the temperature of the particles and the velocity of the gas.

Furthermore, this work will present the results of simulations under different operating conditions (temperature and pressure of the gas) and particles' compositions, which will help to understand the interplay between the different variables and predict the conditions that maximize reduction while minimizing the required process time.

References

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