SisAl Pilot

SisAl Pilot Project
Innovative pilot for Silicon production with low environmental impact using secondary Aluminium and silicon raw materials

Enjoy reading the SisAl Pilot newsletter!

Latest progresses on tests and numerical modelling of the SisAl Pilot process

The first one and a half year has passed In the SisAl Pilot project without any large physical meetings. Despite the lack of interaction with the whole team many achievements have been successfully reached in the project. NTNU and RWTH have done lab scale experiments as input to the pilot trials at Elkem RWTH, Mintek and Fundiciones Rey. As you will read more about in this newsletter, Elkem has already performed 18 pilot trials with raw materials obtained from the project partners (Erimsa, Hydro, Wacker and Elkem). Slags from pilot trials at Elkem have been sent to the hydrometallurgical partners (NTUA and Mytilenous) for further processing and >98% pure Si metal has been sent to Sintef and Silicor to be used in the production of high purity silicon ingots in the project. Fundiciones Rey has done tests with material from Befesa to prepare for their pilot trials in 2022. Theoretical models for the pyrometallurgical pilots are under development by SIMTEC and ITMATI. Also, HZDR has done a first model of the whole SisAl Pilot process in HSC Sim, which is used as input to the LCA team at NTNU and the business models done by BNW. The project has been presented at Infacon, RawMat, ECOMONDO The Green Technology Expo and at a workshop called “Towards a more sustainable alumina production in Europe.” In November the whole project team will meet for the first time at RWTH and discuss the progress in the project and prepare for the upcoming review meeting.

Pilot campaign at Elkem successfully completed

Tests at Elkem started in May 2021, and per November 1st, a total of 20 tests have been performed (2 hot-commissioning tests + 18 scheduled tests). A 600 kW induction furnace and a robot for handling of hot and heavy equipment, have been used throughout the pilot tests.

Tests have been conducted as separate batches run in campaigns of two or four tests; recipes for each batch were calculated and decided by the project team at NTNU.

For slag smelting, the following raw materials were used: Pre-fused slag with SiO_2/CaO ratio approximately 50/50, quartz fines (SiO_2) from partner Erimsa + commercial lime (CaO). Some tests were performed with both pre-fused slag and quartz + lime.

As Aluminium (Al) sources for reduction, Elkem tests have been performed with pure Al blocks, pressed Al shavings and Al dross. All Aluminium sources were supplied from Hydro.

Four tests were designed to check the refining effect of sculls on SisAl produced silicon. Sculls were supplied by Wacker. The results were convincing in terms of purity of the silicon after refining.

From an operational aspect, all tests performed as planned. No major problems or unexpected process deviations occurred. A typical test campaign comprised 4 separate tests for 2 days (48 consecutive hours) manned with 2 operators on each shift and one process engineer during tapping. Prior to the tests, preparation of raw materials was performed. During tests, slag samples were collected at predefined intervals to check the process kinetics. Results and observations indicate that the aluminothermic reduction is quite rapid under the experimental conditions at Elkem.

Charging of raw materials to the induction furnace at Elkem

Casting of SisAl slag at Elkem pilot

The role of stirring in aluminothermic reduction of silica

The SisAl Pilot project is an innovative pilot that is aimed at silicon production based on principles of circular economy. In particular, the use of secondary aluminium and silica raw materials with a subsequent aluminothermic reduction of silicon constitute the core of the project. In comparison with already well developed carbothermic reduction route, the use of secondary aluminium significantly reduces the CO2 emissions. Such metallurgical processes with low environmental impact are studied in this project both experimentally and numerically.

The role of ITMATI and SIMTEC – the numerical modelling partners of the SisAl Pilot project – is to support and guide the experimental work through modelling. Development and validation of numerical models of relevant physical and chemical processes that occur in lab-scale induction and electric arc furnaces will move us towards a better understanding and optimization of those processes and will allow us to optimize the lab-scale furnaces and ultimately to extrapolate some guidelines for designing an industrial-scale equipment.

This task is not simple. A direct numerical modelling of the SisAl Pilot process is complicated due to multiple couplings between different physical and chemical phenomena, such as heat and mass transport, gas and liquid convection, chemical reaction, phenomena in the electric arc plasma, interaction of electric currents with magnetic fields, thermal radiation, materials vaporization, and the effects of non-linear material properties. This newsletter presents some insights about the aluminothermic reduction of silica, obtained through numerical modelling of heat and mass transport phenomena in metal and slag phases at a laboratory scale.

Aluminothermic reduction is exothermic and contributes to the heating of the metal-slag system as soon as the reaction has started. On the one hand, this heating can be dangerous, as local temperature rise can damage the crucible; on the other hand it can be beneficial, as it helps to keep the system in a molten state and to prevent its solidification. The total power of the exothermic heat source is directly defined by the reaction rate. Thus, it is important to understand what defines the global reaction rate, and how to control it in order to stay in an optimal temperature range.

