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RESEARCH ARTICLE

REVISED Separation Time of Aluminothermic Reduction Products for Sustainable Silicon Production

[version 2; peer review: 2 approved, 1 approved with reservations]

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Abstract

Background

This work was carried out within the framework of the SisAl Pilot project, which is devoted to the environmentally friendly production of silicon. This new method relies on the aluminothermic reduction of quartz in slag, offering a more sustainable alternative to the traditional reduction of silica with carbon in submerged arc furnaces.

Methods

The process takes place in a rotary kiln producing silicon (Si) and alumina slag (actually, a CaO – Al2O3 slag), which must be separated at the end to extract the silicon. This separation process is analyzed through mathematical modelling and numerical simulation, as it is of industrial interest to know how much time it takes for Si and CaO – Al2O3 slag to separate once the process has ended. Generally, a multiphase flow model is used to estimate the separation time of the two components once aluminothermic reduction has ended.

Results

Several scenarios are considered for the numerical simulation of the separation time, namely different initial configurations and material properties of both fluids are covered. Moreover, the separation times obtained with two distinct multiphase flow models -VOF (volume of

Open Peer Review

Approval Status ✓ ✓ ?

	1	2	3
version 2 (revision) 03 Jan 2025	✓ view	✓ view	? view
version 1 20 Nov 2024	? view	? view	

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2. **Zulfiadi Zulhan**, Bandung Institute of Technology, Bandung, Indonesia
3. **Mita Dasog**, Dalhousie University, Halifax, Canada

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fluid) and Eulerian- are compared.

Conclusions

The separation times resulting from simulations using the multiphase Eulerian model are more realistic compared to those from the VOF model, which clearly tends to underestimate separation times. Furthermore, apart from the selected multiphase flow model, the density difference between silicon and alumina slag plays a critical role in determining the separation time.

Plain language summary

The traditional production of silicon involves a large amount of carbon dioxide emissions into the atmosphere. To improve this situation, the SisAl Pilot project proposes a new, eco-friendly method that aims to produce silicon and alumina slag as a by-product in a more sustainable manner. This work utilizes mathematical modelling and numerical simulation to estimate the separation time of silicon from slag, with the goal of extracting only high-purity silicon.

Keywords

mathematical modelling, numerical simulation, rotary kiln, aluminothermic reduction, multiphase flow, separation time

H2020 This article is included in the Horizon 2020 gateway.

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Author roles: Bullón J: Conceptualization, Writing – Review & Editing; **Crego Ó**: Methodology, Software; **Ferrín JL**: Investigation, Methodology, Writing – Review & Editing; **Gómez D**: Investigation, Methodology, Writing – Review & Editing; **Martínez I**: Software, Writing – Original Draft Preparation; **Pérez-Pérez LJ**: Methodology, Software

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REVISED **Amendments from Version 1**

The article introduction has been completed and improved by adding new relevant references on silicon production, as well as the economical aspects of the SisAl Pilot project have also been addressed. In addition, the simplification of not considering possible aluminium impurities in the final silicon products is clarified in the introduction. Moreover, the temperature of the slag and silicon mixture, at which the material properties were measured, is now pointed out in the text. Finally, a remark concerning the possibility of new alternative methods to improve the separation time is considered in the conclusions.

Any further responses from the reviewers can be found at the end of the article

1. Introduction

Silicon is a crucial material in European industries, and its production is of great significance to many countries. Traditionally, silicon has been produced by reducing silica with carbon in submerged arc furnaces (SAF)[1]. The operation of SAFs is detailed and analysed in 2 and 3, where there is already an awareness of the need to reduce pollutant emissions when performing the classical process for silicon production. Moreover, in 4 the efficiency of the process both from theoretical and industrial viewpoints is addressed.

The aforementioned typical production process involves high amounts of CO_2 emissions. The SisAl Pilot project[5,6] proposes a novel aluminothermic reduction process to achieve a more environmentally friendly alternative. The project suggests a more sustainable way for silicon production by making a transition from the usual process in SAFs and eliminating the need for raw carbon materials, thereby lowering CO_2 emissions. The SisAl Pilot project is exploring this method to produce decarbonized silicon while also recycling aluminium from dross and scrap. This process can be carried out in different types of furnaces, including electric arc, induction, and rotary kilns. The last type is considered in this study, namely, a gas rotary furnace placed at Fundiciones Rey (FRey) facilities in Spain. After several years of project work, the results obtained allow us to be optimistic about the feasibility of producing silicon with this method on an industrial scale, both from a technical and economic point of view.

In the aluminothermic reduction process, the SisAl reaction mechanism takes place:

$$SiO_2\,(CaO - SiO_2\,\text{slag}) + \frac{4}{3}Al \rightarrow Si + \frac{2}{3}Al_2O_3\,(CaO - Al_2O_3\,\text{slag}).$$

As a result of the aluminothermic reduction, Si and $CaO - Al_2O_3$ slag are obtained, and they need to be separated to obtain the purest possible silicon. Notice that the final silicon samples can contain some impurities which were not considered for the sake of simplicity. The main goal of this work was to estimate the time required for both fluids to completely separate after the end of the aluminothermic reduction.

To achieve this objective, the separation process was mathematically modelled according to the Navier-Stokes equations and adequate multiphase flow models. Then, numerical simulations of the separation process were carried out under various scenarios, including different initial conditions, material properties, and multiphase models.

This paper is organized as follows. In Section 2, the methodology followed through this work is presented, including a description of the industrial problem, the geometry of the rotary furnace and the physical properties of the materials involved. The proposed mathematical model is also described. Section 3 presents the main numerical results. Finally, in Section 4, conclusions regarding the obtained results are presented.

2. Methods

In this section, the methodology followed in this work is detailed. More precisely, the industrial problem related to the aluminothermic reduction in the rotary kiln and the mathematical modelling proposed to estimate the separation time are described.

Problem description

The gas rotary furnace considered in this study is made of a cylindrical steel vessel lined with a thick refractory coating, which rolls around its axial direction following two turned rings that act as guides. To enhance the mixing and homogenize the temperature of the partially molten materials, the furnace can be rotated using an electrical motor. A longitudinal view of the furnace and its main dimensions are shown in Figure 1.

During operation, on one side of the furnace, the exhaust gas collection hood remained open, and the opposite side was closed with a lid that included an oxy-fuel burner in its center. The burner injected natural gas and oxygen to generate an intense flame. The furnace can be tilted to facilitate the loading of the solid material and discharge of the melted material once the melting process is completed.

The simulation of the separation time assumes that the aluminothermic reduction has finished; therefore, neither combustion inside the furnace nor slag melting were considered in this process. Once the reaction had ended, a multiphase flow with two fluids, Si and $CaO - Al_2O_3$, was considered, and their evolution over time was analyzed.

First, the geometry of the load in the rotary furnace was determined. This is the computational domain of the simulation, which mainly depends on the inclination angle of the furnace and burden volume. The two possible rotation movements of the furnace during operation are depicted in Figure 2.

To determine the position of the charge, the relevant rotation angle was measured with respect to the horizontal plane, as the rotation along the largest furnace dimension was not considered. Thus, once the rotation with respect to the

horizontal plane and burden volume are given, the geometry of the charge can be obtained. Note that the computational domain is the charge inside the furnace, not including air or the furnace itself, as shown in Figure 3.

Several charge geometries for different rotation angles are shown in Figure 4. The charge geometry used in the simulations corresponded to an inclination of 5°.

In principle, a 3D simulation considering Si, CaO – Al_2O_3 and air is desirable; however, the computational cost makes it unaffordable. The problem can be modelled, in a very good approximation, by a 2D model and by only considering the geometry of the charge corresponding to Si and CaO – Al_2O_3 in a longitudinal cut of the 3D domain. The proposed 2D computational domain and corresponding finite volume mesh for an inclination of 5° are shown in Figure 5.