The final composition of the metal and slag phases is another important indicator of the SisAl Pilot process efficiency. The goal of the project is to maximize the silicon output. Theoretically, the equilibrium composition of phases is defined by the kinetics of aluminothermic reduction that takes place at the interface between immiscible metal and slag phases. However, the time to reach the equilibrium in a whole system depends also on how quickly chemical species are transported across the phases bulk. Both the reaction kinetics and the transport of chemical species, such as diffusion and convection, define the global reaction rate and indicate the required duration of this process to reach a certain phases composition. Numerical computations suggest that, in the absence of stirring, natural convection may substantially contribute to the transport of reacting species and, thus, accelerate the aluminothermic reduction. The intensity of natural convection depends on the liquid layer stability in the Earth’s gravitational field.

As far as slag is denser than metal, it prefers to stay below the metal layer. Aluminothermic reduction at the layers' interface changes the local density of both metal and slag phases by increasing their temperature and by modifying their chemical composition. This results in vertical density gradients across metal and slag layers. When material density is increasing with height, it is an unstable configuration, where heavier liquid is above the lighter one, and they try to exchange their places, resulting in a convective Rayleigh-Taylor instability that mixes the layer. When density gradient is such that heavier liquid is below the lighter one, it is a stable system, and no natural convection appears in this case. In case of the metal layer, the temperature rise at the metal-slag interface destabilises the layer, while composition change caused by the chemical reaction stabilises it. In the slag layer, the situation is opposite: the temperature rise at the metal-slag interface stabilizes the layer, while the composition change destabilizes it, since slag density increases during aluminothermic reduction. In terms of convective instability in both the metal and the slag layers, composition change is competing with the temperature rise. As numerical simulations show, see Figure 1, the composition change dominates the temperature rise in the metal phase, and the metal layer remains stable. In the slag layer, there are two visible sublayers: the unstable one immediately below the metal-slag interface, where composition change dominates the temperature rise; and the stable one beneath it, where temperature rise dominates the composition change. The presence of stable layer in the slag domain reduces the volume mixed by natural convection, and thus reduces the global reaction rate, which is mostly limited

by the transport of reagents towards the metal-slag interface and not by the reaction kinetics at the interface.

By numerically deactivating the stabilizing mechanism in the slag layer, namely by keeping system isothermal, one can increase the size of mixed region, thus increasing the global reaction rate, as can be seen by comparing black and grey lines in Figure 2.

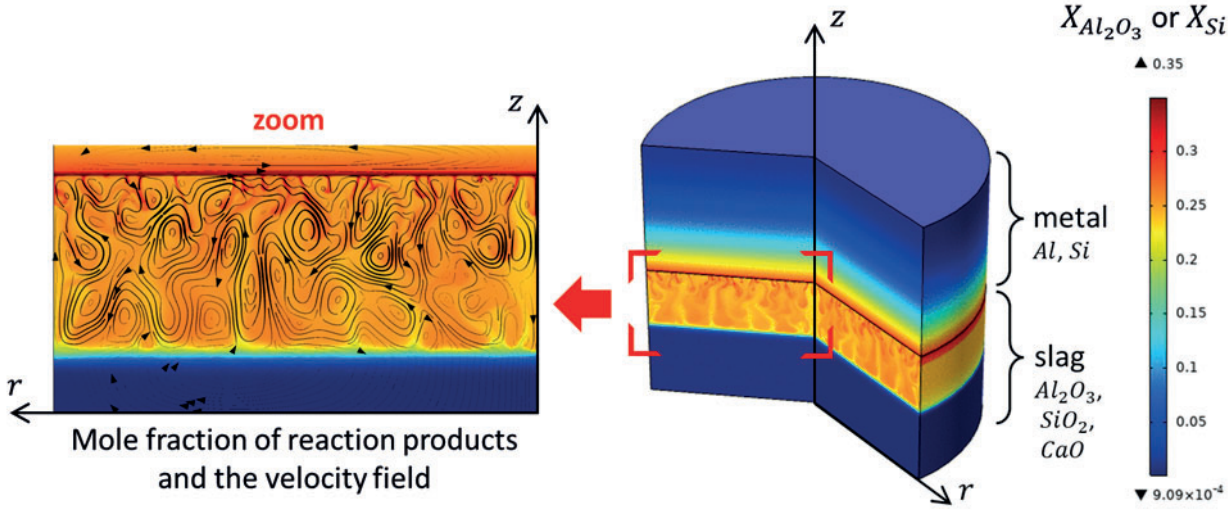

Figure 1: Mole fraction (X_(Al_2 O_3), X_Si) and velocity fields for diffuse interface model with natural soluto- and thermo-gravitational convection after a reaction time of 10000 s.