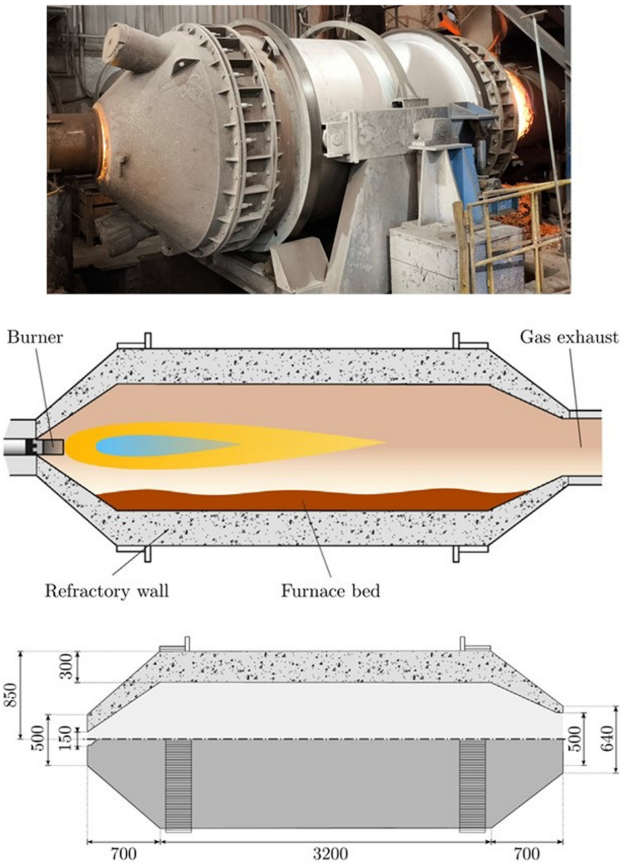

Figure 1. Rotary furnace at FRey (top), schematic diagram (center) and dimensions in mm (bottom).

The physical properties needed for Si and CaO – Al_2O_3 are density and viscosity, which are summarized in Table 1. The mixture is considered at 1400 °C and the material properties at this temperature were extracted from experimental measurements carried out by our partners in the SisAl Project.

Note that both the density and viscosity of the silicon were modified to account for the fact that the furnace is commonly used to melt iron at FRey facilities; therefore, the final slag composition would be contaminated by iron adhering to the furnace walls.

Mathematical modelling

The separation problem within the charge domain was modelled using a transient hydrodynamic model. Specifically, the averaged Navier-Stokes equations and the K – ω SST turbulence model are considered in addition to an adequate multiphase flow model. The mass and momentum conservation equations are given by:

$$\operatorname{div}(\mathbf{v}) = 0,$$

$$\frac{\partial}{\partial t}(\rho\mathbf{v}) + \operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v}) = -\operatorname{grad}(p) - \operatorname{div}\left((\mu+\mu_T)\left[2\mathbf{D}(\mathbf{v}) - \frac{2}{3}\operatorname{div}(\mathbf{v})\mathbf{I}\right] - \frac{2}{3}\rho K\mathbf{I}\right),$$

where $\mathbf{v}$ is the fluid velocity, p is the pressure, μ_T is the turbulent viscosity, $\mathbf{D}(\mathbf{v})$ is the symmetric part of the velocity gradient, and $\mathbf{I}$ is the identity tensor.

Moreover, the K – ω SST turbulence model[7,8] involves two additonal equations for the turbulent kinetic energy, K, and the specific rate of dissipation, ω:

$$\frac{\partial}{\partial t}(\rho K) + \operatorname{div}(\rho K\mathbf{v}) = \operatorname{div}(\Gamma_K \operatorname{grad} K) + \tilde{G}_K - Y_K,$$

$$\frac{\partial}{\partial t}(\rho\omega) + \operatorname{div}(\rho\omega\mathbf{v}) = \operatorname{div}(\Gamma_\omega \operatorname{grad}\omega) + G_\omega - Y_\omega + D_\omega.$$

In the previous equations, $\tilde{G}_K$ represents the generation of turbulence kinetic energy due to mean velocity gradients,

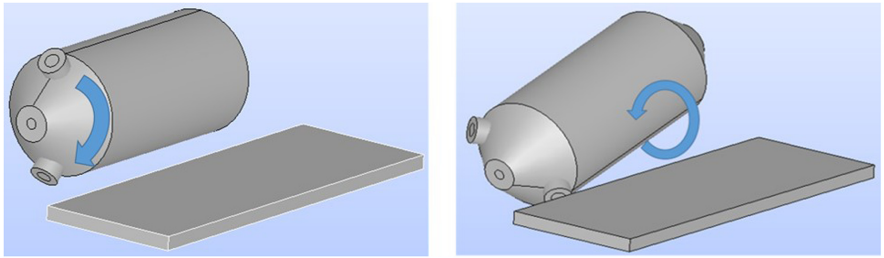

Figure 2. Possible rotation movements of the rotary furnace.

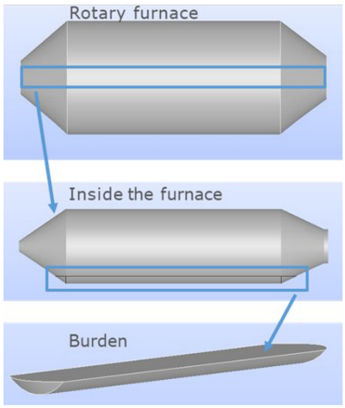

Figure 3. Location of the computational domain inside the rotary furnace.

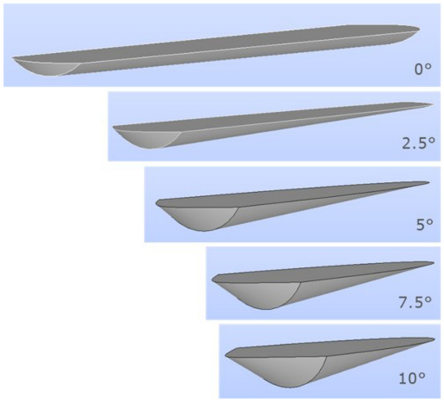

Figure 4. Charge geometry depending on the rotation angle for a given burden volume.

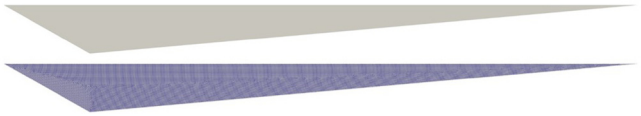

Figure 5. Computational domain (top) and mesh (bottom).

Table 1. Densities and viscosities considered for Si and CaO – Al_2O_3 in the simulations at 1400 °C.

	Si	CaO – Al_2O_3
Density, ρ (kg m^{-3})	3240	2500
Viscosity, μ (Pa s)	5.82E-4	0.1353

G_ω represents the generation of ω; Y_K and Y_ω represent the dissipation of K and ω; Γ_K and Γ_ω represent the effective diffusivity of K and ω; and D_ω is the cross-diffusion term.

With respect to the boundary conditions, zero-shear stress was considered on the top free surface, and no-slip conditions were considered on the walls.

In addition to the conservation equations and turbulence modelling, an adequate multiphase model is required to properly model the separation of both fluids. There are two main multiphase models that use different mathematical descriptions: the VOF model (see 9) and the Eulerian model. The VOF model can handle several immiscible fluids by solving a single set of momentum equations and by tracking the volume fraction of each fluid throughout the domain. On the other hand, the Eulerian option can also model several fluids but the momentum and continuity equations are considered for each phase separately. The VOF model is suitable for flows with a clearly defined phase interface, as both phases are non-interpenetrating and cannot be mixed. In contrast, the Eulerian model assumes that the two continuous phases form an interpenetrating continuum.

As a first approach, the VOF model is considered because its complexity and computational cost are less expensive than those of the Eulerian model. The general idea is to consider the initial distribution of Si and Al_2O_3 on the charge, simulate the evolution of both fluids until they are conveniently separated, and determine the time required to reach the final state. After this time, a denser fluid should be placed at the bottom of the charge.

3. Numerical results

The proposed model was solved using commercial software ANSYS Fluent 2022 R2[10]. It employs a cell-centered finite volume method to discretize the conservation equations. The coupling of the velocity and pressure was achieved using the SIMPLE iterative algorithm. Least-squares cell-based schemes are considered to handle the diffusive terms, whereas second-order upwind schemes are utilized for the treatment of convective terms. Pressure interpolation was performed using PRESTO! scheme. Time discretization was performed using a second-order implicit scheme. For a more in-depth understanding of these numerical schemes, interested readers are encouraged to refer to 11 for further details.

Before the 2D resolution of the hydrodynamic model, a 3D test was considered only for demonstration purposes (see Figure 6). As expected, several weeks of computational time were required to advance only a few seconds of real-time simulation, despite the poor meshing considered.

Different scenarios were considered for the 2D simulations with respect to the multiphase flow model, material properties, and initial configurations of both fluids in the computational domain. The cases addressed in this study are summarized in Table 2.

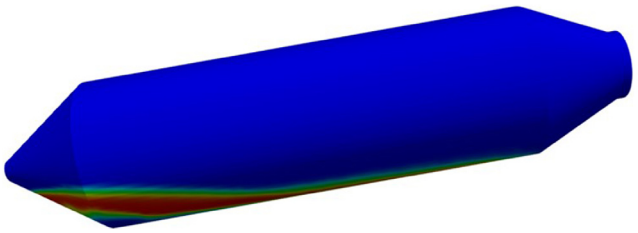

Figure 6. 3D simulation, including air, Si and CaO – Al_2O_3 slag, which is computationally unaffordable.