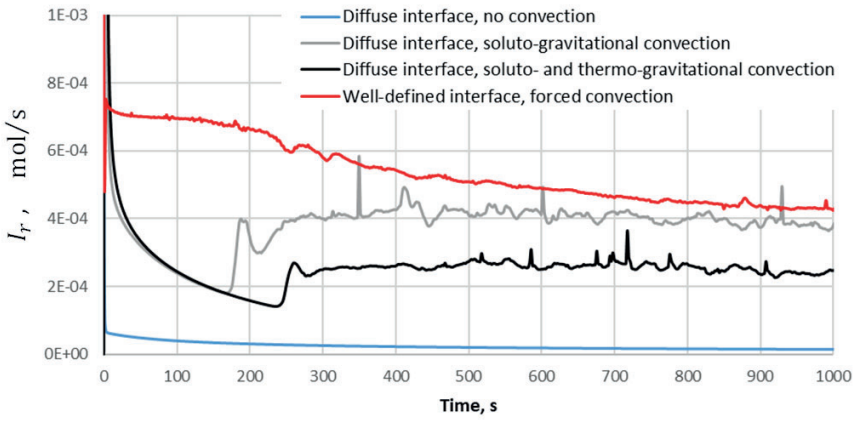

Figure 2: Global reaction rate comparison between different numerical models.

The model presented in Figure 1 belongs to the class of diffuse interface models that feature a smooth transition between phases with a continuous change of material properties across the interface. On the one hand, a moving metal-slag interface in such a model helps to naturally generate and maintain a large amount of Rayleigh-Taylor instability vortices. On the other hand, it requires a considerable amount of computational resources and a long computation time. In case of more complex flow regimes, when moving interface is subject to the Kelvin-Helmholtz instability, this type of model becomes prohibitively expensive and inefficient.

Therefore, in order to study the stirring of metal and slag phases by introducing a forced convection into the system, a model of another type has been used: with immobile and well-defined interface between metal and slag layers, which hinders the instability generation and speeds up computations. Forcing a particular stirring flow, see Figure 3, allowed to further increase the global reaction rate, as can be seen by comparing grey and red lines in Figure 2.

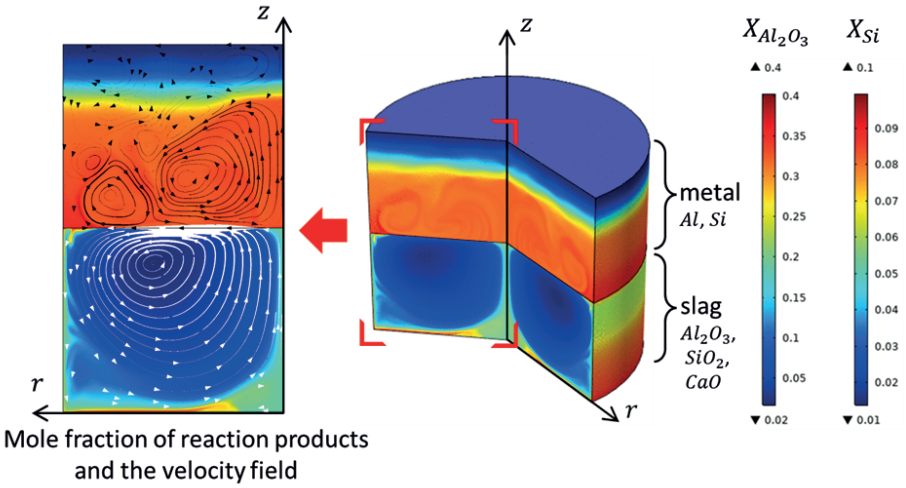

Figure 3: Mole fraction (X_(Al_2 O_3), X_Si) and velocity fields from the well-defined interface model with forced convection at the metal-slag interface, after a reaction time of 2000 s.

On the other extremity, by artificially eliminating the convection from the model and keeping only the diffusion as a species transport mechanism in the phases' bulk, results in a considerable drop of the global reaction rate, see blue line in Figure 2. Such process would require days for any significant advancement of the chemical reaction. This result demonstrates a critical importance of phases stirring, either by natural or forced convection, for the process of aluminothermic reduction.

In conclusion, thanks to a specific consideration of each component of the transport phenomena in the numerical model, we have successfully estimated the impact of each one on the global reaction rate. Models demonstrate a crucial importance of the slag and metal stirring for the process of aluminothermic reduction of silica. To optimize the process, a major interest on the stirring should be taken into account

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PNO
INNOVATION ENGINEERING

Contact us

PROJECT COORDINATOR
Gabriella Tranell
gabriella.tranell@ntnu.no

ADMIN MANAGER
Maria Wallin
maria.wallin@ntnu.no

EXPLOITATION MANAGER
Torstein Haarberg
th@bnw-energy.com

DISSEMINATION MANAGER
Valentina Cinti
v.cinti@ciaotech.com

www.twitter.com/SisalPilot

www.linkedin.com/company/sisal-pilot-project

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