Table 2. Characteristics of the different scenarios considered.

Scenario	Multiphase model	Initial configuration	Material properties
Case 1	VOF	Horizontal separation (Si on top)	Table 1
Case 2	VOF	Vertical separation	Table 1
Case 3	VOF	Horizontal separation (Si on top)	μ = 3.45 Pa s (CaO-Al_2O_3)
Case 4	VOF	Horizontal separation (Si on top)	μ = 3.45 × 10^{-4} Pa s (CaO-Al_2O_3)
Case 5	Eulerian	Horizontal separation (Si on top)	Table 1
Case 6	Eulerian	Homogeneous mixture	Table 1
Case 7	Eulerian	Homogeneous mixture	ρ = 2570 kg m^{-3} (Si); ρ = 2600 kg m^{-3} (CaO-Al_2O_3)

First, the least favorable initial condition for the VOF model is considered, with a denser fluid (Si) on top at the initial time of the simulation, as shown in Figure 7.



Figure 7. Case 1: initial configuration with Si on top.

The evolution of the simulation with the previous initial condition is shown in Figure 8, giving rise to a complete separation after 30 s.

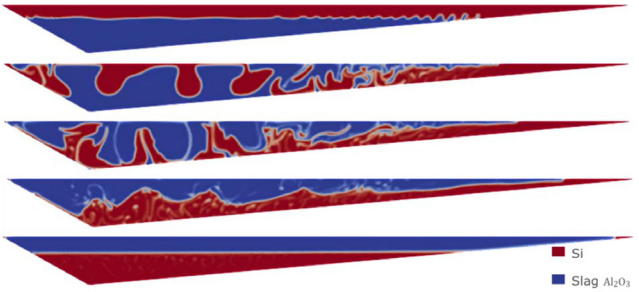

Figure 8. Case 1: complete separation after 30 s (bottom image).

Different initial conditions can be considered, for instance, a vertical initial separation between the two fluids, as depicted in Figure 9.



Figure 9. Case 2: initial configuration with vertical separation.

Although the initial condition is different from that of Case 1, the evolution of the simulation ends with a complete separation after 30 s, as shown in Figure 10.



Figure 10. Case 2: complete separation after 30 s (bottom).

Sensitivity analyses were performed using the VOF model. In particular, starting from the least favorable initial condition (the same as in Case 1), extreme values for slag CaO – Al_2O_3 viscosity were considered, as this value is difficult to obtain from experimental measurements. In Figure 11 and Figure 12 the evolution for both Case 3 and Case 4 is shown, where different values of the slag CaO – Al_2O_3 viscosity were considered.

It is observed that in all the simulations carried out with the VOF model, both Si and CaO – Al_2O_3 are fully separated after 30 s, regardless of the initial conditions or viscosities. Because this separation time is much shorter than the expected time for this type of process, we will change the multiphase VOF model for the Eulerian model.

Therefore, we consider the horizontal initial condition of Case 1, but for the Eulerian model, where the denser fluid (Si) is on top at the initial time of the simulation. The evolution of the separation of the two fluids is shown in Figure 13. After 30 min of simulation, the two fluids were almost completely separated.

Moreover, using the Eulerian model, it is possible to consider an initial homogeneous mixture of Si and CaO – Al_2O_3. This is probably the most realistic and unfavorable initial condition for the separation process, and it cannot be considered when employing the VOF model. The evolution of the separation under this initial condition is shown in Figure 14. It was necessary to wait for at least 60 min to obtain an almost complete separation between Si and CaO – Al_2O_3.

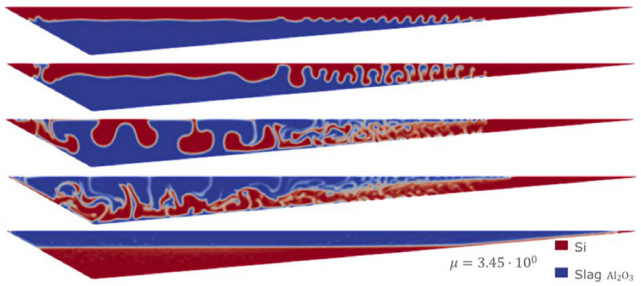

Figure 11. Case 3: complete separation after 30 s (bottom) for μ_{slag} = 3.45 Pa s.

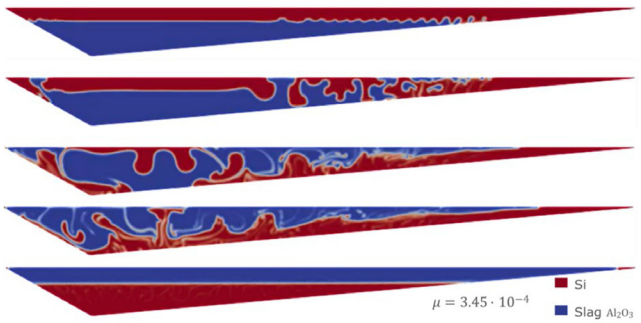

Figure 12. Case 4: complete separation after 30 s (bottom) for μ_{slag} = 3.45×10^{-4} Pa s.

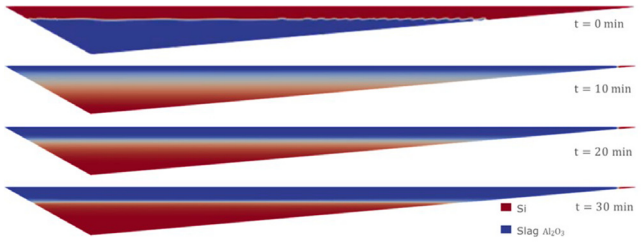

Figure 13. Case 5: complete separation after 30 min (bottom).

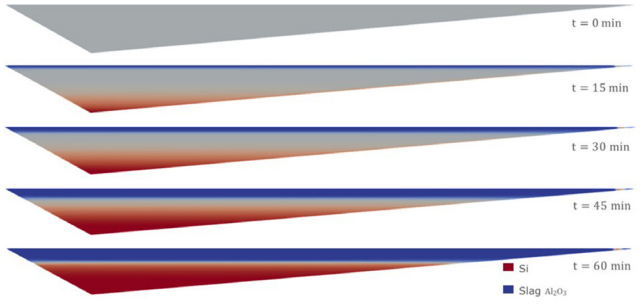

Figure 14. Case 6: complete separation after 60 min (bottom).

The separation times resulting from the Eulerian model are much higher than those obtained with the VOF model, and seem more realistic according to the knowledge obtained from the plant experience.

However, it is well known that the difference in densities between Si and CaO – Al_2O_3 is the key factor in controlling the separation time, which is more important than any other parameter. This can be appreciated in the following simulation using the Eulerian model, starting from the homogeneous mixture condition and with the densities of both fluids modified to 2570 kg m^{-3} for Si and 2600 kg m^{-3} for CaO – Al_2O_3. As shown in Figure 15, after 10 min of simulation, almost no separation was observed. This is because of the similarity of both densities, which leads to extremely long separation times.

4. Conclusions

Once the aluminothermic reduction process in the rotary furnace has finished, it is of industrial interest to determine how long it will take for silicon and alumina slag to separate and ensure that only silicon is cast. To meet this requirement, own code was developed to calculate the geometry of the charge inside the furnace based on its geometry, inclination, and mass of charge. After determining the geometry, a multiphase flow model was applied to estimate the separation time of the two components after the reduction process. The separation time was simulated under different conditions including different material properties, initial conditions, and multiphase models. The results obtained with the multiphase Eulerian model are more realistic than those obtained with the VOF model, which has an obvious tendency to underestimate the separation times.

As is clear from the simulations, apart from the selected multiphase flow model, the density difference between silicon and alumina slag plays a critical role in determining the separation time.

Finally, it is important to note that for industrial purposes it would the best to have a separation time as short as possible, but our aim in this work is only to study the separation time due to density differences and viscosity effects. A further step could involve the analysis of novel separation methods that could eventually optimize the separation time.

Ethics and consent

Ethics and consent were not required for this study.



Figure 15. Case 7: no separation after 10 minutes when densities are almost equal.

Data and software availability

No data associated with this article. The numerical simulations in this work were performed using ANSYS Fluent 2022 R2. An open source alternative could be OpenFOAM[12], which is capable of doing similar tasks as those performed in this work.

Acknowledgements

The authors are particularly grateful to Fundiciones Rey for facilitating the experimental data, and for their continuous support and valuable discussions throughout the project.

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https://www.openfoam.com/

Open Peer Review

Current Peer Review Status: ✔ ✔ ?

Version 2

Reviewer Report 03 February 2025

https://doi.org/10.21956/openreseurope.20838.r49487

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Mita Dasog
Dalhousie University, Halifax, Nova Scotia, Canada

The study investigates the separation process of Si and CaO-Al_2O_3 slag in the SisAl Pilot project's aluminothermic reduction method using mathematical modeling and numerical simulation. By comparing two multiphase flow models, the results indicate that the Eulerian model provides more realistic separation times than the VOF model, which tends to underestimate them. As alternatives to carbothermal reduction are currently being explored, it is important to demonstrate the commercial feasibility of alternative reduction methods.

The paper can benefit from further clarifications and responses to the following queries:
1. The temperature of the mixture was considered to be 1400°C, as obtained from the experimental work. Is this temperature measured at the surface of the mixture or assumed to be uniform throughout? Rotary kilns are known to have a radial thermal gradient, which is likely to be more pronounced during the separation step when the kiln is not rotating. If this temperature corresponds to the surface, how would a thermal gradient affect the viscosity and, consequently, the calculations?

2.Can the authors explain why a 5-degree inclination was chosen for the simulations?

3.While the effect of viscosity was investigated using the VOF model, it was not examined with the Eulerian model. Can the authors clarify why this was the case?

4. A discussion on the accuracy or error margin in the time values predicted using the Eulerian model would be beneficial to readers.

5. There is a typographical error in Table 1: In the third column label, the numbers in Al_2O_3 should be subscripted.

Is the work clearly and accurately presented and does it cite the current literature?
Yes

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
Yes

If applicable, is the statistical analysis and its interpretation appropriate?
I cannot comment. A qualified statistician is required.

Are all the source data underlying the results available to ensure full reproducibility?
No source data required

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Reviewer Report 10 January 2025

https://doi.org/10.21956/openreseurope.20838.r49461

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Zulfiadi Zulhan
Bandung Institute of Technology, Bandung, Indonesia

I have reviewed the manuscript, and I confirm that most of the revisions suggested have been implemented by the authors. Therefore, I recommend that the manuscript be accepted for indexing.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Partly

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?

Partly

Are all the source data underlying the results available to ensure full reproducibility?
Partly

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Reviewer Report 08 January 2025

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Navneet Singh Randhawa
CSIR-National Metallurgical Laboratory, Jharkhand, India

The revised article may be accepted.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Partly

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?
Partly

Are all the source data underlying the results available to ensure full reproducibility?
Partly

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard.

Version 1

Reviewer Report 18 December 2024

https://doi.org/10.21956/openreseurope.20381.r46985

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Zulfiadi Zulhan
Bandung Institute of Technology, Bandung, Indonesia

The manuscript is part of the SisAl project to produce environmentally friendly silicon metal using SiO_2-CaO slag as raw material. The manuscript focuses on the separation of silicon from CaO-Al_2O_3 slag.

However, the manuscript does not provide information regarding the temperature of the silicon separation process and the CaO-Al_2O_3 slag, including viscosity and density data of silicon and CaO-Al_2O_3 slag at what temperature? What are the data sources for Table 1 and Table 2?

What was the environmental condition during heating with the burner—was it reductive or oxidative?

Generally, there is a possibility of excess aluminum entering the silicon, which has not been considered. Is the produced metal always pure without aluminum in it?

I am not an expert in CFD calculations, but verification is usually required from simulation calculations using CFD (Computational Fluid Dynamics), for example, using a water model!

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Partly

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?
Not applicable

Are all the source data underlying the results available to ensure full reproducibility?
Partly

Are the conclusions drawn adequately supported by the results?
Partly

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: High temperatures metals processing, ironmaking & steelmaking, ferronickel smelting, tin smelting, magnesium production by metallothermic, carbothermic reduction, hydrogen and methane reduction, hydrogen plasma smelting reduction.

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 21 Dec 2024

Iván Martínez Suárez

We want to thank the reviewer for reading the manuscript so carefully and for the given remarks, which we believe allowed us to improve the paper. In what follows we briefly comment the suggestions and questions that were made.

- *The manuscript does not provide information regarding the temperature of the silicon separation process and the CaO-Al_2O_3 slag, including viscosity and density data of silicon and CaO-Al_2O_3 slag at what temperature? What are the data sources for Table 1 and Table 2?*

The temperature considered for the mixture of slag and silicon is about 1400 ºC. Viscosity and density data at that temperature are shown in Table 1 and were provided by our experimental partners in the SisAl Project. This point has been clarified in the text. Concerning Table 2, different scenarios are proposed for simulation purposes. The material properties in Table 2 which are not included in Table 1 are only for simulation and comparison between scenarios.

- *What was the environmental condition during heating with the burner—was it reductive or oxidative?*

The furnace at FRey facilities is equipped with an oxy-combustion natural gas burner using pure oxygen as oxidizer.

- *Generally, there is a possibility of excess aluminum entering the silicon, which has not been considered. Is the produced metal always pure without aluminum in it?*

In different experimental tests in plant, some impurities were observed in the final produced silicon, which would require further refining processes to achieve optimal purity. Of course, these impurities could affect the final separation time of the components of the mixture, although our aim in this work is to make an initial approximation from a less detailed perspective. This point was clarified in the introduction.

- *Verification of simulation calculations using CFD (Computational Fluid Dynamics), for example, using a water model.*

It would be optimal to be able to measure the separation time in plant, but this is difficult to

do accurately due to the daily production needs of our industrial partner and further work would be needed. Nevertheless, the results obtained with the Eulerian model are in line with the results of close observation in plant.

Competing Interests: No competing interests were disclosed.

Reviewer Report 16 December 2024

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Navneet Singh Randhawa
CSIR-National Metallurgical Laboratory, Jharkhand, India

The manuscript reports the numerical simulation work on the Separation Time of Aluminothermic Reduction Products for Sustainable Silicon Production. This work is industrially relevant and would interest researchers in this field. The manuscript may be indexed after revision with the following comments.
The relevant literature on silicon reproduction should be thoroughly presented and compared with the present work.
The economic aspect of the aluminothermic process is lacking in the manuscript. A bride account may be given.
The method may be elaborated so that the researched would understand and follow the approach.
The optimal separation time determined by the model should be mentioned and discussed.

Is the work clearly and accurately presented and does it cite the current literature?
Partly

Is the study design appropriate and does the work have academic merit?
Yes

Are sufficient details of methods and analysis provided to allow replication by others?
Partly

If applicable, is the statistical analysis and its interpretation appropriate?
I cannot comment. A qualified statistician is required.

Are all the source data underlying the results available to ensure full reproducibility?
No

Are the conclusions drawn adequately supported by the results?

Yes

Competing Interests: No competing interests were disclosed.

Reviewer Expertise: Valorization of metallurgical wastes and by-products. Computational thermodynamics for Extractive Metallurgy. Extraction of metal values from primary and secondary. resources. Pilotscale evaluation of metal extraction processes

I confirm that I have read this submission and believe that I have an appropriate level of expertise to confirm that it is of an acceptable scientific standard, however I have significant reservations, as outlined above.

Author Response 21 Dec 2024

Iván Martínez Suárez

We want to thank the reviewer for reading the manuscript so carefully and for the given remarks, which we believe allowed us to improve the paper. In what follows we briefly comment the suggestions that were made.

- *The relevant literature on silicon reproduction should be thoroughly presented and compared with the present work.*

Information regarding this issue has been enriched and completed in the article introduction, including the addition of relevant references on silicon production.

- *The economic aspect of the aluminothermic process is lacking in the manuscript. A bride account may be given.*

The economic aspects of the aluminothermic process have mainly been addressed by specialized partners of the SisAl Pilot Project. Nevertheless, in pooling the conclusions of the different partners, it was agreed that the production of silicon through aluminothermic reduction would be feasible on an industrial scale both from a technical and an economic point of view. A remark was added in the introduction to clarify this point.

- *The method may be elaborated so that the researched would understand and follow the approach.*

Our aim when describing the methods was to provide a guide that regular users who are familiar with CFD simulation could follow, including standard mathematical models in a 2D computational domain. The simulations were performed by using the software Ansys Fluent 2022 R2 and the accessible open source alternative, OpenFOAM, was also recommended.

- *The optimal separation time determined by the model should be mentioned and discussed.*

The separation time of the slag and the silicon is analysed under different simulation scenarios, including different material properties, initial conditions and multiphase models. As an insight of these simulations, the Eulerian model is the one that best fits the separation times observed in plant. For industrial purposes it would the best to have a separation time as short as possible, but our aim in this work is only to study the separation time due to density differences and viscosity effects. A further step could involve the analysis of novel separation methods that could eventually optimize the separation time. A remark has been added to the conclusions to clarify this point.

Competing Interests: No competing interests were disclosed.